



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:15 PM GMT

PDB ID : 4V95
Title : Crystal structure of YAEJ bound to the 70S ribosome
Authors : Gagnon, M.G.; Seetharaman, S.V.; Bulkley, D.P.; Steitz, T.A.
Deposited on : 2012-01-27
Resolution : 3.20 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

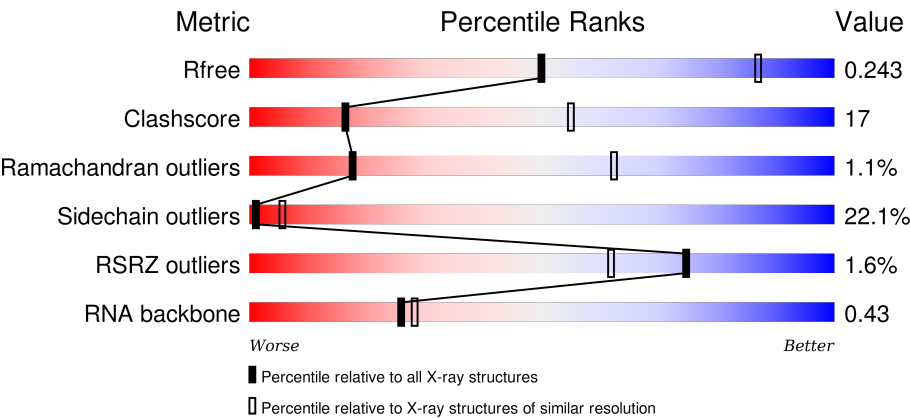
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.






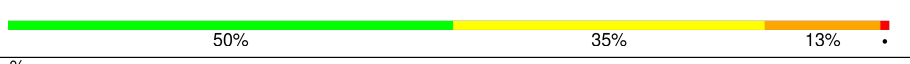
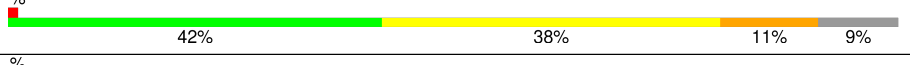
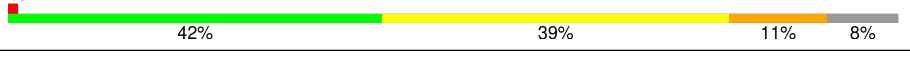
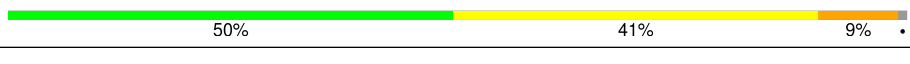

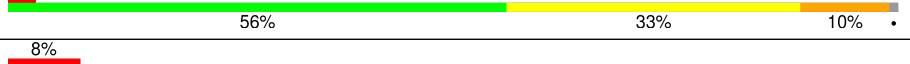








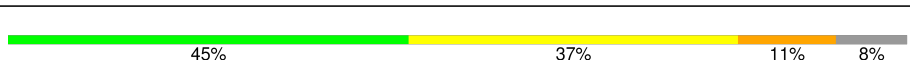
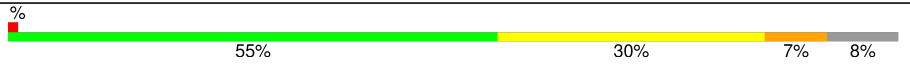


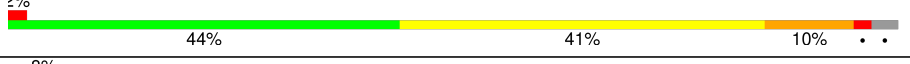



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1124 (3.24-3.16) |
| Clashscore | 102246 | 1024 (3.22-3.18) |
| Ramachandran outliers | 100387 | 1004 (3.22-3.18) |
| Sidechain outliers | 100360 | 1003 (3.22-3.18) |
| RSRZ outliers | 91569 | 1129 (3.24-3.16) |
| RNA backbone | 2183 | 1079 (3.70-2.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 | AA | 1522 | <div><div>2%</div><div><div></div><div>25%</div><div>43%</div><div>23%</div><div>6%</div><div></div></div><div></div></div> |
| 1 | CA | 1522 | <div><div>2%</div><div><div></div><div>29%</div><div>43%</div><div>20%</div><div></div><div></div></div><div></div></div> |
| 2 | AB | 256 | <div><div></div><div><div></div><div>36%</div><div>42%</div><div>12%</div><div></div><div>9%</div></div><div></div></div> |
| 2 | CB | 256 | <div><div>4%</div><div><div></div><div>31%</div><div>49%</div><div>11%</div><div></div><div>8%</div></div><div></div></div> |


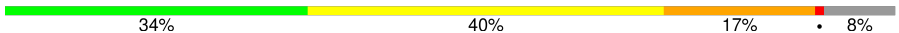
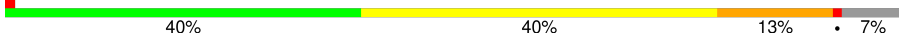


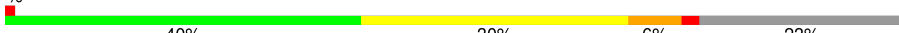
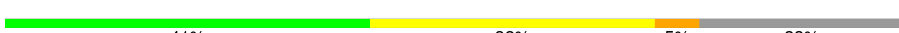









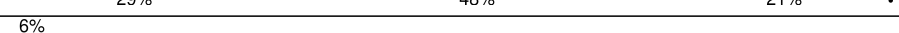



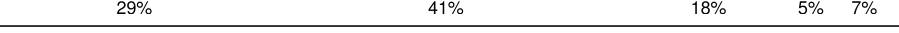
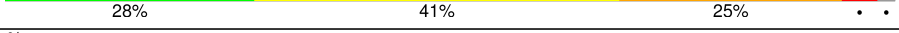
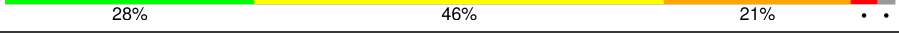


Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | AC | 239 |  |
| 3 | CC | 239 |  |
| 4 | AD | 209 |  |
| 4 | CD | 209 |  |
| 5 | AE | 162 |  |
| 5 | CE | 162 |  |
| 6 | AF | 101 |  |
| 6 | CF | 101 |  |
| 7 | AG | 156 |  |
| 7 | CG | 156 |  |
| 8 | AH | 138 |  |
| 8 | CH | 138 |  |
| 9 | AI | 128 |  |
| 9 | CI | 128 |  |
| 10 | AJ | 105 |  |
| 10 | CJ | 105 |  |
| 11 | AK | 129 |  |
| 11 | CK | 129 |  |
| 12 | AL | 132 |  |
| 12 | CL | 132 |  |
| 13 | AM | 126 |  |
| 13 | CM | 126 |  |
| 14 | AN | 61 |  |
| 14 | CN | 61 |  |
| 15 | AO | 89 |  |



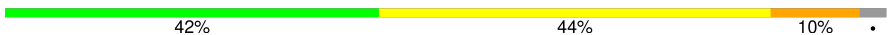




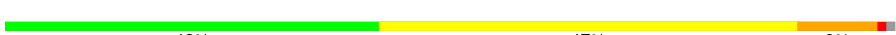



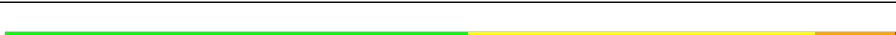

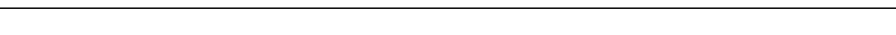
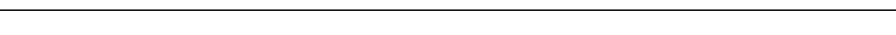
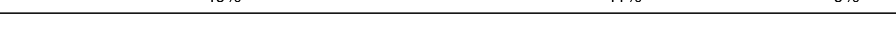

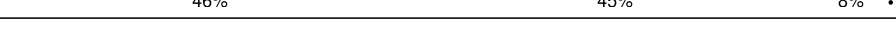







Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | CO | 89 |  |
| 16 | AP | 88 |  |
| 16 | CP | 88 |  |
| 17 | AQ | 105 |  |
| 17 | CQ | 105 |  |
| 18 | AR | 88 |  |
| 18 | CR | 88 |  |
| 19 | AS | 93 |  |
| 19 | CS | 93 |  |
| 20 | AT | 106 |  |
| 20 | CT | 106 |  |
| 21 | AU | 27 |  |
| 21 | CU | 27 |  |
| 22 | AY | 140 |  |
| 23 | AV | 77 |  |
| 23 | CV | 77 |  |
| 24 | AX | 16 |  |
| 24 | CX | 16 |  |
| 25 | BA | 2915 |  |
| 25 | DA | 2915 |  |
| 26 | BB | 122 |  |
| 26 | DB | 122 |  |
| 27 | BD | 276 |  |
| 27 | DD | 276 |  |
| 28 | BE | 206 |  |









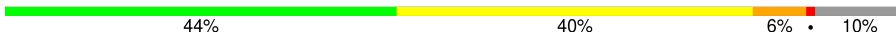
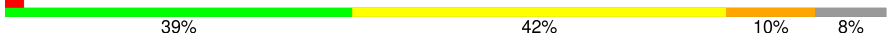
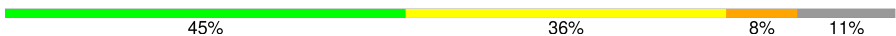
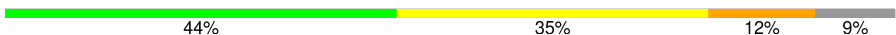













Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | DE | 206 |  |
| 29 | BF | 210 |  |
| 29 | DF | 210 |  |
| 30 | BG | 182 |  |
| 30 | DG | 182 |  |
| 31 | BH | 180 |  |
| 31 | DH | 180 |  |
| 32 | BI | 148 |  |
| 32 | DI | 148 |  |
| 33 | BN | 140 |  |
| 33 | DN | 140 |  |
| 34 | BO | 122 |  |
| 34 | DO | 122 |  |
| 35 | BP | 150 |  |
| 35 | DP | 150 |  |
| 36 | BQ | 141 |  |
| 36 | DQ | 141 |  |
| 37 | BR | 118 |  |
| 37 | DR | 118 |  |
| 38 | BS | 112 |  |
| 38 | DS | 112 |  |
| 39 | BT | 146 |  |
| 39 | DT | 146 |  |
| 40 | BU | 118 |  |
| 40 | DU | 118 |  |

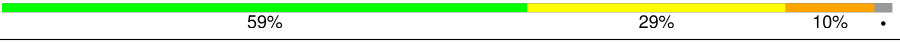

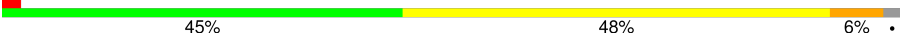


Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 41 | BV | 101 |  |
| 41 | DV | 101 |  |
| 42 | BW | 113 |  |
| 42 | DW | 113 |  |
| 43 | BX | 96 |  |
| 43 | DX | 96 |  |
| 44 | BY | 110 |  |
| 44 | DY | 110 |  |
| 45 | BZ | 206 |  |
| 45 | DZ | 206 |  |
| 46 | B0 | 85 |  |
| 46 | D0 | 85 |  |
| 47 | B1 | 98 |  |
| 47 | D1 | 98 |  |
| 48 | B2 | 72 |  |
| 48 | D2 | 72 |  |
| 49 | B3 | 60 |  |
| 49 | D3 | 60 |  |
| 50 | B4 | 71 |  |
| 50 | D4 | 71 |  |
| 51 | B5 | 60 |  |
| 51 | D5 | 60 |  |
| 52 | B6 | 54 |  |
| 52 | D6 | 54 |  |
| 53 | B7 | 49 |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 53 | D7 | 49 |  |
| 54 | B8 | 65 |  |
| 54 | D8 | 65 |  |
| 55 | B9 | 37 |  |
| 55 | D9 | 37 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | AA | 1604 | - | - | - | X |
| 56 | MG | AA | 1607 | - | - | - | X |
| 56 | MG | AA | 1619 | - | - | - | X |
| 56 | MG | AA | 1626 | - | - | - | X |
| 56 | MG | AA | 1628 | - | - | - | X |
| 56 | MG | AA | 1630 | - | - | - | X |
| 56 | MG | AA | 1631 | - | - | - | X |
| 56 | MG | AA | 1635 | - | - | - | X |
| 56 | MG | AA | 1636 | - | - | - | X |
| 56 | MG | AA | 1642 | - | - | - | X |
| 56 | MG | AA | 1644 | - | - | - | X |
| 56 | MG | AA | 1645 | - | - | - | X |
| 56 | MG | AA | 1648 | - | - | - | X |
| 56 | MG | AA | 1650 | - | - | - | X |
| 56 | MG | AA | 1659 | - | - | - | X |
| 56 | MG | AA | 1663 | - | - | - | X |
| 56 | MG | AA | 1683 | - | - | - | X |
| 56 | MG | AA | 1685 | - | - | - | X |
| 56 | MG | AA | 1687 | - | - | - | X |
| 56 | MG | AA | 1711 | - | - | - | X |
| 56 | MG | AA | 1726 | - | - | - | X |
| 56 | MG | AA | 1728 | - | - | - | X |
| 56 | MG | AA | 1735 | - | - | - | X |
| 56 | MG | AA | 1739 | - | - | - | X |
| 56 | MG | AA | 1754 | - | - | - | X |
| 56 | MG | AA | 1771 | - | - | - | X |
| 56 | MG | AA | 1776 | - | - | - | X |
| 56 | MG | AA | 1782 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | AA | 1786 | - | - | - | X |
| 56 | MG | AA | 1797 | - | - | - | X |
| 56 | MG | AA | 1800 | - | - | - | X |
| 56 | MG | AA | 1806 | - | - | - | X |
| 56 | MG | AA | 1809 | - | - | - | X |
| 56 | MG | AA | 1822 | - | - | - | X |
| 56 | MG | AA | 1838 | - | - | - | X |
| 56 | MG | AA | 1842 | - | - | - | X |
| 56 | MG | AA | 1845 | - | - | - | X |
| 56 | MG | AA | 1872 | - | - | - | X |
| 56 | MG | AA | 1874 | - | - | - | X |
| 56 | MG | AA | 1897 | - | - | - | X |
| 56 | MG | AA | 1919 | - | - | - | X |
| 56 | MG | AD | 302 | - | - | - | X |
| 56 | MG | AV | 101 | - | - | - | X |
| 56 | MG | B1 | 101 | - | - | - | X |
| 56 | MG | B2 | 102 | - | - | - | X |
| 56 | MG | B3 | 101 | - | - | - | X |
| 56 | MG | BA | 3012 | - | - | - | X |
| 56 | MG | BA | 3014 | - | - | - | X |
| 56 | MG | BA | 3029 | - | - | - | X |
| 56 | MG | BA | 3030 | - | - | - | X |
| 56 | MG | BA | 3035 | - | - | - | X |
| 56 | MG | BA | 3038 | - | - | - | X |
| 56 | MG | BA | 3043 | - | - | - | X |
| 56 | MG | BA | 3045 | - | - | - | X |
| 56 | MG | BA | 3048 | - | - | - | X |
| 56 | MG | BA | 3051 | - | - | - | X |
| 56 | MG | BA | 3052 | - | - | - | X |
| 56 | MG | BA | 3056 | - | - | - | X |
| 56 | MG | BA | 3059 | - | - | - | X |
| 56 | MG | BA | 3061 | - | - | - | X |
| 56 | MG | BA | 3064 | - | - | - | X |
| 56 | MG | BA | 3069 | - | - | - | X |
| 56 | MG | BA | 3073 | - | - | - | X |
| 56 | MG | BA | 3076 | - | - | - | X |
| 56 | MG | BA | 3077 | - | - | - | X |
| 56 | MG | BA | 3084 | - | - | - | X |
| 56 | MG | BA | 3092 | - | - | - | X |
| 56 | MG | BA | 3098 | - | - | - | X |
| 56 | MG | BA | 3123 | - | - | - | X |
| 56 | MG | BA | 3124 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | BA | 3134 | - | - | - | X |
| 56 | MG | BA | 3145 | - | - | - | X |
| 56 | MG | BA | 3154 | - | - | - | X |
| 56 | MG | BA | 3156 | - | - | - | X |
| 56 | MG | BA | 3165 | - | - | - | X |
| 56 | MG | BA | 3166 | - | - | - | X |
| 56 | MG | BA | 3169 | - | - | - | X |
| 56 | MG | BA | 3183 | - | - | - | X |
| 56 | MG | BA | 3188 | - | - | - | X |
| 56 | MG | BA | 3193 | - | - | - | X |
| 56 | MG | BA | 3199 | - | - | - | X |
| 56 | MG | BA | 3200 | - | - | - | X |
| 56 | MG | BA | 3203 | - | - | - | X |
| 56 | MG | BA | 3204 | - | - | - | X |
| 56 | MG | BA | 3209 | - | - | - | X |
| 56 | MG | BA | 3210 | - | - | - | X |
| 56 | MG | BA | 3211 | - | - | - | X |
| 56 | MG | BA | 3218 | - | - | - | X |
| 56 | MG | BA | 3220 | - | - | - | X |
| 56 | MG | BA | 3221 | - | - | - | X |
| 56 | MG | BA | 3224 | - | - | - | X |
| 56 | MG | BA | 3225 | - | - | - | X |
| 56 | MG | BA | 3227 | - | - | - | X |
| 56 | MG | BA | 3233 | - | - | - | X |
| 56 | MG | BA | 3243 | - | - | - | X |
| 56 | MG | BA | 3248 | - | - | - | X |
| 56 | MG | BA | 3250 | - | - | - | X |
| 56 | MG | BA | 3252 | - | - | - | X |
| 56 | MG | BA | 3254 | - | - | - | X |
| 56 | MG | BA | 3317 | - | - | - | X |
| 56 | MG | BA | 3340 | - | - | - | X |
| 56 | MG | BA | 3366 | - | - | - | X |
| 56 | MG | BA | 3367 | - | - | - | X |
| 56 | MG | BA | 3374 | - | - | - | X |
| 56 | MG | BA | 3375 | - | - | - | X |
| 56 | MG | BA | 3376 | - | - | - | X |
| 56 | MG | BA | 3383 | - | - | - | X |
| 56 | MG | BA | 3390 | - | - | - | X |
| 56 | MG | BA | 3408 | - | - | - | X |
| 56 | MG | BA | 3410 | - | - | - | X |
| 56 | MG | BA | 3411 | - | - | - | X |
| 56 | MG | BA | 3419 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | BA | 3437 | - | - | - | X |
| 56 | MG | BA | 3450 | - | - | - | X |
| 56 | MG | BA | 3453 | - | - | - | X |
| 56 | MG | BA | 3455 | - | - | - | X |
| 56 | MG | BA | 3467 | - | - | - | X |
| 56 | MG | BA | 3477 | - | - | - | X |
| 56 | MG | BA | 3484 | - | - | - | X |
| 56 | MG | BA | 3488 | - | - | - | X |
| 56 | MG | BA | 3548 | - | - | - | X |
| 56 | MG | BA | 3550 | - | - | - | X |
| 56 | MG | BA | 3571 | - | - | - | X |
| 56 | MG | BA | 3581 | - | - | - | X |
| 56 | MG | BA | 3582 | - | - | - | X |
| 56 | MG | BA | 3602 | - | - | - | X |
| 56 | MG | BA | 3614 | - | - | - | X |
| 56 | MG | BA | 3648 | - | - | - | X |
| 56 | MG | BA | 3654 | - | - | - | X |
| 56 | MG | BA | 3675 | - | - | - | X |
| 56 | MG | BA | 3676 | - | - | - | X |
| 56 | MG | BA | 3682 | - | - | - | X |
| 56 | MG | BA | 3687 | - | - | - | X |
| 56 | MG | BA | 3700 | - | - | - | X |
| 56 | MG | BA | 3702 | - | - | - | X |
| 56 | MG | BA | 3732 | - | - | - | X |
| 56 | MG | BA | 3753 | - | - | - | X |
| 56 | MG | BA | 3759 | - | - | - | X |
| 56 | MG | BA | 3766 | - | - | - | X |
| 56 | MG | BA | 3770 | - | - | - | X |
| 56 | MG | BA | 3782 | - | - | - | X |
| 56 | MG | BA | 3791 | - | - | - | X |
| 56 | MG | BA | 3805 | - | - | - | X |
| 56 | MG | BA | 3809 | - | - | - | X |
| 56 | MG | BA | 3837 | - | - | - | X |
| 56 | MG | BA | 3853 | - | - | - | X |
| 56 | MG | BA | 3854 | - | - | - | X |
| 56 | MG | BA | 3868 | - | - | - | X |
| 56 | MG | BA | 3872 | - | - | - | X |
| 56 | MG | BA | 3875 | - | - | - | X |
| 56 | MG | BA | 3887 | - | - | - | X |
| 56 | MG | BA | 3894 | - | - | - | X |
| 56 | MG | BB | 201 | - | - | - | X |
| 56 | MG | BB | 213 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | BD | 301 | - | - | - | X |
| 56 | MG | BD | 302 | - | - | - | X |
| 56 | MG | BD | 303 | - | - | - | X |
| 56 | MG | BE | 301 | - | - | - | X |
| 56 | MG | BF | 305 | - | - | - | X |
| 56 | MG | BG | 201 | - | - | - | X |
| 56 | MG | BP | 201 | - | - | - | X |
| 56 | MG | BR | 201 | - | - | - | X |
| 56 | MG | BU | 201 | - | - | - | X |
| 56 | MG | BV | 201 | - | - | - | X |
| 56 | MG | CA | 1602 | - | - | - | X |
| 56 | MG | CA | 1605 | - | - | - | X |
| 56 | MG | CA | 1606 | - | - | - | X |
| 56 | MG | CA | 1608 | - | - | - | X |
| 56 | MG | CA | 1612 | - | - | - | X |
| 56 | MG | CA | 1621 | - | - | - | X |
| 56 | MG | CA | 1625 | - | - | - | X |
| 56 | MG | CA | 1628 | - | - | - | X |
| 56 | MG | CA | 1637 | - | - | - | X |
| 56 | MG | CA | 1647 | - | - | - | X |
| 56 | MG | CA | 1656 | - | - | - | X |
| 56 | MG | CA | 1679 | - | - | - | X |
| 56 | MG | CA | 1682 | - | - | - | X |
| 56 | MG | CA | 1690 | - | - | - | X |
| 56 | MG | CA | 1691 | - | - | - | X |
| 56 | MG | CA | 1692 | - | - | - | X |
| 56 | MG | CA | 1693 | - | - | - | X |
| 56 | MG | CA | 1697 | - | - | - | X |
| 56 | MG | CA | 1705 | - | - | - | X |
| 56 | MG | CA | 1706 | - | - | - | X |
| 56 | MG | CA | 1722 | - | - | - | X |
| 56 | MG | CA | 1726 | - | - | - | X |
| 56 | MG | CA | 1732 | - | - | - | X |
| 56 | MG | CA | 1737 | - | - | - | X |
| 56 | MG | CA | 1743 | - | - | - | X |
| 56 | MG | CA | 1745 | - | - | - | X |
| 56 | MG | CA | 1753 | - | - | - | X |
| 56 | MG | CA | 1761 | - | - | - | X |
| 56 | MG | CA | 1778 | - | - | - | X |
| 56 | MG | CA | 1788 | - | - | - | X |
| 56 | MG | D0 | 101 | - | - | - | X |
| 56 | MG | D1 | 101 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | D6 | 102 | - | - | - | X |
| 56 | MG | D6 | 103 | - | - | - | X |
| 56 | MG | D7 | 101 | - | - | - | X |
| 56 | MG | DA | 3017 | - | - | - | X |
| 56 | MG | DA | 3018 | - | - | - | X |
| 56 | MG | DA | 3021 | - | - | - | X |
| 56 | MG | DA | 3024 | - | - | - | X |
| 56 | MG | DA | 3029 | - | - | - | X |
| 56 | MG | DA | 3030 | - | - | - | X |
| 56 | MG | DA | 3041 | - | - | - | X |
| 56 | MG | DA | 3044 | - | - | - | X |
| 56 | MG | DA | 3045 | - | - | - | X |
| 56 | MG | DA | 3047 | - | - | - | X |
| 56 | MG | DA | 3051 | - | - | - | X |
| 56 | MG | DA | 3054 | - | - | - | X |
| 56 | MG | DA | 3059 | - | - | - | X |
| 56 | MG | DA | 3068 | - | - | - | X |
| 56 | MG | DA | 3074 | - | - | - | X |
| 56 | MG | DA | 3075 | - | - | - | X |
| 56 | MG | DA | 3079 | - | - | - | X |
| 56 | MG | DA | 3080 | - | - | - | X |
| 56 | MG | DA | 3087 | - | - | - | X |
| 56 | MG | DA | 3097 | - | - | - | X |
| 56 | MG | DA | 3100 | - | - | - | X |
| 56 | MG | DA | 3101 | - | - | - | X |
| 56 | MG | DA | 3109 | - | - | - | X |
| 56 | MG | DA | 3121 | - | - | - | X |
| 56 | MG | DA | 3123 | - | - | - | X |
| 56 | MG | DA | 3124 | - | - | - | X |
| 56 | MG | DA | 3127 | - | - | - | X |
| 56 | MG | DA | 3141 | - | - | - | X |
| 56 | MG | DA | 3142 | - | - | - | X |
| 56 | MG | DA | 3146 | - | - | - | X |
| 56 | MG | DA | 3153 | - | - | - | X |
| 56 | MG | DA | 3156 | - | - | - | X |
| 56 | MG | DA | 3168 | - | - | - | X |
| 56 | MG | DA | 3172 | - | - | - | X |
| 56 | MG | DA | 3175 | - | - | - | X |
| 56 | MG | DA | 3178 | - | - | - | X |
| 56 | MG | DA | 3192 | - | - | - | X |
| 56 | MG | DA | 3197 | - | - | - | X |
| 56 | MG | DA | 3198 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | DA | 3218 | - | - | - | X |
| 56 | MG | DA | 3244 | - | - | - | X |
| 56 | MG | DA | 3249 | - | - | - | X |
| 56 | MG | DA | 3250 | - | - | - | X |
| 56 | MG | DA | 3251 | - | - | - | X |
| 56 | MG | DA | 3264 | - | - | - | X |
| 56 | MG | DA | 3273 | - | - | - | X |
| 56 | MG | DA | 3274 | - | - | - | X |
| 56 | MG | DA | 3277 | - | - | - | X |
| 56 | MG | DA | 3284 | - | - | - | X |
| 56 | MG | DA | 3285 | - | - | - | X |
| 56 | MG | DA | 3286 | - | - | - | X |
| 56 | MG | DA | 3312 | - | - | - | X |
| 56 | MG | DA | 3317 | - | - | - | X |
| 56 | MG | DA | 3321 | - | - | - | X |
| 56 | MG | DA | 3325 | - | - | - | X |
| 56 | MG | DA | 3341 | - | - | - | X |
| 56 | MG | DA | 3347 | - | - | - | X |
| 56 | MG | DA | 3353 | - | - | - | X |
| 56 | MG | DA | 3354 | - | - | - | X |
| 56 | MG | DA | 3357 | - | - | - | X |
| 56 | MG | DA | 3369 | - | - | - | X |
| 56 | MG | DA | 3386 | - | - | - | X |
| 56 | MG | DA | 3393 | - | - | - | X |
| 56 | MG | DA | 3399 | - | - | - | X |
| 56 | MG | DA | 3403 | - | - | - | X |
| 56 | MG | DA | 3417 | - | - | - | X |
| 56 | MG | DA | 3419 | - | - | - | X |
| 56 | MG | DA | 3427 | - | - | - | X |
| 56 | MG | DA | 3433 | - | - | - | X |
| 56 | MG | DA | 3447 | - | - | - | X |
| 56 | MG | DA | 3450 | - | - | - | X |
| 56 | MG | DA | 3451 | - | - | - | X |
| 56 | MG | DA | 3452 | - | - | - | X |
| 56 | MG | DA | 3459 | - | - | - | X |
| 56 | MG | DA | 3460 | - | - | - | X |
| 56 | MG | DA | 3461 | - | - | - | X |
| 56 | MG | DA | 3486 | - | - | - | X |
| 56 | MG | DA | 3510 | - | - | - | X |
| 56 | MG | DA | 3515 | - | - | - | X |
| 56 | MG | DA | 3525 | - | - | - | X |
| 56 | MG | DA | 3530 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | DA | 3536 | - | - | - | X |
| 56 | MG | DA | 3537 | - | - | - | X |
| 56 | MG | DA | 3539 | - | - | - | X |
| 56 | MG | DA | 3540 | - | - | - | X |
| 56 | MG | DA | 3550 | - | - | - | X |
| 56 | MG | DA | 3552 | - | - | - | X |
| 56 | MG | DA | 3553 | - | - | - | X |
| 56 | MG | DA | 3558 | - | - | - | X |
| 56 | MG | DA | 3567 | - | - | - | X |
| 56 | MG | DA | 3572 | - | - | - | X |
| 56 | MG | DA | 3576 | - | - | - | X |
| 56 | MG | DA | 3585 | - | - | - | X |
| 56 | MG | DA | 3586 | - | - | - | X |
| 56 | MG | DA | 3598 | - | - | - | X |
| 56 | MG | DA | 3599 | - | - | - | X |
| 56 | MG | DA | 3600 | - | - | - | X |
| 56 | MG | DA | 3601 | - | - | - | X |
| 56 | MG | DA | 3615 | - | - | - | X |
| 56 | MG | DA | 3624 | - | - | - | X |
| 56 | MG | DA | 3625 | - | - | - | X |
| 56 | MG | DA | 3627 | - | - | - | X |
| 56 | MG | DA | 3629 | - | - | - | X |
| 56 | MG | DA | 3632 | - | - | - | X |
| 56 | MG | DA | 3646 | - | - | - | X |
| 56 | MG | DA | 3666 | - | - | - | X |
| 56 | MG | DA | 3677 | - | - | - | X |
| 56 | MG | DA | 3679 | - | - | - | X |
| 56 | MG | DA | 3692 | - | - | - | X |
| 56 | MG | DB | 201 | - | - | - | X |
| 56 | MG | DB | 203 | - | - | - | X |
| 56 | MG | DD | 302 | - | - | - | X |
| 56 | MG | DD | 303 | - | - | - | X |
| 56 | MG | DE | 302 | - | - | - | X |
| 56 | MG | DE | 303 | - | - | - | X |
| 56 | MG | DF | 302 | - | - | - | X |
| 56 | MG | DQ | 202 | - | - | - | X |
| 56 | MG | DT | 203 | - | - | - | X |
| 56 | MG | DV | 201 | - | - | - | X |

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 284877 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 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1466 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 31513 | 14026 | 5840 | 10181 | 1466 | | | |
| 1 | CA | 1461 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 31406 | 13979 | 5822 | 10145 | 1460 | | | |

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1809 | 1157 | 322 | 325 | 5 | | | |
| 2 | CB | 235 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1817 | 1160 | 325 | 327 | 5 | | | |

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | AC | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1434 | 896 | 277 | 260 | 1 | | | |
| 3 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1453 | 908 | 280 | 264 | 1 | | | |

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | AD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1520 | 960 | 283 | 272 | 5 | | | |
| 4 | CD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1537 | 968 | 287 | 276 | 6 | | | |

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 699 | 204 | 198 | 4 | | | |
| 5 | CE | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1115 | 706 | 206 | 199 | 4 | | | |

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 781 | 495 | 137 | 146 | 3 | | | |
| 6 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 784 | 496 | 137 | 148 | 3 | | | |

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1152 | 716 | 222 | 208 | 6 | | | |
| 7 | CG | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1149 | 715 | 222 | 206 | 6 | | | |

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 665 | 188 | 190 | 2 | | | |
| 8 | CH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1049 | 667 | 188 | 192 | 2 | | | |

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9 | AI | 125 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 863 | 542 | 164 | 157 | | | | |
| 9 | CI | 125 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 849 | 531 | 161 | 157 | | | | |

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 10 | AJ | 96 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 659 | 408 | 131 | 120 | | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10 | CJ | 96 | Total | C | N | O | | | |
| | | | 657 | 407 | 129 | 121 | 0 | 0 | 0 |

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 11 | AK | 115 | Total | C | N | O | S | | |
| | | | 843 | 524 | 160 | 156 | 3 | 0 | 0 |
| 11 | CK | 114 | Total | C | N | O | S | | |
| | | | 828 | 516 | 155 | 154 | 3 | 0 | 0 |

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 12 | AL | 122 | Total | C | N | O | S | | |
| | | | 909 | 570 | 179 | 159 | 1 | 0 | 0 |
| 12 | CL | 122 | Total | C | N | O | S | | |
| | | | 905 | 567 | 178 | 159 | 1 | 0 | 0 |

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 13 | AM | 115 | Total | C | N | O | S | | |
| | | | 814 | 503 | 166 | 144 | 1 | 0 | 0 |
| 13 | CM | 112 | Total | C | N | O | S | | |
| | | | 784 | 486 | 159 | 138 | 1 | 0 | 0 |

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 14 | AN | 59 | Total | C | N | O | S | | |
| | | | 473 | 300 | 98 | 71 | 4 | 0 | 0 |
| 14 | CN | 59 | Total | C | N | O | S | | |
| | | | 469 | 297 | 97 | 71 | 4 | 0 | 0 |

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | | |
| | | | 724 | 453 | 143 | 126 | 2 | 0 | 0 |
| 15 | CO | 88 | Total | C | N | O | S | | |
| | | | 724 | 453 | 143 | 126 | 2 | 0 | 0 |

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 646 | 413 | 122 | 110 | 1 | | | |
| 16 | CP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 661 | 421 | 126 | 113 | 1 | | | |

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |
| 17 | CQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 819 | 525 | 150 | 142 | 2 | | | |

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | AR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 514 | 329 | 98 | 87 | | | |
| 18 | CR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 514 | 329 | 98 | 87 | | | |

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 19 | AS | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 560 | 351 | 108 | 99 | 2 | | | |
| 19 | CS | 75 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 529 | 332 | 102 | 93 | 2 | | | |

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 438 | 154 | 120 | 2 | | | |
| 20 | CT | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 773 | 476 | 162 | 133 | 2 | | | |

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | CU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 180 | 112 | 41 | 27 | | | |

- Molecule 22 is a protein called YAEJ.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | AY | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1031 | 638 | 204 | 187 | 2 | | | |

- Molecule 23 is a RNA chain called P-site fMet-tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23 | AV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |
| 23 | CV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 24 | AX | 6 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 131 | 59 | 27 | 39 | 6 | | | |
| 24 | CX | 6 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 131 | 59 | 27 | 39 | 6 | | | |

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25 | BA | 2752 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59281 | 26384 | 11101 | 19045 | 2751 | | | |
| 25 | DA | 2722 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 58627 | 26093 | 10971 | 18843 | 2720 | | | |

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | BB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |
| 26 | DB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2131 | 1346 | 422 | 360 | 3 | | | |
| 27 | DD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 982 | 297 | 270 | 6 | | | |
| 28 | DE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 982 | 297 | 270 | 6 | | | |

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | BF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1576 | 1005 | 297 | 272 | 2 | | | |
| 29 | DF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1578 | 1007 | 297 | 272 | 2 | | | |

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1368 | 879 | 242 | 244 | 3 | | | |
| 30 | DG | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1361 | 874 | 241 | 243 | 3 | | | |

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | BH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1317 | 837 | 243 | 236 | 1 | | | |
| 31 | DH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1317 | 837 | 243 | 236 | 1 | | | |

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BI | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1066 | 687 | 184 | 194 | 1 | | | |
| 32 | DI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1057 | 682 | 182 | 192 | 1 | | | |

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 717 | 207 | 184 | 4 | | | |
| 33 | DN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 717 | 207 | 184 | 4 | | | |

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 923 | 583 | 168 | 168 | 4 | | | |
| 34 | DO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 923 | 583 | 168 | 168 | 4 | | | |

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 703 | 229 | 196 | 3 | | | |
| 35 | DP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 703 | 229 | 196 | 3 | | | |

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | BQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 36 | DQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | DR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 38 | BS | 110 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 865 | 544 | 172 | 149 | | | | |
| 38 | DS | 110 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 873 | 550 | 174 | 149 | | | | |

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BT | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1072 | 672 | 215 | 184 | 1 | | | |
| 39 | DT | 130 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1058 | 663 | 212 | 182 | 1 | | | |

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 40 | DU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BV | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 766 | 493 | 139 | 133 | 1 | | | |
| 41 | DV | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 770 | 496 | 140 | 133 | 1 | | | |

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 175 | 153 | 2 | | | |
| 42 | DW | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 552 | 171 | 152 | 2 | | | |

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 483 | 134 | 124 | 1 | | | |
| 43 | DX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 732 | 477 | 130 | 124 | 1 | | | |

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 503 | 145 | 131 | 6 | | | |
| 44 | DY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 781 | 502 | 145 | 128 | 6 | | | |

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BZ | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1454 | 929 | 256 | 267 | 2 | | | |
| 45 | DZ | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1451 | 925 | 253 | 270 | 3 | | | |

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | B0 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 594 | 368 | 125 | 100 | 1 | | | |
| 46 | D0 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 607 | 376 | 126 | 104 | 1 | | | |

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | B1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 745 | 469 | 144 | 131 | 1 | | | |
| 47 | D1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 745 | 469 | 144 | 131 | 1 | | | |

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | B2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |
| 48 | D2 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 584 | 361 | 118 | 103 | 2 | | | |

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49 | B3 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 458 | 293 | 87 | 78 | | | | |
| 49 | D3 | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 290 | 86 | 77 | | | | |

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B4 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 349 | 223 | 57 | 64 | 5 | | | |
| 50 | D4 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 349 | 223 | 57 | 64 | 5 | | | |

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 286 | 90 | 74 | 5 | | | |
| 51 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 451 | 283 | 89 | 74 | 5 | | | |

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 278 | 90 | 77 | 4 | | | |
| 52 | D6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 437 | 272 | 84 | 77 | 4 | | | |

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | B7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | D7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 402 | 248 | 97 | 55 | 2 | | | |

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 326 | 99 | 82 | 2 | | | |
| 54 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 326 | 99 | 82 | 2 | | | |

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55 | B9 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 297 | 182 | 66 | 46 | 3 | | | |
| 55 | D9 | 35 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 292 | 180 | 65 | 44 | 3 | | | |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | BA | 896 | Total | Mg | 0 | 0 |
| | | | 896 | 896 | | |
| 56 | AK | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DQ | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | DF | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | CV | 10 | Total | Mg | 0 | 0 |
| | | | 10 | 10 | | |
| 56 | B8 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | BE | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | DU | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | B1 | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | CD | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | BP | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | DR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | CA | 219 | Total 219 | Mg 219 | 0 | 0 |
| 56 | B5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | BB | 30 | Total 30 | Mg 30 | 0 | 0 |
| 56 | BT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | D8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BF | 7 | Total 7 | Mg 7 | 0 | 0 |
| 56 | AV | 18 | Total 18 | Mg 18 | 0 | 0 |
| 56 | BX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B2 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | AA | 348 | Total 348 | Mg 348 | 0 | 0 |
| 56 | BQ | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | D6 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | CX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | D7 | 1 | Total 1 | Mg 1 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | AD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | DD | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | CT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | D0 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | BG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | AI | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | BY | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | DE | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | B3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | BR | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | DA | 696 | Total 696 | Mg 696 | 0 | 0 |
| 56 | B7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BV | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | DO | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | BO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | D1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BZ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | D5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BD | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | AT | 1 | Total 1 | Mg 1 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 56 | DT | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | B0 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | AY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DB | 16 | Total 16 | Mg 16 | 0 | 0 |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57 | B5 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | B4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | AD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | CD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | B9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | BY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | DY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | D5 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | D4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | AN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | CN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | D6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | B6 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 58 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 58 | AA | 372 | Total 372 | O 372 | 0 | 0 |
| 58 | AD | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | AE | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | AI | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | AK | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | AL | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | AN | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | AT | 5 | Total 5 | O 5 | 0 | 0 |
| 58 | AY | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | AV | 16 | Total 16 | O 16 | 0 | 0 |
| 58 | AX | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | BA | 1491 | Total 1491 | O 1491 | 0 | 0 |
| 58 | BB | 46 | Total 46 | O 46 | 0 | 0 |
| 58 | BD | 10 | Total 10 | O 10 | 0 | 0 |
| 58 | BE | 5 | Total 5 | O 5 | 0 | 0 |
| 58 | BF | 5 | Total 5 | O 5 | 0 | 0 |
| 58 | BG | 5 | Total 5 | O 5 | 0 | 0 |
| 58 | BH | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | BN | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | BO | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | BP | 9 | Total 9 | O 9 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 58 | BQ | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | BR | 7 | Total 7 | O 7 | 0 | 0 |
| 58 | BT | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | BU | 7 | Total 7 | O 7 | 0 | 0 |
| 58 | BV | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | BW | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | BX | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | BY | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | B0 | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | B1 | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | B3 | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | B6 | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | B7 | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | B8 | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | B9 | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | CA | 330 | Total 330 | O 330 | 0 | 0 |
| 58 | CB | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | CC | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | CD | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | CE | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | CK | 2 | Total 2 | O 2 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 58 | CL | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | CN | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | CO | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | CQ | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | CT | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | CV | 13 | Total 13 | O 13 | 0 | 0 |
| 58 | CX | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | DA | 1028 | Total 1028 | O 1028 | 0 | 0 |
| 58 | DB | 40 | Total 40 | O 40 | 0 | 0 |
| 58 | DD | 8 | Total 8 | O 8 | 0 | 0 |
| 58 | DE | 11 | Total 11 | O 11 | 0 | 0 |
| 58 | DF | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | DG | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | DN | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | DO | 5 | Total 5 | O 5 | 0 | 0 |
| 58 | DP | 4 | Total 4 | O 4 | 0 | 0 |
| 58 | DR | 5 | Total 5 | O 5 | 0 | 0 |
| 58 | DT | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | DW | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | DY | 2 | Total 2 | O 2 | 0 | 0 |

Continued on next page...

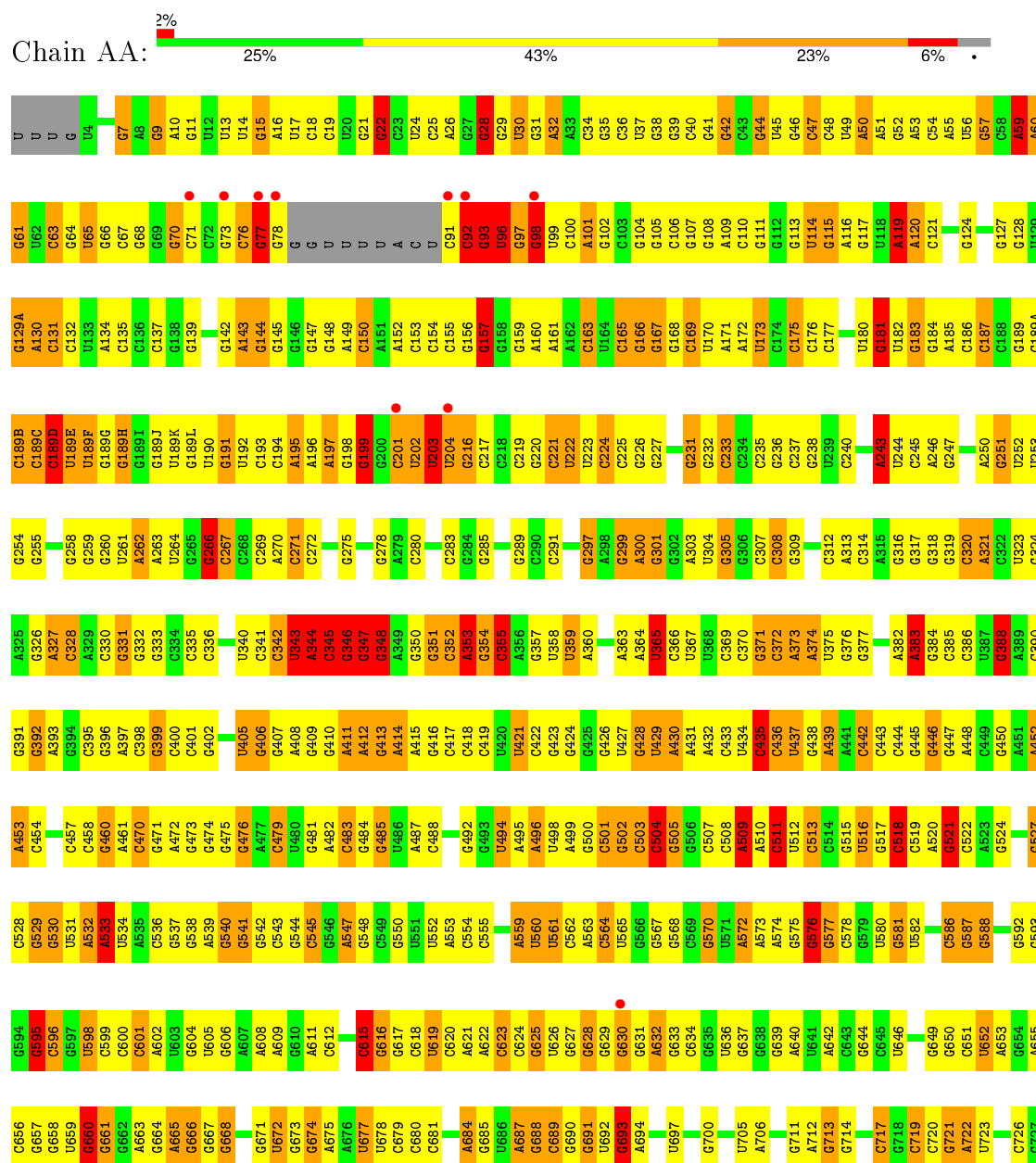
Continued from previous page...

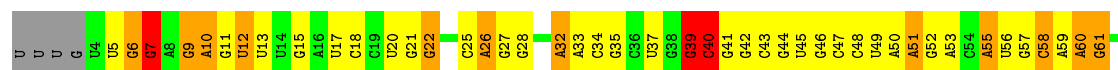
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 58 | D1 | 3 | Total 3 | O 3 | 0 | 0 |
| 58 | D3 | 1 | Total 1 | O 1 | 0 | 0 |
| 58 | D6 | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | D7 | 2 | Total 2 | O 2 | 0 | 0 |
| 58 | D8 | 4 | Total 4 | O 4 | 0 | 0 |

3 Residue-property plots

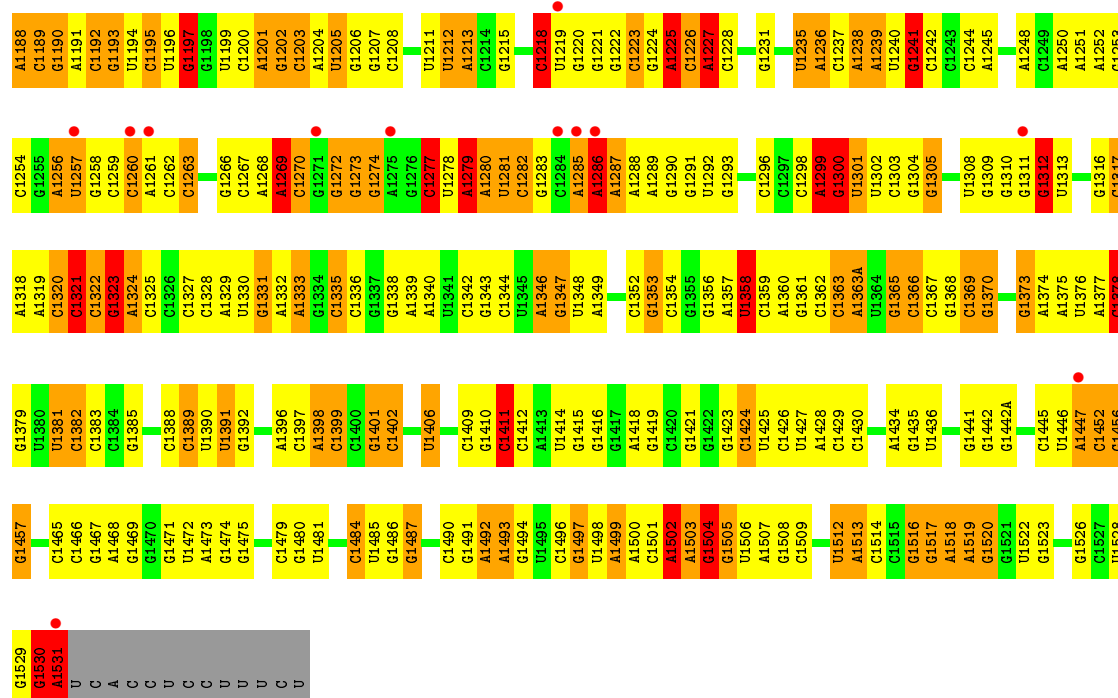
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 16S Ribosomal RNA

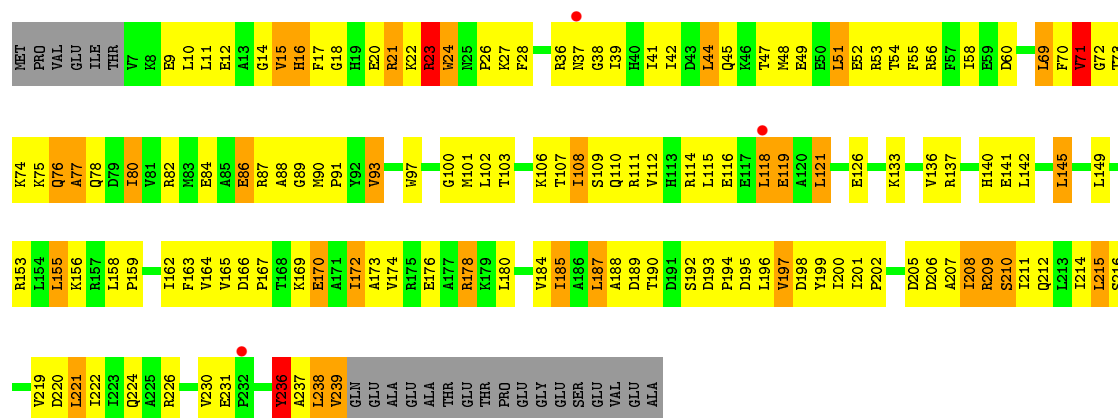




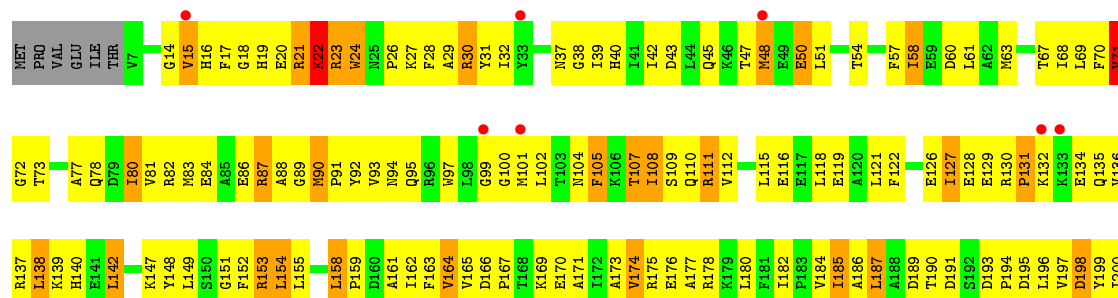
| | | | | | | | | | | | | | |
|-------|-------|------|------|------|------|------|------|------|------|------|------|-------|-------|
| A1123 | U1056 | C934 | A872 | U801 | C732 | A648 | G576 | C511 | U427 | U296 | C218 | G148 | G64 |
| G1124 | G1057 | A936 | A873 | A802 | A733 | G649 | G577 | U512 | G428 | G297 | C219 | A149 | U65 |
| U1125 | G1058 | C936 | G874 | G803 | G734 | G650 | C578 | C513 | U429 | A298 | G220 | G150 | G66 |
| U1126 | C1059 | A937 | C875 | U804 | C735 | A653 | G579 | C518 | A431 | C300 | C221 | C153 | G67 |
| G1127 | A1060 | A938 | C876 | C805 | C736 | G656 | U580 | C519 | A432 | A303 | U222 | G154 | G68 |
| C1128 | U1061 | C939 | G877 | C806 | A737 | G657 | G581 | A520 | C433 | U304 | G223 | C155 | G69 |
| C1129 | U1062 | C940 | G878 | C810 | C738 | G658 | U582 | G521 | U434 | G305 | G227 | A160 | C70 |
| A1130 | C1063 | G941 | C879 | C811 | U740 | G659 | C586 | G522 | C435 | G306 | G227 | A161 | C71 |
| G1131 | G1064 | G942 | C880 | C812 | G741 | G662 | G587 | A523 | C436 | G307 | G232 | A162 | C72 |
| C1132 | U1065 | U943 | G881 | U813 | G742 | G663 | G588 | G524 | U437 | C308 | G233 | C163 | C73 |
| G1133 | C1066 | G944 | C882 | U814 | G743 | G664 | G589 | C525 | C438 | G309 | C234 | U164 | G76 |
| C1134 | A1067 | A945 | C883 | A814 | C744 | G665 | C590 | G526 | A439 | G310 | C235 | C165 | G |
| G1135 | U1068 | A946 | U884 | A815 | C745 | G666 | C591 | G527 | A441 | G311 | G236 | G | G |
| U1136 | C1069 | G947 | G885 | A816 | C746 | G667 | U591 | G528 | C442 | C312 | G237 | G168 | G |
| C1137 | U1070 | C948 | G886 | C817 | U750 | G671 | G592 | G530 | C443 | C313 | C237 | G | U |
| G1138 | C1071 | G949 | G887 | G818 | U751 | G672 | G593 | U531 | C444 | A314 | C240 | A171 | U |
| C1139 | U1072 | G950 | G888 | A819 | C754 | G673 | G594 | A532 | C445 | G315 | C241 | A172 | U |
| G1140 | G1073 | G951 | G889 | U820 | G755 | G674 | C596 | A533 | C446 | G316 | C242 | U173 | U |
| C1141 | U1074 | G952 | G890 | G821 | C756 | A675 | G597 | U534 | C447 | G317 | C243 | A174 | A |
| G1142 | C1075 | A959 | U891 | C826 | C757 | A676 | U598 | A535 | C450 | G318 | U244 | C175 | C |
| C1143 | U1076 | U960 | A892 | U827 | U757 | G677 | C599 | C536 | U451 | G319 | C245 | C176 | U |
| G1144 | G1077 | U961 | C993 | A828 | G758 | U677 | C600 | G537 | A452 | A321 | A246 | C177 | C |
| C1145 | U1078 | G962 | G894 | G829 | A759 | U678 | C601 | G538 | A453 | G324 | G247 | C | C |
| A1146 | G1079 | G963 | G895 | G830 | G760 | C679 | A602 | A539 | A454 | A325 | A250 | U180 | G93 |
| C1147 | U1080 | A964 | U905 | G831 | G763 | G682 | U603 | G540 | G455 | A326 | A251 | U181 | U96 |
| U1148 | G1081 | A965 | C899 | U832 | C764 | G683 | G604 | G541 | G456 | A327 | U252 | U182 | G97 |
| C1149 | U1082 | G966 | A900 | C833 | G765 | A684 | U605 | A542 | A461 | G328 | U253 | C186 | G98 |
| U1150 | C1083 | C967 | A901 | U834 | C766 | G685 | G606 | C543 | C470 | A329 | G254 | C187 | U99 |
| C1151 | G1084 | A968 | G902 | C834 | A766 | U686 | A607 | G544 | C471 | C330 | G255 | C188 | C100 |
| U1152 | U1085 | C969 | G903 | U835 | A767 | G687 | A608 | G545 | G472 | G331 | U256 | C189 | A101 |
| C1153 | C1086 | G970 | C904 | G836 | A768 | G688 | G609 | G546 | C473 | C332 | G257 | G190 | G105 |
| G1154 | U1087 | G971 | U906 | G837 | G769 | G689 | G610 | A547 | C474 | A333 | G258 | C189B | C106 |
| U1155 | C1088 | C972 | G906 | C838 | C770 | G690 | C611 | G548 | C475 | C337 | A262 | C189D | G112 |
| G1156 | U1089 | G973 | A907 | U839 | G773 | G691 | C612 | G549 | C476 | C338 | A263 | U189E | G113 |
| C1157 | A1093 | A974 | A908 | C840 | G774 | G692 | G616 | U551 | C477 | C339 | G267 | U189F | U114 |
| G1158 | G1094 | A975 | A909 | U841 | G775 | G693 | G617 | G552 | C481 | U404 | G267 | G190G | G115 |
| U1159 | U1095 | C976 | C910 | C843 | G776 | A694 | C618 | U553 | C482 | G405 | C267 | G190H | A116 |
| G1160 | C1096 | A977 | U911 | C849 | G777 | G711 | U619 | C555 | C483 | G406 | C267 | G190I | G117 |
| C1161 | U1097 | C978 | C912 | U850 | A777 | G712 | C620 | C556 | C484 | G407 | C267 | G190L | U118 |
| C1162 | G1098 | G979 | A913 | G851 | G778 | G713 | A621 | G557 | C485 | A408 | A270 | U189L | C271 |
| U1168 | C1100 | C980 | A914 | U852 | C779 | G714 | G622 | G558 | C486 | G409 | C272 | G190 | A120 |
| A1169 | G1101 | U981 | A915 | G853 | A780 | G715 | G623 | G559 | C487 | G410 | A273 | C121 | C123 |
| C1170 | C1102 | C982 | G916 | G854 | A781 | A715 | C624 | A560 | C488 | G411 | A274 | C193 | G124 |
| U1171 | U1103 | A983 | G917 | C855 | A782 | G716 | G625 | U561 | C489 | G350 | G275 | C194 | U125 |
| G1174 | C1104 | C984 | A918 | C856 | C783 | G717 | G626 | G562 | C490 | A351 | G281 | A195 | G126 |
| A1175 | G1107 | G985 | A919 | G857 | G784 | G718 | G629 | C563 | C491 | C352 | G282 | A197 | G129A |
| C1176 | U1108 | A986 | U920 | C858 | A785 | C719 | G630 | A564 | C492 | A353 | C283 | G198 | A130 |
| G1177 | C1109 | G987 | U921 | A859 | G786 | G720 | G631 | G565 | C493 | G354 | C284 | G199 | C131 |
| U1178 | U1110 | C988 | G922 | A860 | U788 | G721 | A632 | U566 | C494 | A355 | G285 | G200 | C132 |
| C1179 | C1112 | C989 | A923 | G861 | U789 | A722 | G633 | G567 | C495 | C356 | G286 | C201 | G144 |
| G1175 | G1113 | G990 | C924 | C862 | A790 | G723 | G634 | G568 | C496 | A357 | G289 | U202 | G145 |
| A1176 | U1114 | U991 | G925 | U863 | G791 | U724 | G635 | G569 | A496 | C357 | G290 | U203 | G146 |
| C1177 | C1115 | U992 | G926 | A864 | A792 | G725 | G636 | C570 | C497 | G358 | G291 | G216 | G147 |
| G1178 | G1116 | G993 | G927 | A865 | U793 | G726 | G637 | G571 | C498 | A360 | G292 | C217 | |
| U1179 | U1117 | C994 | G928 | C866 | C795 | G727 | G638 | A572 | C499 | G361 | G292 | | |
| A1180 | C1118 | A994 | G929 | G867 | C796 | A728 | G644 | A573 | C500 | G362 | | | |
| C1181 | G1119 | C995 | C930 | C868 | C797 | U729 | G645 | A574 | C501 | A363 | | | |
| U1182 | U1120 | G996 | C931 | G869 | C798 | G730 | U646 | A575 | C502 | G364 | | | |
| G1183 | C1121 | C997 | C932 | G870 | C799 | A731 | U647 | G576 | C503 | A365 | | | |
| A1184 | U1122 | G998 | G933 | U871 | G800 | G732 | C647 | | | | | | |

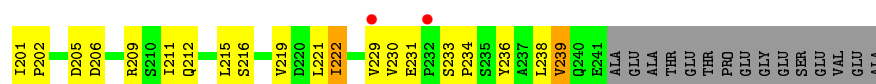


• Molecule 2: 30S Ribosomal Protein S2

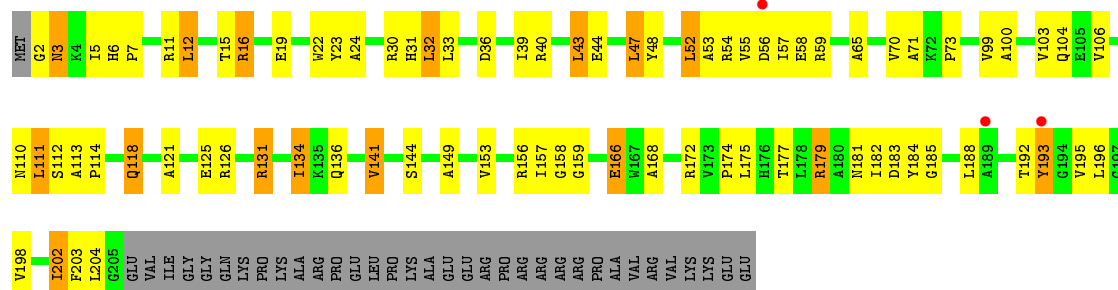


• Molecule 2: 30S Ribosomal Protein S2

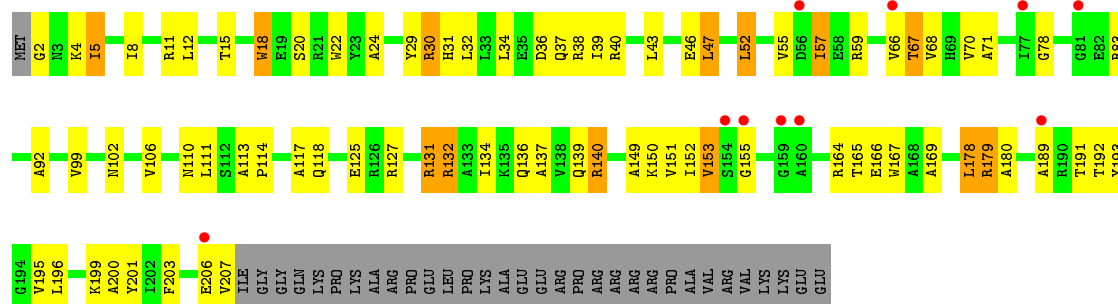




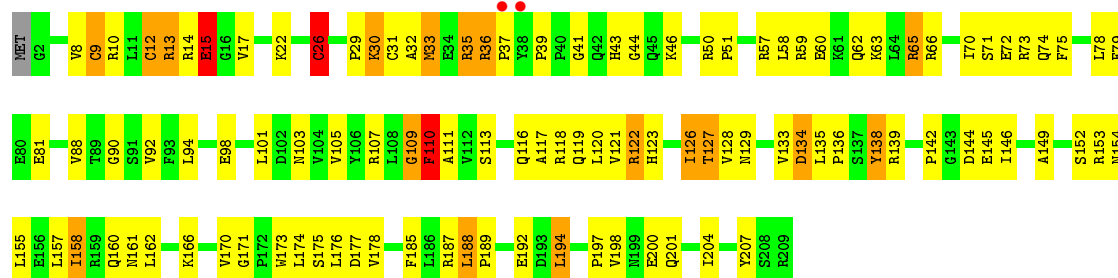
• Molecule 3: 30S Ribosomal Protein S3



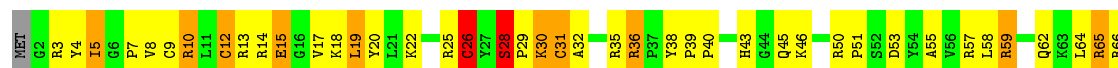
• Molecule 3: 30S Ribosomal Protein S3

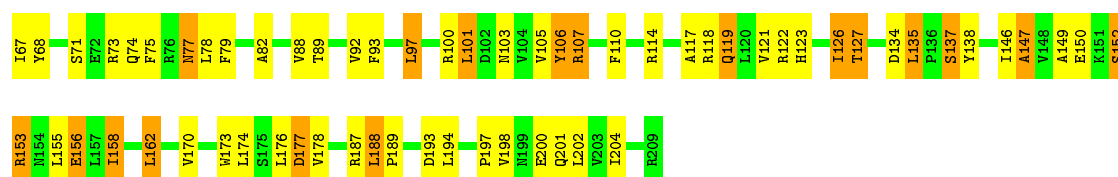


• Molecule 4: 30S Ribosomal Protein S4

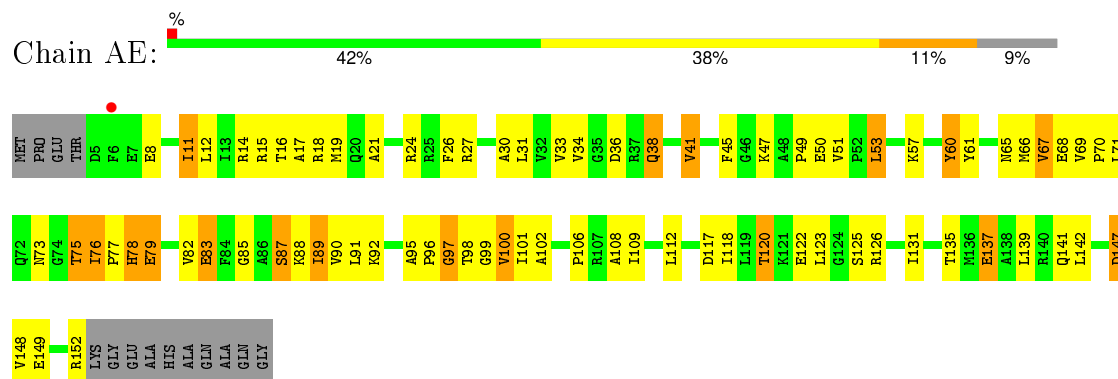


• Molecule 4: 30S Ribosomal Protein S4

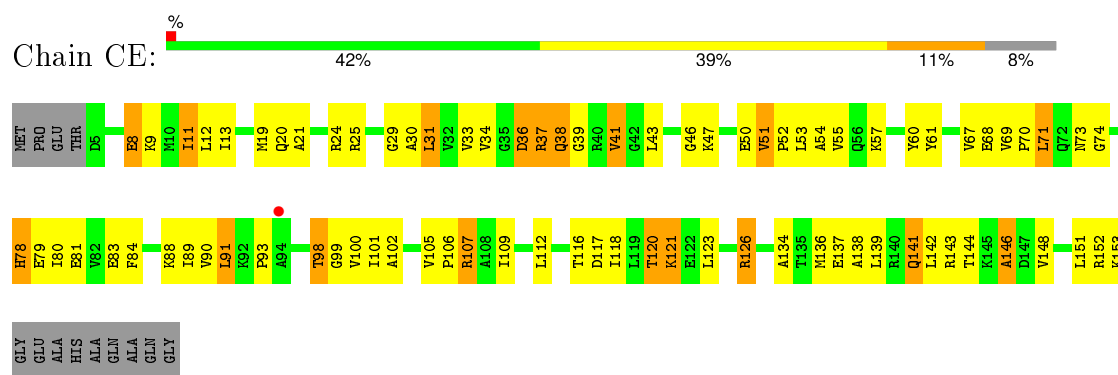




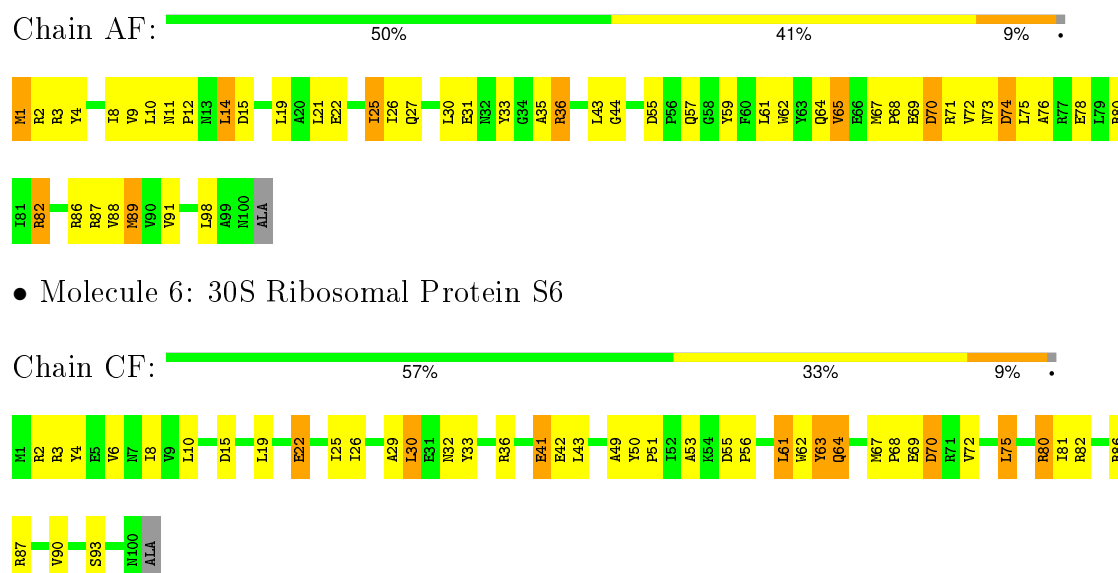
• Molecule 5: 30S Ribosomal Protein S5



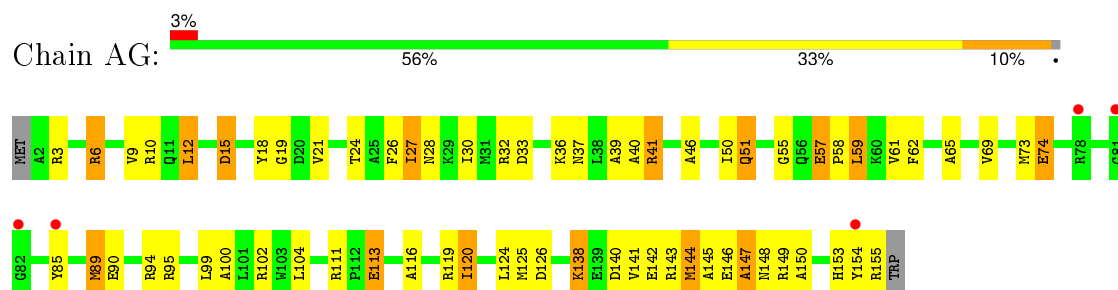
• Molecule 5: 30S Ribosomal Protein S5



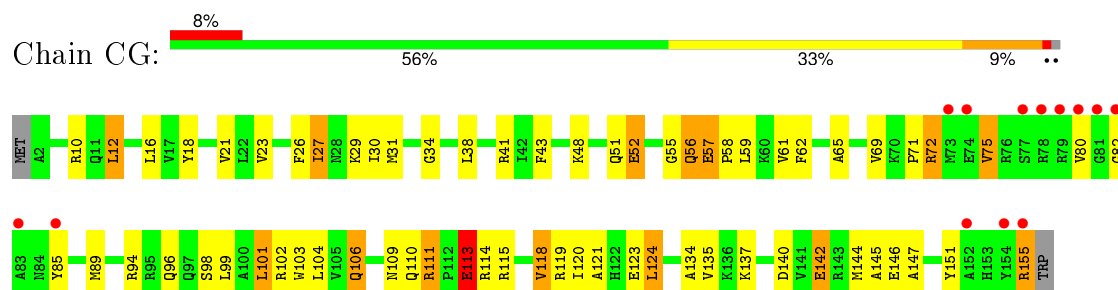
• Molecule 6: 30S Ribosomal Protein S6



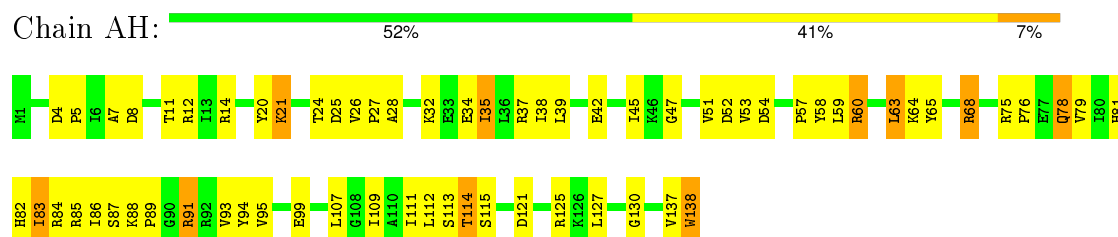
- Molecule 7: 30S Ribosomal Protein S7



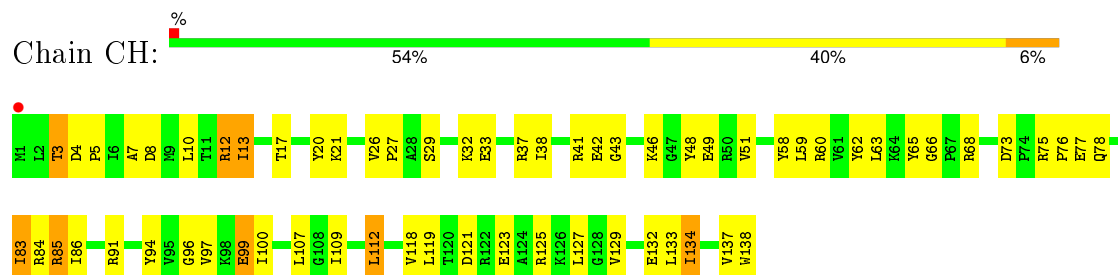
- Molecule 7: 30S Ribosomal Protein S7



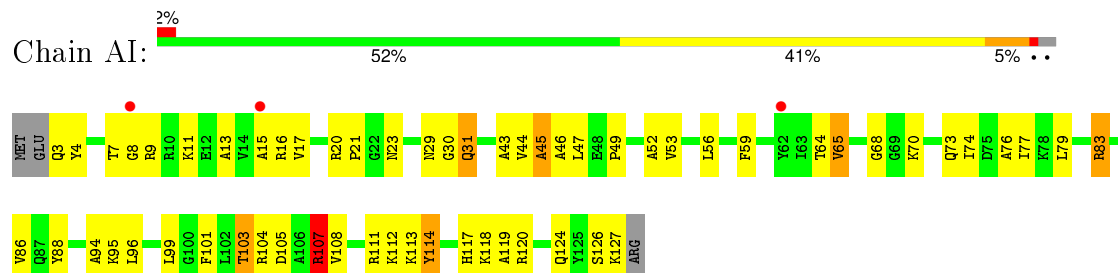
- Molecule 8: 30S Ribosomal Protein S8



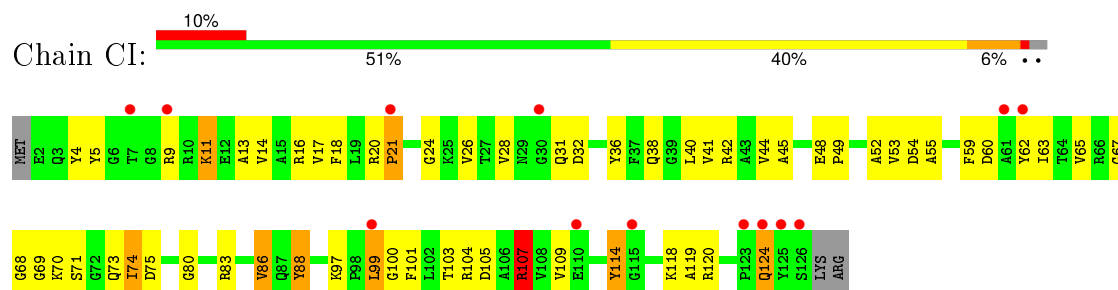
- Molecule 8: 30S Ribosomal Protein S8



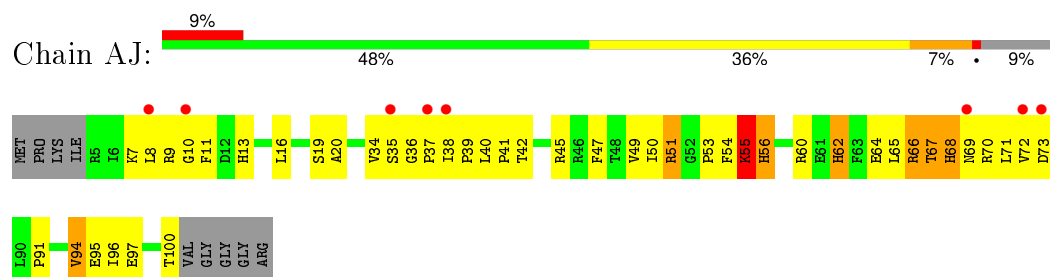
- Molecule 9: 30S Ribosomal Protein S9



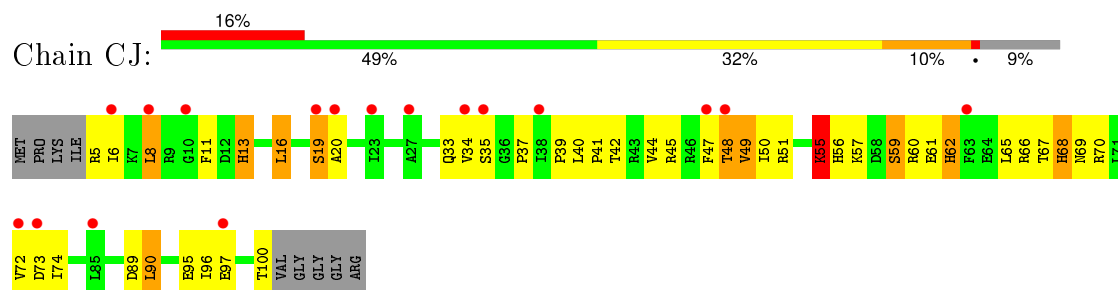
- Molecule 9: 30S Ribosomal Protein S9



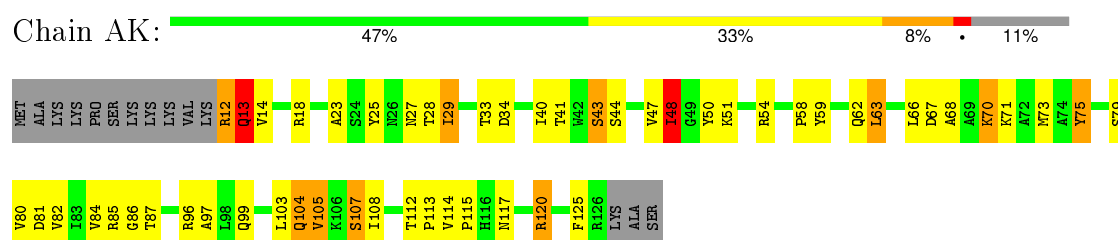
- Molecule 10: 30S Ribosomal Protein S10



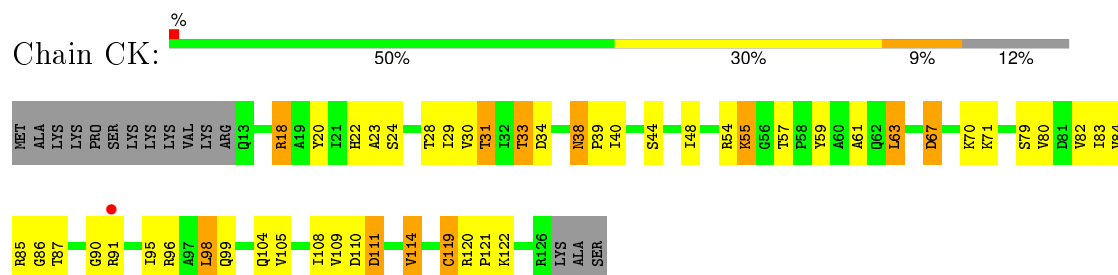
- Molecule 10: 30S Ribosomal Protein S10



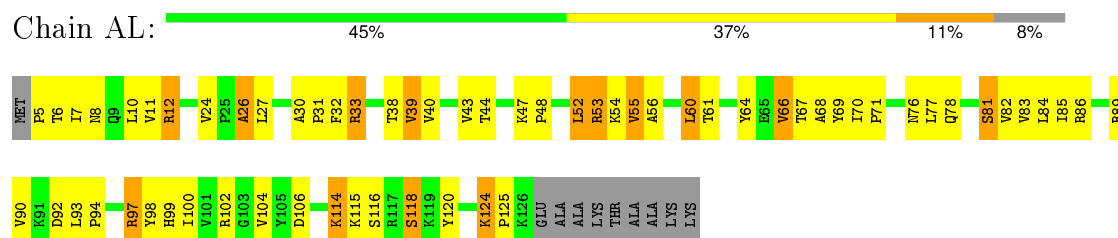
- Molecule 11: 30S Ribosomal Protein S11



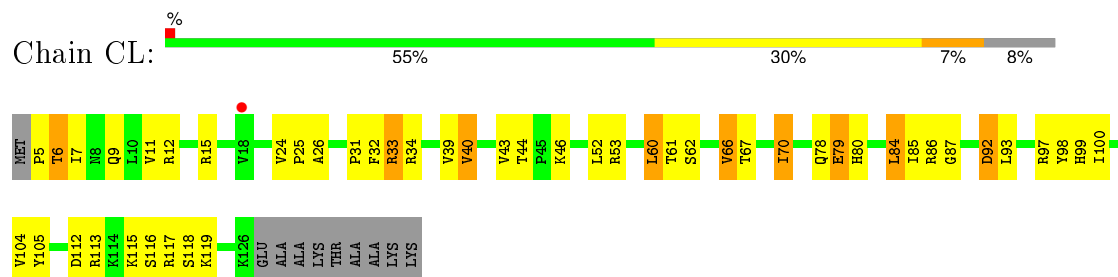
- Molecule 11: 30S Ribosomal Protein S11



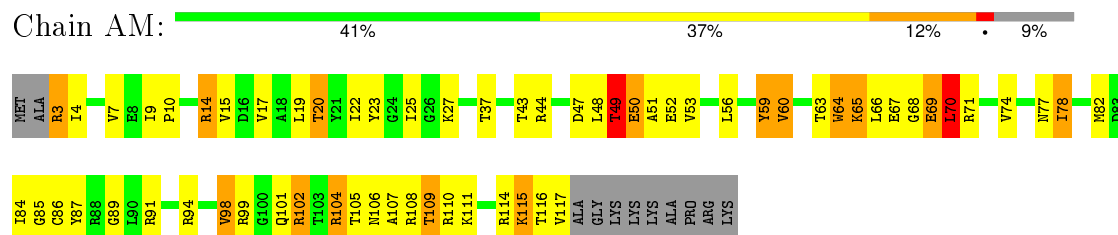
- Molecule 12: 30S Ribosomal Protein S12



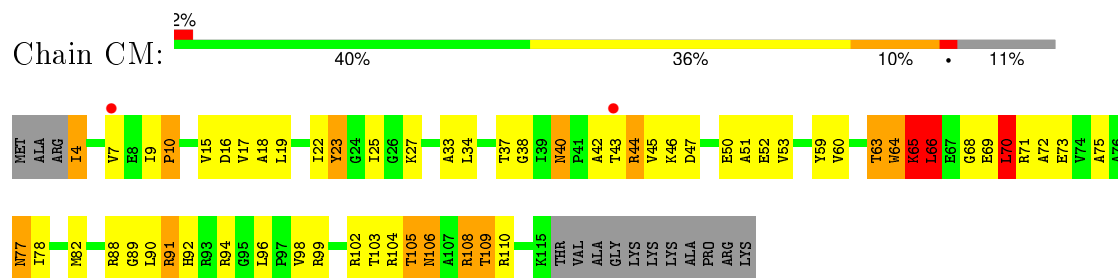
- Molecule 12: 30S Ribosomal Protein S12



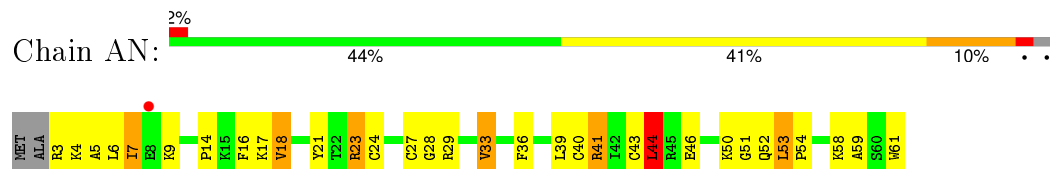
- Molecule 13: 30S Ribosomal Protein S13



- Molecule 13: 30S Ribosomal Protein S13



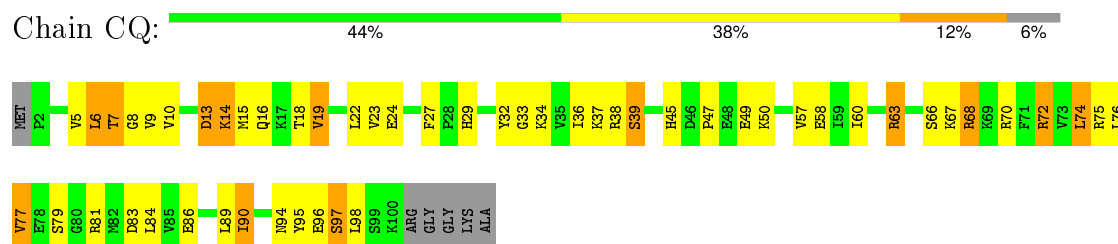
- Molecule 14: 30S Ribosomal Protein S14



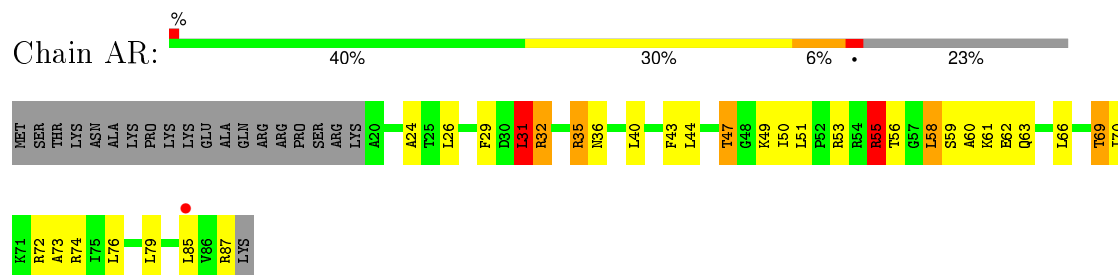
- Molecule 14: 30S Ribosomal Protein S14



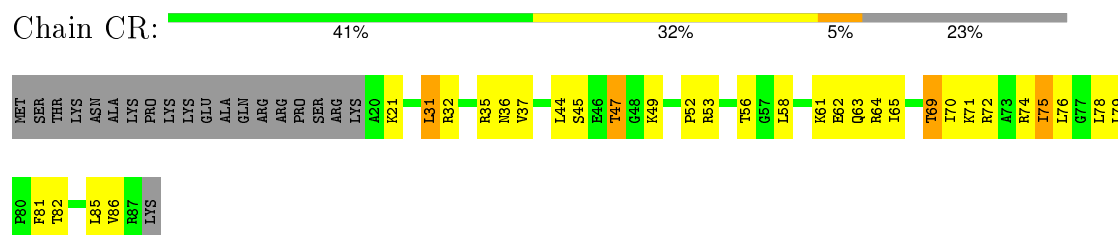
- Molecule 17: 30S Ribosomal Protein S17



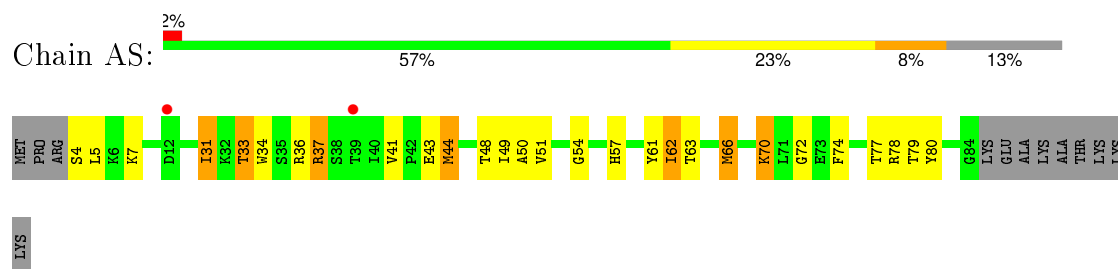
- Molecule 18: 30S Ribosomal Protein S18



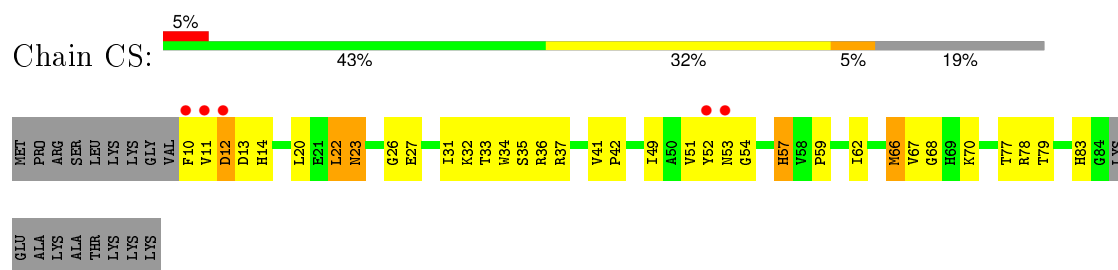
- Molecule 18: 30S Ribosomal Protein S18



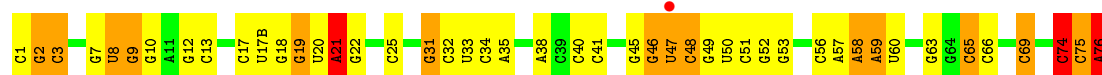
- Molecule 19: 30S Ribosomal Protein S19



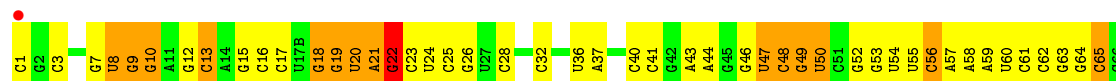
- Molecule 19: 30S Ribosomal Protein S19



- Molecule 20: 30S Ribosomal Protein S20



• Molecule 23: P-site fMet-tRNA



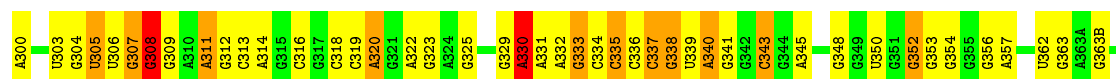
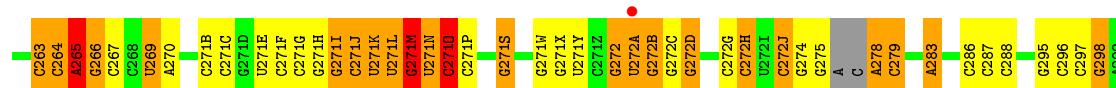
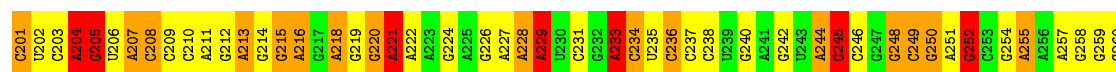
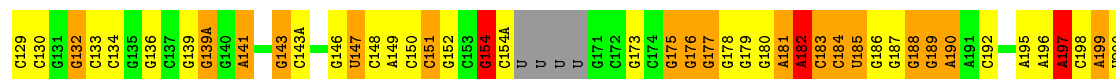
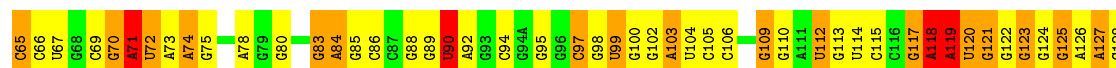
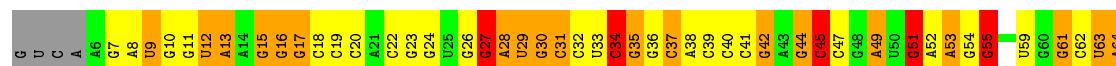
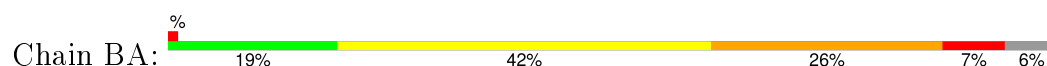
• Molecule 24: mRNA



• Molecule 24: mRNA

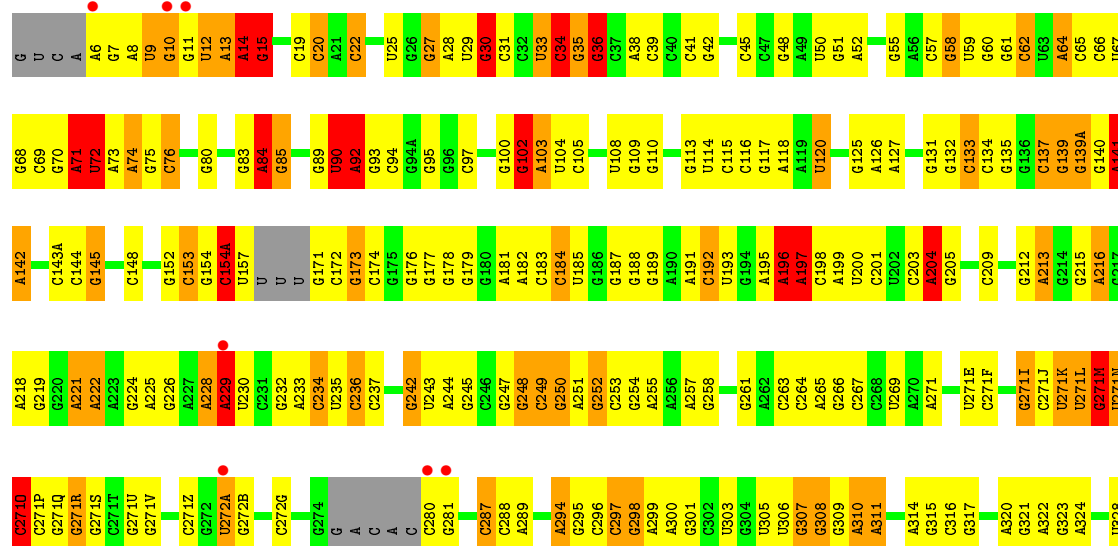


• Molecule 25: 23S Ribosomal RNA



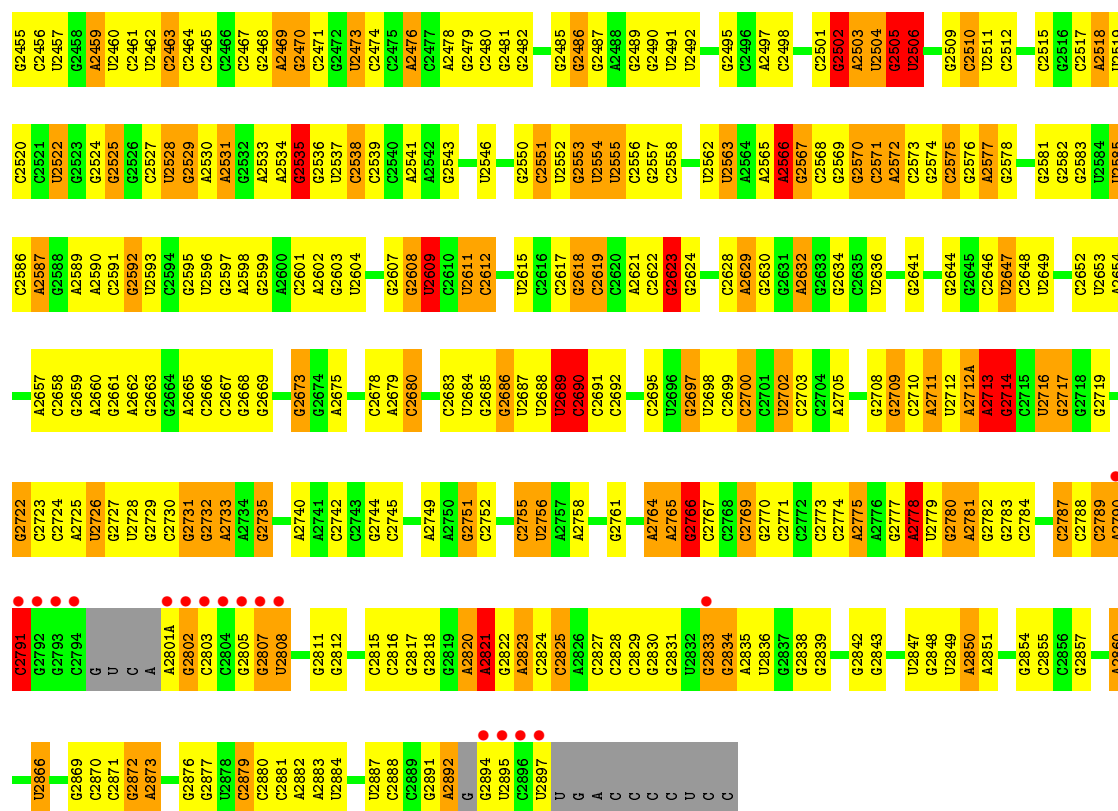


| | | | | | | | | | | | |
|-------|-------|---|-------|-------|-------|-------|-------|--------|-------|--------|-------|
| G2270 | U2197 | G | U2076 | A2015 | C1887 | A1812 | C1751 | C1598 | U | G1470 | G1343 |
| G2271 | A2198 | C | A2077 | U2016 | G1888 | G1813 | C1752 | C1599 | A | A1471 | G1344 |
| A2272 | C2200 | C | U2078 | U2017 | A1889 | G1814 | G1753 | C1600 | C | A1472 | G1345 |
| G2273 | C2201 | C | U2079 | G2018 | G1890 | A1815 | G1754 | C1601 | G | G1473 | G1346 |
| G2274 | C2202 | C | G2081 | A2019 | C1893 | G1816 | A1755 | U1602 | G1537 | | G1347 |
| G2275 | C2203 | C | A2082 | A2020 | G1958 | G1817 | G1756 | A1603 | G1538 | | G1348 |
| G2276 | U2203 | C | G2082 | C2021 | A1960 | U1818 | U1757 | C1604 | G1539 | C1476 | G1349 |
| G2277 | C2205 | C | G2083 | U2022 | G1961 | U1819 | G1758 | C1605 | U1540 | A1477 | A1349 |
| G2278 | A2206 | U | G2084 | G2023 | C1962 | U1820 | A1759 | G1606 | G1541 | G1478 | C1350 |
| G2279 | C2207 | C | C2085 | U2024 | U1963 | G1823 | G1760 | C1607 | A1542 | G1479 | C1351 |
| G2280 | A2208 | C | U2086 | C2025 | G1964 | C1761 | A1608 | C1608 | C1543 | G1480 | U1352 |
| G2281 | C2209 | G | C2087 | G2026 | C1965 | A1762 | U1671 | A1609 | A1544 | U1481 | A1353 |
| G2282 | U2218 | G | G2088 | G2027 | A1901 | A1825 | G1763 | U1672 | A1545 | G1482 | A1354 |
| G2283 | G2220 | G | U2089 | U2028 | C1967 | G1826 | G1764 | U1673 | C1546 | G1484 | A1355 |
| G2284 | | U | G2090 | G2029 | G1968 | C1827 | C1765 | G1674 | C1547 | G1485 | |
| G2285 | G2223 | U | U2091 | A2030 | G1969 | G1828 | U1766 | C1612 | C1548 | A1486 | G1358 |
| G2286 | A2224 | G | U2092 | G2031 | A1970 | A1829 | C1767 | G1613 | C1549 | G1487 | A1359 |
| A2287 | A2225 | G | G2093 | G2032 | A1971 | C1830 | U1768 | A1614 | C1550 | U1488 | A1360 |
| G2288 | C2226 | G | U2094 | A2033 | G1972 | G1831 | G1769 | G1621 | C1551 | U1489 | A1361 |
| A2289 | A2227 | G | C2095 | U2034 | U1973 | C1832 | G1770 | G1622 | G1552 | A1490 | C1362 |
| G2290 | G2228 | G | U2096 | U2035 | C1974 | U1833 | G1771 | G1623 | A1553 | G1491 | C1363 |
| U2291 | C2229 | G | G2097 | G2036 | G1975 | U1834 | G1772 | G1624 | A1554 | G1492 | G1364 |
| C2292 | G2230 | A | U2098 | G2037 | U1976 | G1835 | A1773 | G1625 | A1555 | C1493 | A1365 |
| C2293 | C2231 | G | U2099 | G2038 | A1977 | C1836 | C1774 | G1626 | C1556 | A1494 | G1366 |
| C2294 | U2232 | G | G2100 | C2039 | A1978 | C1837 | U1775 | U1627 | C1557 | A1495 | A1367 |
| C2295 | U2233 | C | G2101 | G2040 | G1979 | C1838 | G1776 | U1628 | A1558 | A1496 | G1368 |
| G2296 | G2234 | U | U2102 | U2041 | G1980 | G1839 | U1777 | U1629 | C1559 | U1497 | G1369 |
| G2297 | C2235 | C | A2042 | A2042 | A1918 | U1840 | U1778 | C1631 | G1560 | C1498 | C1370 |
| G2298 | A2236 | C | G2098 | G2043 | C1981 | A1841 | U1779 | C1632 | G1561 | G1499 | G1371 |
| G2299 | C2237 | C | C2044 | C2044 | C1982 | G1843 | G1780 | G1633 | G1562 | G1500 | U1372 |
| G2300 | G2238 | U | C2045 | C2045 | C1983 | C1844 | G1781 | U1632 | G1563 | C1501 | C1373 |
| G2301 | G2239 | G | G2046 | G2046 | G1984 | G1845 | C1782 | U1633 | C1564 | C1502 | G1374 |
| | G2240 | G | | | U1924 | G1846 | C1783 | U1634 | C1565 | U1503 | C1375 |
| G2304 | A2241 | A | U | G2049 | C1988 | A1847 | A1784 | C1635 | C1566 | C1504 | G1376 |
| A2305 | G2242 | A | G | A2050 | C1989 | A1848 | U1785 | C1636 | A1567 | G1505 | G1377 |
| G2306 | U2243 | U | C | A2051 | U1926 | G1849 | A1786 | A1631A | G1568 | G1441 | A1378 |
| G2307 | U2244 | A | C | G2052 | A1927 | G1850 | C1787 | G1633 | A1569 | A1507 | A1379 |
| G2308 | U2245 | A | U | G2053 | U1928 | G1851 | C1788 | G1634 | A1570 | G1444 | G1380 |
| A2309 | G2246 | A | A | A2054 | G1929 | A1854 | U1789 | U1635 | A1571 | C1509 | G1381 |
| G2310 | A2247 | C | G | C2055 | U1930 | G1855 | C1790 | C1636 | A1572 | A1509A | G1382 |
| A2311 | G2248 | C | G | G2056 | U1931 | G1856 | U1791 | A1637 | G1573 | A1509B | C1383 |
| U2312 | U2249 | C | A | A2057 | G1932 | G1857 | G1792 | C1637 | G1510 | G1447 | A1384 |
| C2313 | C2250 | C | U | A2058 | C1933 | G1858 | C1793 | U1638 | C1511 | G1448 | G1385 |
| C2314 | G2251 | C | U | A2059 | G1934 | A1859 | U1794 | U1639 | G1577 | A1449 | C1386 |
| G2315 | G2252 | U | G | A2060 | A1936 | G1862 | C1795 | C1640 | U1578 | G1450 | G1387 |
| G2316 | G2253 | G | U | G2061 | A1937 | G1862 | U1796 | G1642 | A1579 | G1450A | G1388 |
| C2317 | C2254 | G | U | A2062 | A1938 | G1863 | C1797 | G1647 | U1518 | U1453 | U1390 |
| G2318 | G2255 | C | G | C2063 | A1939 | U1864 | U1798 | U1648 | G1519 | G1455 | U1391 |
| G2319 | G2256 | G | G | G2064 | U1940 | G1865 | G1799 | G1649 | G1520 | G1456 | A1392 |
| A2320 | U2257 | G | A | C2065 | C1941 | C1866 | C1800 | G1650 | G1523 | A1457 | A1393 |
| G2321 | C2258 | A | U | G2066 | C1942 | A1876 | G1801 | G1651 | G1524 | C1458 | U1394 |
| G2322 | G2259 | G | G | G2067 | C2006 | A1877 | A1802 | G1652 | A1586 | C1459 | A1395 |
| G2323 | C2260 | C | C | U2068 | G1945 | C1877 | C1803 | C1653 | A1587 | G1460 | U1396 |
| C2324 | G2261 | C | C | G2069 | U1946 | C1878 | A1804 | G1654 | C1588 | A1461 | U1397 |
| G2325 | U2262 | U | U | G2070 | C2007 | C1879 | C1805 | A1654 | G1592 | G1464 | C1398 |
| G2326 | C2263 | G | U | A2071 | G1948 | U1880 | U1806 | U1739 | G1593 | C1465 | G1399 |
| A2327 | U2265 | U | U | G2072 | U2011 | G1883 | G1807 | C1655 | G1594 | G1466 | G1400 |
| G2328 | G2266 | G | G | G2073 | A2012 | A1884 | | C1657 | G1595 | G1467 | G1401 |
| A2329 | U2267 | A | A | U2074 | U1951 | A1885 | A1810 | G1658 | C1531 | C1467 | C1402 |
| G2330 | A2269 | A | A | U2075 | A2014 | C1886 | G1811 | U1659 | A1597 | G | C1403 |



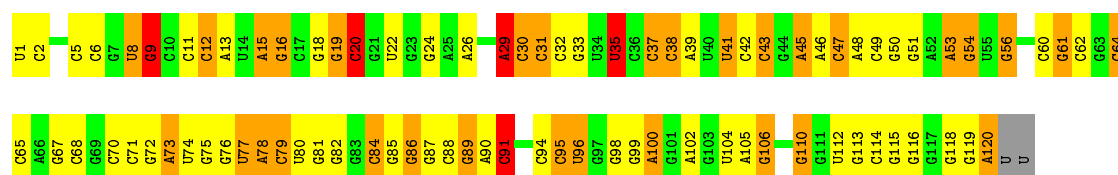


WORLDWIDE
PDB
PROTEIN DATA BANK



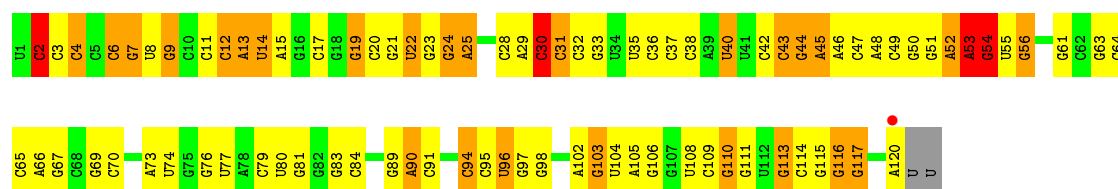
● Molecule 26: 5S Ribosomal RNA

Chain BB: 28% 41% 25%



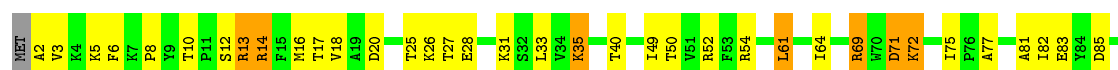
● Molecule 26: 5S Ribosomal RNA

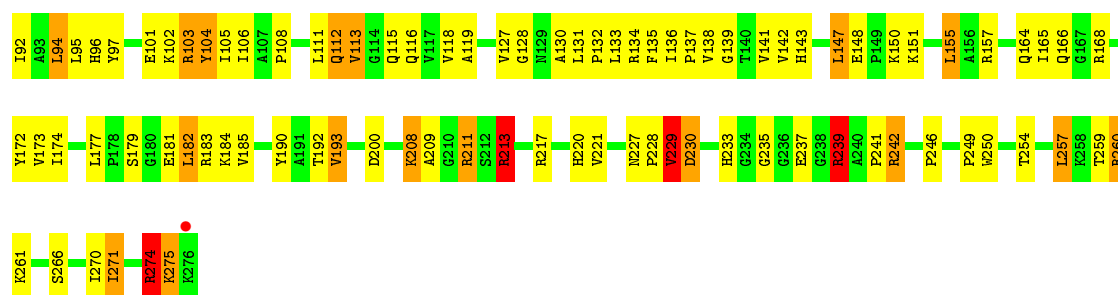
Chain DB: 28% 46% 21%



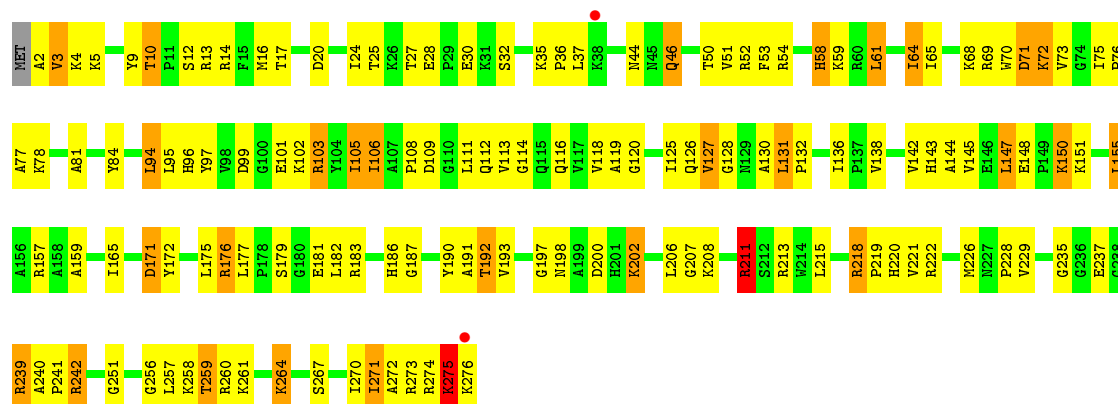
● Molecule 27: 50S Ribosomal Protein L2

Chain BD: 55% 35% 9%

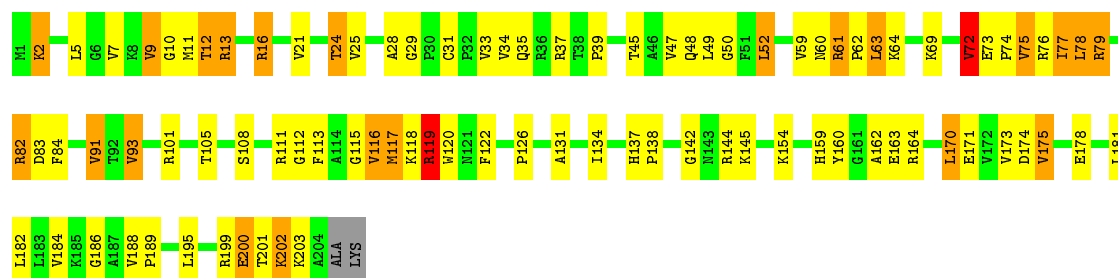




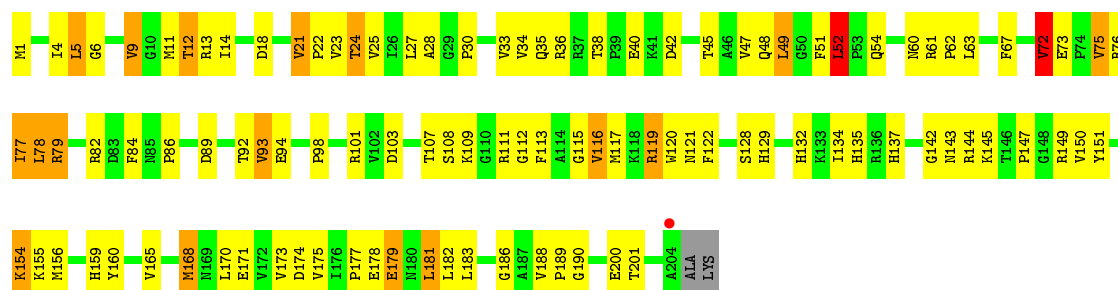
• Molecule 27: 50S Ribosomal Protein L2



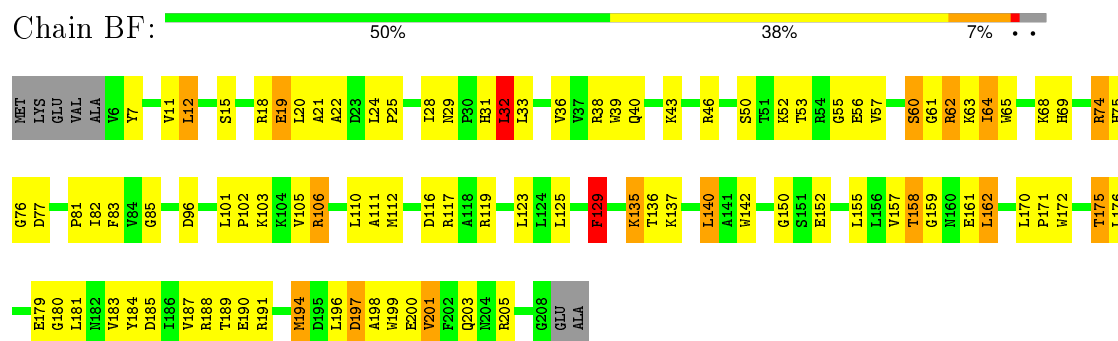
• Molecule 28: 50S Ribosomal Protein L3



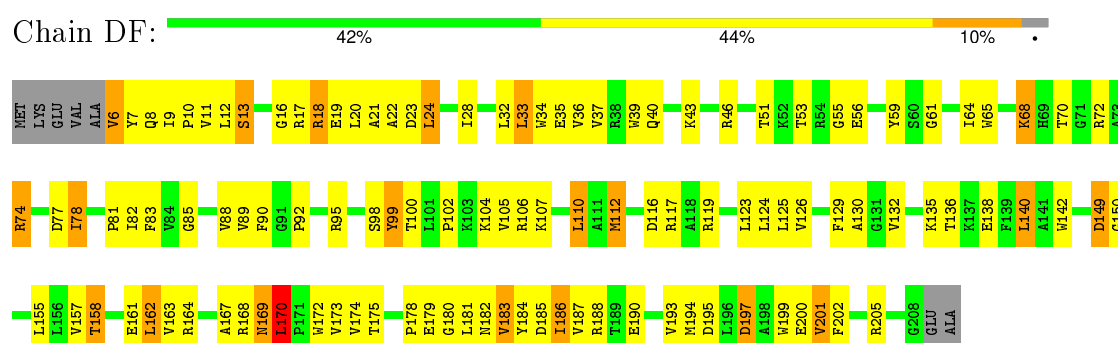
• Molecule 28: 50S Ribosomal Protein L3



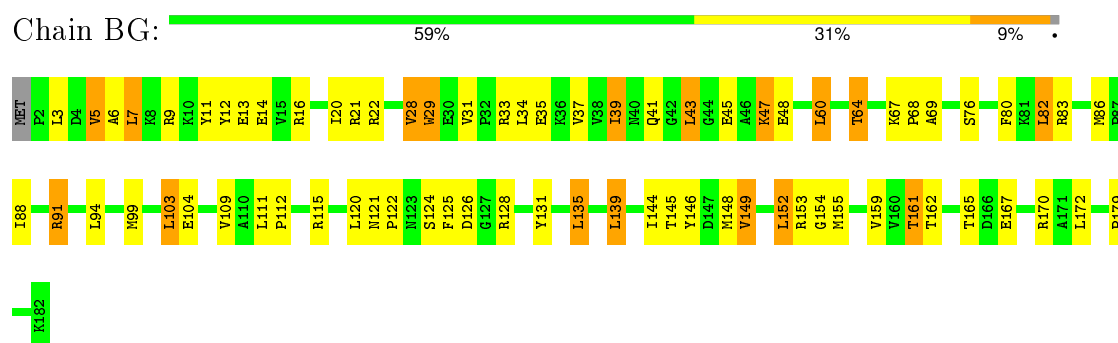
- Molecule 29: 50S Ribosomal Protein L4



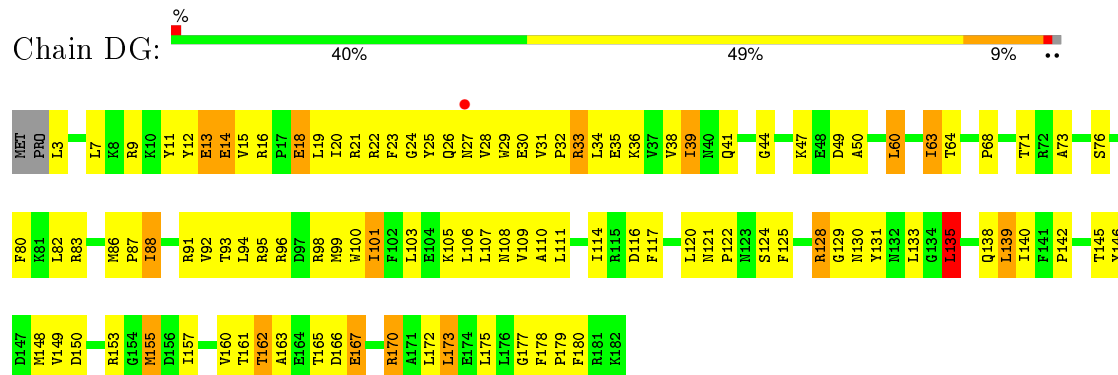
- Molecule 29: 50S Ribosomal Protein L4



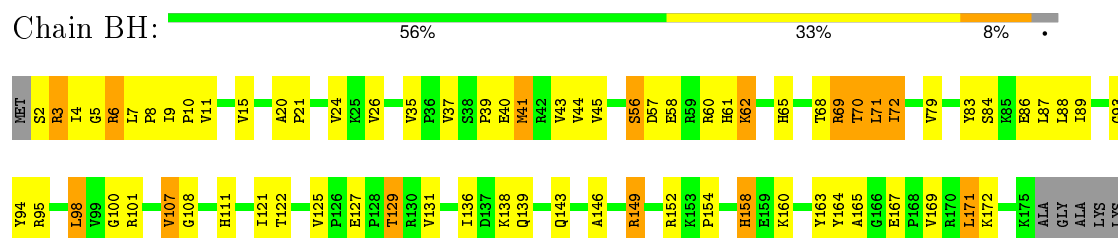
- Molecule 30: 50S Ribosomal Protein L5



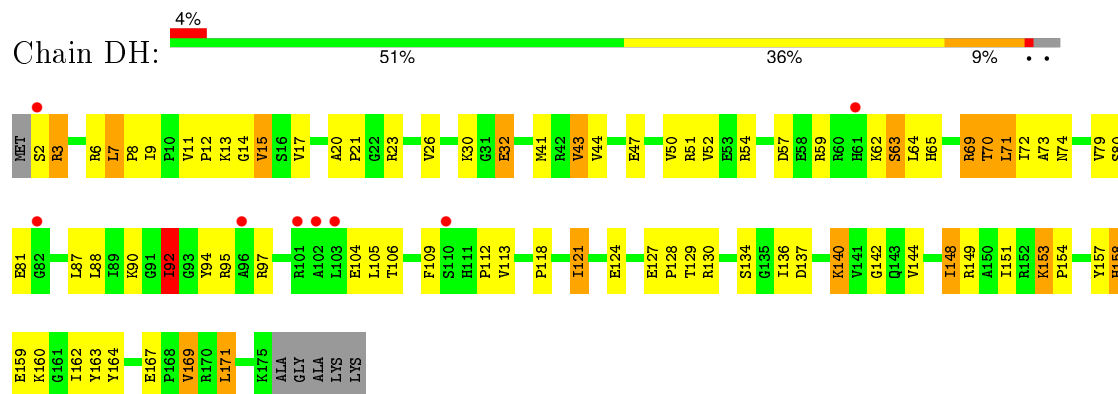
- Molecule 30: 50S Ribosomal Protein L5



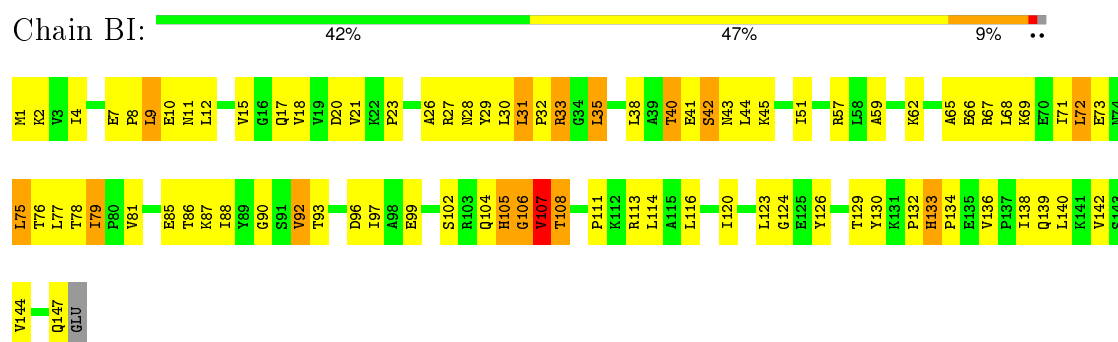
- Molecule 31: 50S Ribosomal Protein L6



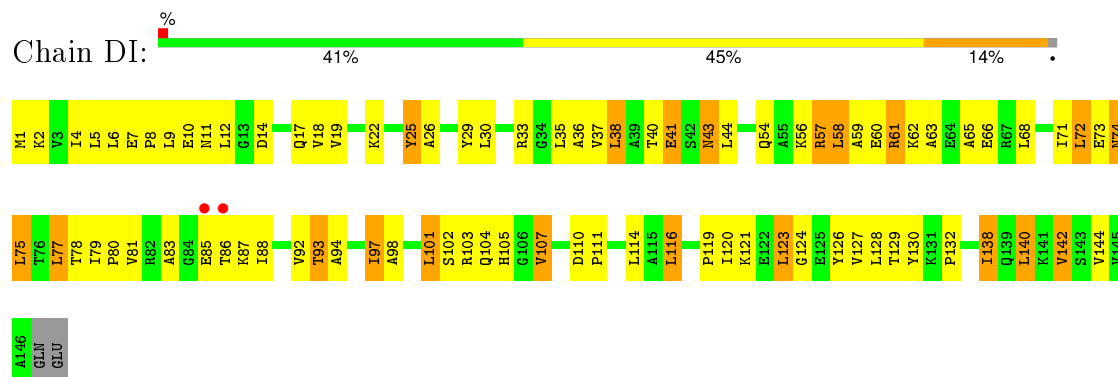
- Molecule 31: 50S Ribosomal Protein L6



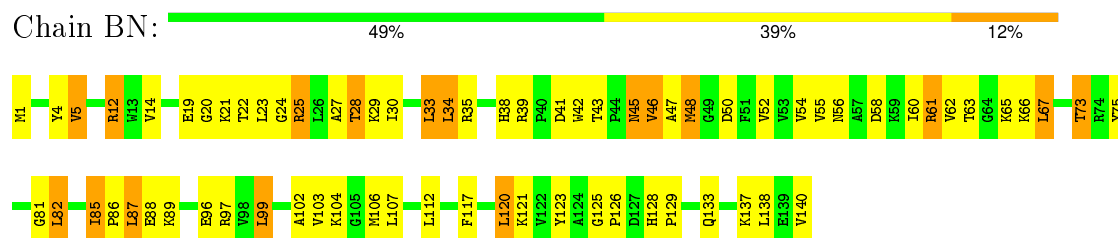
- Molecule 32: 50S Ribosomal Protein L9



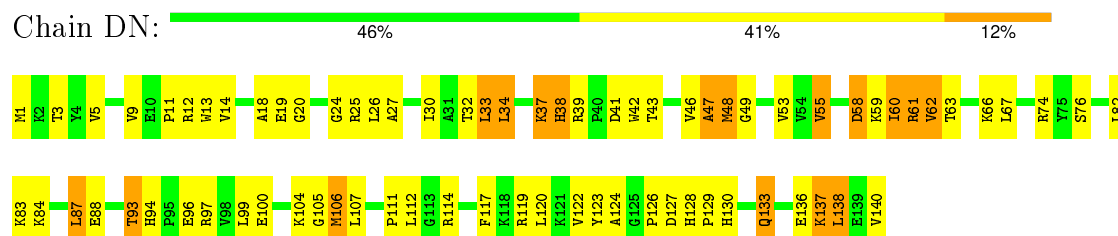
- Molecule 32: 50S Ribosomal Protein L9



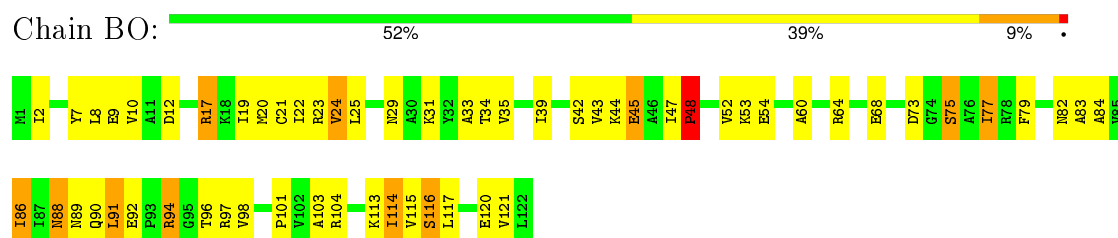
- Molecule 33: 50S Ribosomal Protein L13



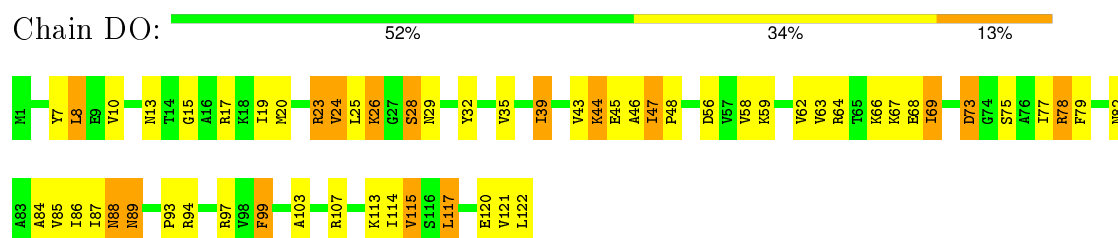
• Molecule 33: 50S Ribosomal Protein L13



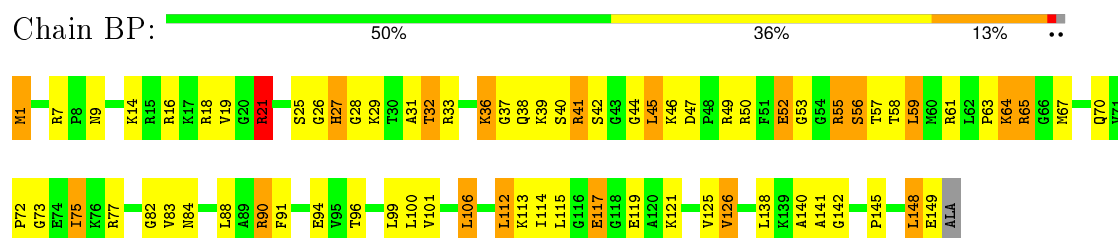
• Molecule 34: 50S Ribosomal Protein L14



• Molecule 34: 50S Ribosomal Protein L14

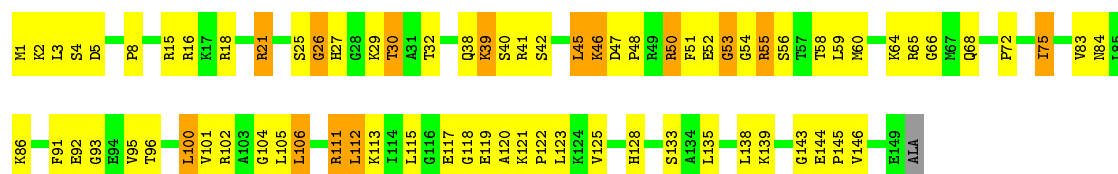


• Molecule 35: 50S Ribosomal Protein L15

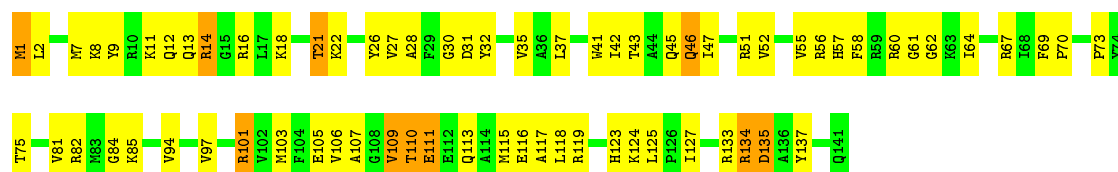


• Molecule 35: 50S Ribosomal Protein L15

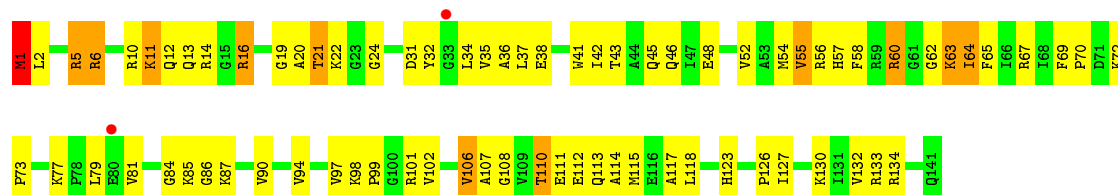




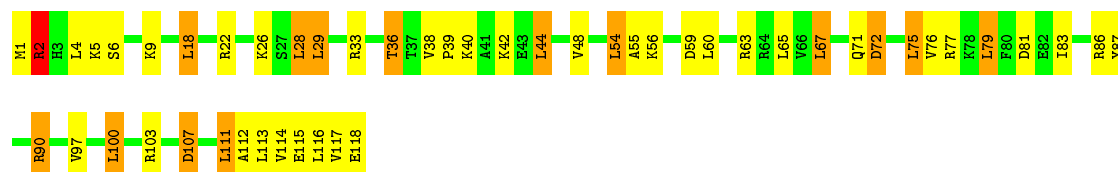
• Molecule 36: 50S Ribosomal Protein L16



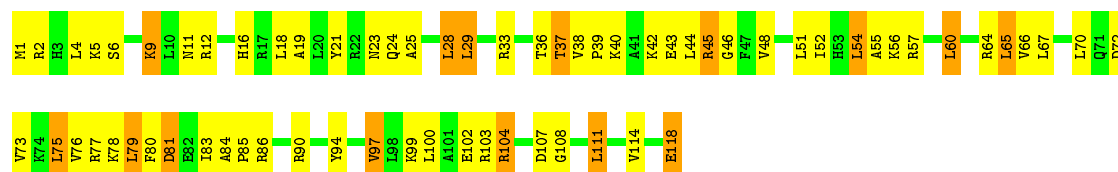
• Molecule 36: 50S Ribosomal Protein L16



• Molecule 37: 50S Ribosomal Protein L17

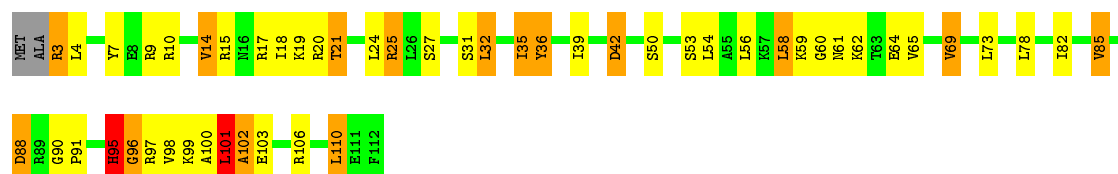


• Molecule 37: 50S Ribosomal Protein L17



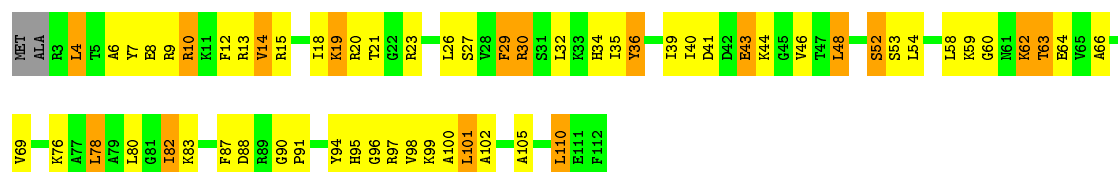
• Molecule 38: 50S Ribosomal Protein L18





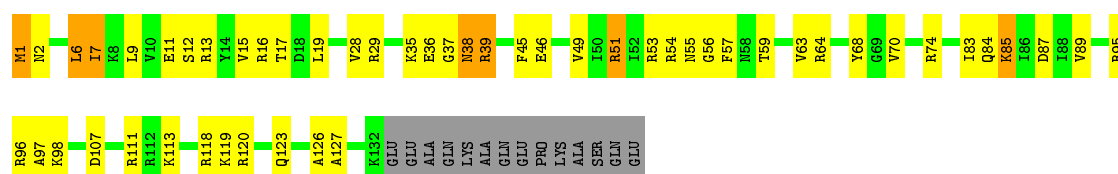
• Molecule 38: 50S Ribosomal Protein L18

Chain DS: 44% 40% 14%



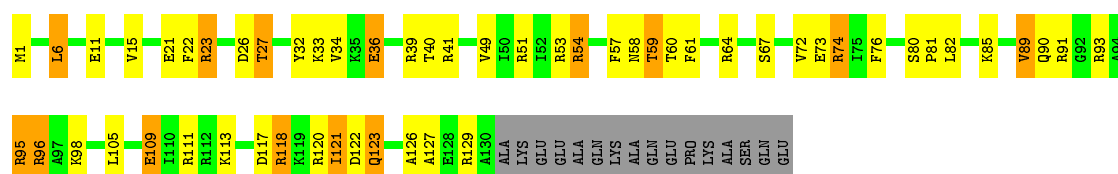
• Molecule 39: 50S Ribosomal Protein L19

Chain BT: 55% 31% 5% 10%



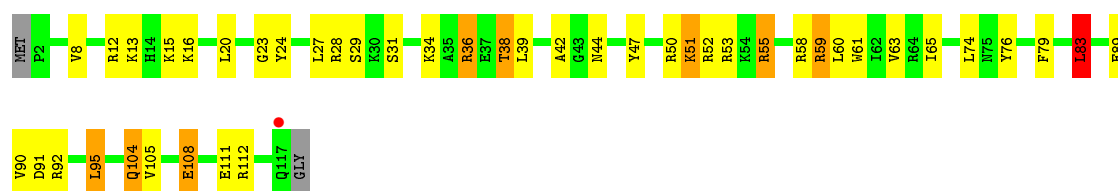
• Molecule 39: 50S Ribosomal Protein L19

Chain DT: 51% 28% 10% 11%



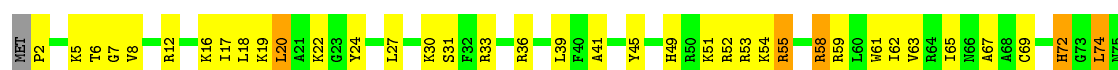
• Molecule 40: 50S Ribosomal Protein L20

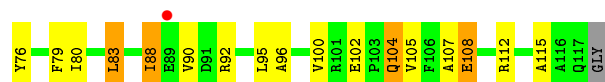
Chain BU: 61% 30% 7% ..



• Molecule 40: 50S Ribosomal Protein L20

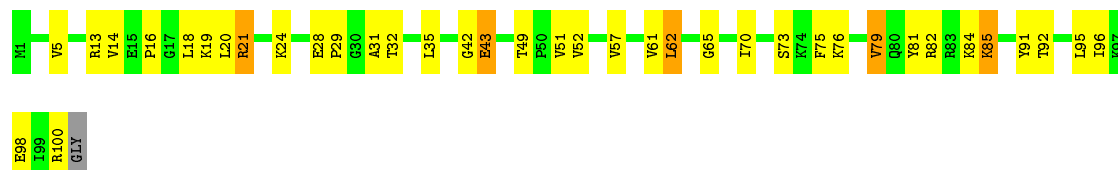
Chain DU: 53% 38% 8%





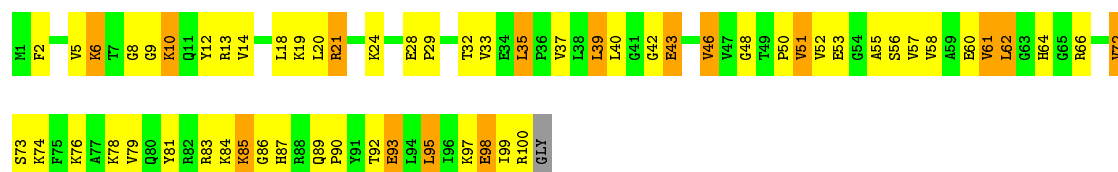
• Molecule 41: 50S Ribosomal Protein L21

Chain BV: 61% 33% 5% •



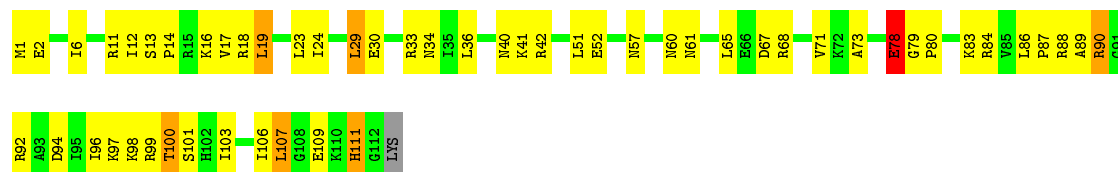
• Molecule 41: 50S Ribosomal Protein L21

Chain DV: 40% 45% 15% •



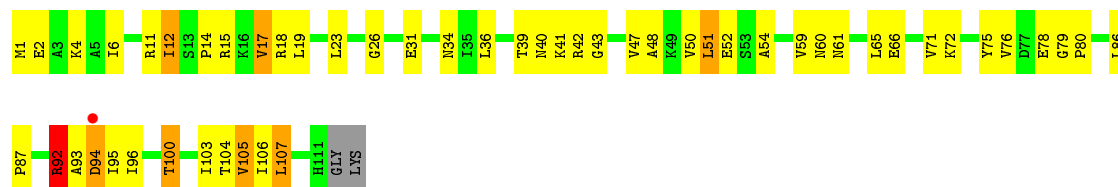
• Molecule 42: 50S Ribosomal Protein L22

Chain BW: 51% 42% 5% ••



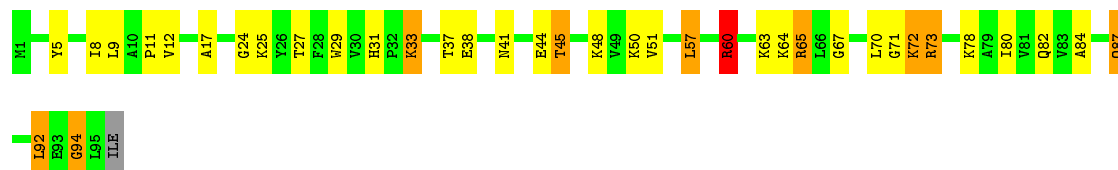
• Molecule 42: 50S Ribosomal Protein L22

Chain DW: 52% 39% 6% ••



• Molecule 43: 50S Ribosomal Protein L23

Chain BX: 60% 28% 9% ••



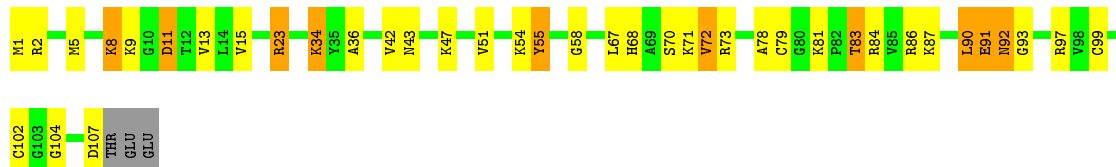
- Molecule 43: 50S Ribosomal Protein L23

Chain DX: 



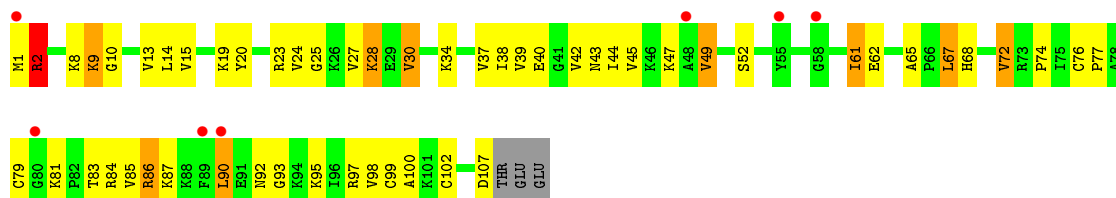
- Molecule 44: 50S Ribosomal Protein L24

Chain BY: 



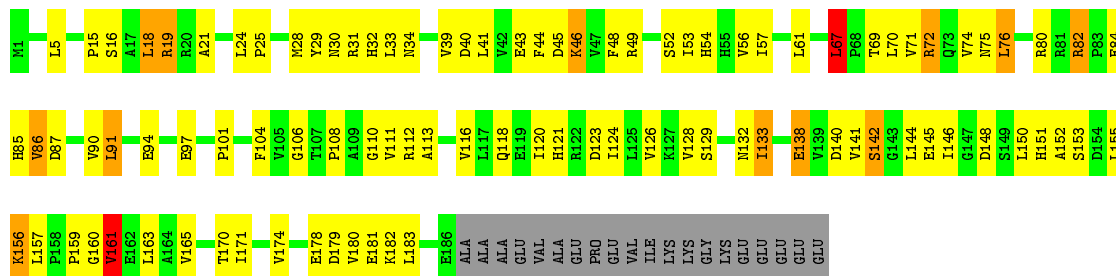
- Molecule 44: 50S Ribosomal Protein L24

Chain DY: 

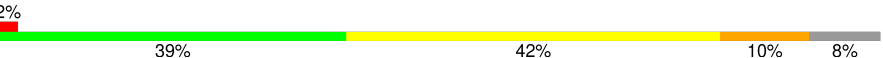


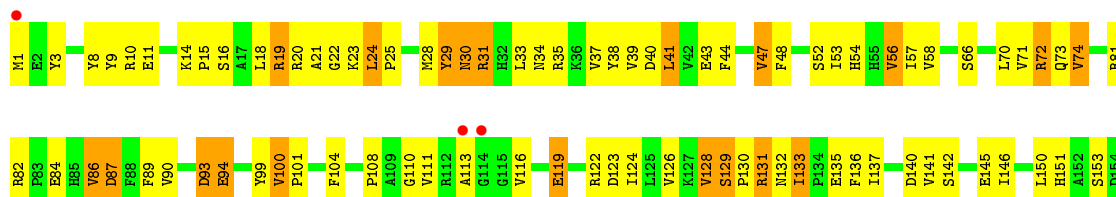
- Molecule 45: 50S Ribosomal Protein L25

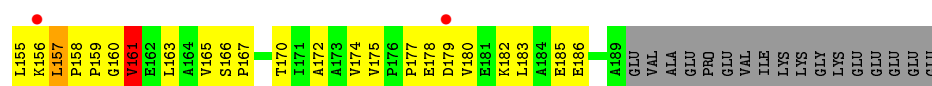
Chain BZ: 



- Molecule 45: 50S Ribosomal Protein L25

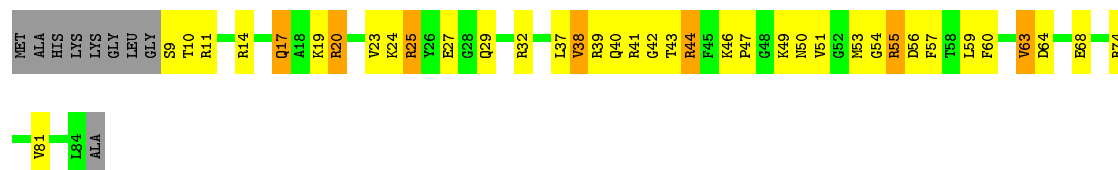
Chain DZ: 





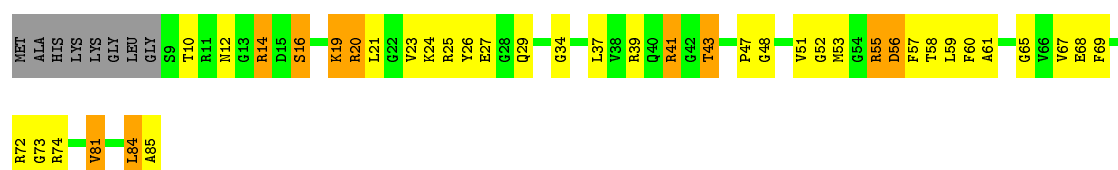
• Molecule 46: 50S Ribosomal Protein L27

Chain B0: 45% 36% 8% 11%



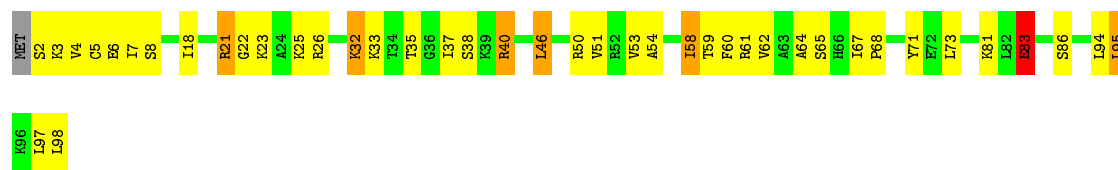
• Molecule 46: 50S Ribosomal Protein L27

Chain D0: 44% 35% 12% 9%



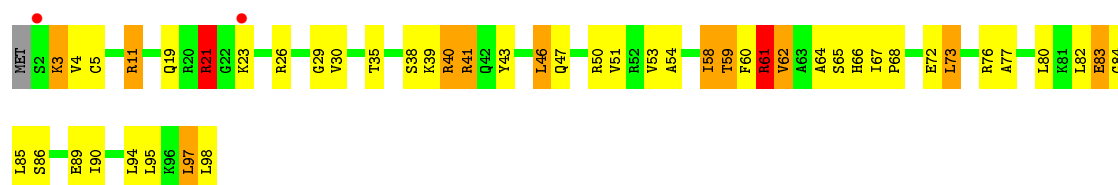
• Molecule 47: 50S Ribosomal Protein L28

Chain B1: 56% 36% 6% ..



• Molecule 47: 50S Ribosomal Protein L28

Chain D1: 2% 50% 36% 11% ..



• Molecule 48: 50S Ribosomal Protein L29

Chain B2: 42% 39% 15% ..



• Molecule 48: 50S Ribosomal Protein L29

- Molecule 52: 50S Ribosomal Protein L33

Chain B6: 



- Molecule 52: 50S Ribosomal Protein L33

Chain D6: 



- Molecule 53: 50S Ribosomal Protein L34

Chain B7: 



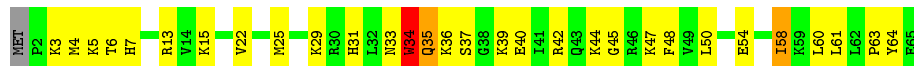
- Molecule 53: 50S Ribosomal Protein L34

Chain D7: 



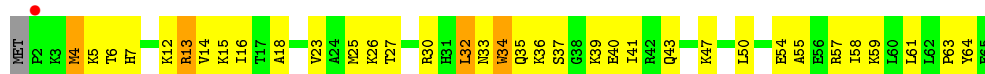
- Molecule 54: 50S Ribosomal Protein L35

Chain B8: 



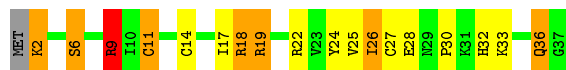
- Molecule 54: 50S Ribosomal Protein L35

Chain D8: 



- Molecule 55: 50S Ribosomal Protein L36

Chain B9: 



- Molecule 55: 50S Ribosomal Protein L36

Chain D9: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.96 Å 448.86 Å 624.20 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 34.91 – 3.20 34.91 – 3.20 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (34.91-3.20) 99.8 (34.91-3.20) | Depositor EDS |
| R_{merge} | 0.28 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.32 (at 3.18 Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.3_928) | Depositor |
| R, R_{free} | 0.188 , 0.245 0.185 , 0.243 | Depositor DCC |
| R_{free} test set | 48022 reflections (5.02%) | DCC |
| Wilson B-factor (Å ²) | 73.8 | Xtriage |
| Anisotropy | 0.161 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 75.2 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Outliers | 0 of 956750 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 284877 | wwPDB-VP |
| Average B, all atoms (Å ²) | 80.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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 | AA | 0.97 | 30/35273 (0.1%) | 1.68 | 779/55046 (1.4%) |
| 1 | CA | 0.89 | 15/35152 (0.0%) | 1.51 | 525/54858 (1.0%) |
| 2 | AB | 0.67 | 3/1844 (0.2%) | 0.87 | 1/2498 (0.0%) |
| 2 | CB | 0.55 | 0/1852 | 0.79 | 1/2510 (0.0%) |
| 3 | AC | 0.56 | 0/1458 | 0.84 | 0/1981 |
| 3 | CC | 0.53 | 0/1477 | 0.75 | 0/2006 |
| 4 | AD | 0.66 | 2/1550 (0.1%) | 0.93 | 4/2106 (0.2%) |
| 4 | CD | 0.70 | 3/1567 (0.2%) | 0.95 | 4/2125 (0.2%) |
| 5 | AE | 0.64 | 0/1121 | 0.90 | 0/1517 |
| 5 | CE | 0.68 | 0/1131 | 0.92 | 0/1529 |
| 6 | AF | 0.62 | 0/794 | 0.86 | 1/1082 (0.1%) |
| 6 | CF | 0.60 | 0/797 | 0.81 | 0/1085 |
| 7 | AG | 0.53 | 0/1169 | 0.73 | 0/1580 |
| 7 | CG | 0.53 | 0/1166 | 0.77 | 0/1576 |
| 8 | AH | 0.63 | 0/1065 | 0.83 | 0/1445 |
| 8 | CH | 0.57 | 0/1069 | 0.80 | 0/1450 |
| 9 | AI | 0.60 | 0/879 | 0.96 | 1/1195 (0.1%) |
| 9 | CI | 0.53 | 0/864 | 0.80 | 1/1177 (0.1%) |
| 10 | AJ | 0.57 | 0/672 | 0.81 | 0/919 |
| 10 | CJ | 0.55 | 0/670 | 0.84 | 0/917 |
| 11 | AK | 0.70 | 0/858 | 0.91 | 1/1163 (0.1%) |
| 11 | CK | 0.58 | 0/843 | 0.77 | 0/1144 |
| 12 | AL | 0.70 | 0/925 | 0.87 | 0/1251 |
| 12 | CL | 0.64 | 0/921 | 0.88 | 0/1247 |
| 13 | AM | 0.66 | 1/824 (0.1%) | 0.92 | 1/1120 (0.1%) |
| 13 | CM | 0.55 | 0/794 | 0.81 | 1/1081 (0.1%) |
| 14 | AN | 0.59 | 0/482 | 0.86 | 2/642 (0.3%) |
| 14 | CN | 0.60 | 0/478 | 0.86 | 0/638 |
| 15 | AO | 0.62 | 0/735 | 0.87 | 1/981 (0.1%) |
| 15 | CO | 0.59 | 0/735 | 0.84 | 0/981 |
| 16 | AP | 0.60 | 0/662 | 0.99 | 3/898 (0.3%) |
| 16 | CP | 0.60 | 0/677 | 0.91 | 0/917 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.70 | 0/836 | 0.90 | 0/1117 |
| 17 | CQ | 0.63 | 0/832 | 0.84 | 1/1113 (0.1%) |
| 18 | AR | 0.64 | 0/519 | 0.96 | 3/699 (0.4%) |
| 18 | CR | 0.59 | 0/519 | 0.79 | 0/699 |
| 19 | AS | 0.51 | 0/574 | 0.83 | 0/781 |
| 19 | CS | 0.46 | 0/543 | 0.73 | 1/740 (0.1%) |
| 20 | AT | 0.57 | 0/716 | 0.82 | 0/947 |
| 20 | CT | 0.62 | 0/776 | 0.85 | 0/1026 |
| 21 | AU | 0.66 | 0/221 | 0.84 | 0/288 |
| 21 | CU | 0.60 | 0/184 | 0.78 | 0/244 |
| 22 | AY | 0.78 | 1/1043 (0.1%) | 1.02 | 5/1399 (0.4%) |
| 23 | AV | 1.07 | 3/1836 (0.2%) | 1.55 | 36/2859 (1.3%) |
| 23 | CV | 0.78 | 1/1836 (0.1%) | 1.29 | 11/2859 (0.4%) |
| 24 | AX | 0.94 | 0/147 | 1.18 | 0/227 |
| 24 | CX | 0.85 | 0/147 | 1.11 | 0/227 |
| 25 | BA | 1.52 | 551/66391 (0.8%) | 2.06 | 3990/103628 (3.9%) |
| 25 | DA | 1.06 | 69/65653 (0.1%) | 1.63 | 1707/102473 (1.7%) |
| 26 | BB | 1.26 | 6/2878 (0.2%) | 1.93 | 156/4490 (3.5%) |
| 26 | DB | 0.88 | 1/2878 (0.0%) | 1.42 | 35/4490 (0.8%) |
| 27 | BD | 1.02 | 3/2181 (0.1%) | 1.14 | 8/2940 (0.3%) |
| 27 | DD | 0.83 | 3/2186 (0.1%) | 0.98 | 2/2944 (0.1%) |
| 28 | BE | 0.96 | 0/1588 | 1.09 | 4/2145 (0.2%) |
| 28 | DE | 0.72 | 0/1588 | 0.90 | 1/2145 (0.0%) |
| 29 | BF | 0.93 | 0/1609 | 0.97 | 2/2177 (0.1%) |
| 29 | DF | 0.64 | 0/1611 | 0.87 | 2/2180 (0.1%) |
| 30 | BG | 0.70 | 1/1393 (0.1%) | 0.92 | 0/1892 |
| 30 | DG | 0.53 | 0/1385 | 0.83 | 1/1881 (0.1%) |
| 31 | BH | 0.84 | 0/1343 | 0.94 | 0/1820 |
| 31 | DH | 0.53 | 0/1343 | 0.76 | 1/1820 (0.1%) |
| 32 | BI | 0.63 | 0/1081 | 0.92 | 2/1477 (0.1%) |
| 32 | DI | 0.59 | 0/1072 | 0.85 | 1/1465 (0.1%) |
| 33 | BN | 1.00 | 0/1139 | 1.10 | 3/1538 (0.2%) |
| 33 | DN | 0.63 | 0/1139 | 0.83 | 0/1538 |
| 34 | BO | 0.96 | 0/933 | 1.03 | 2/1257 (0.2%) |
| 34 | DO | 0.74 | 0/933 | 0.93 | 2/1257 (0.2%) |
| 35 | BP | 0.89 | 0/1148 | 1.09 | 5/1529 (0.3%) |
| 35 | DP | 0.65 | 0/1148 | 0.91 | 2/1529 (0.1%) |
| 36 | BQ | 1.01 | 0/1143 | 1.04 | 4/1527 (0.3%) |
| 36 | DQ | 0.67 | 0/1143 | 0.89 | 1/1527 (0.1%) |
| 37 | BR | 0.90 | 0/982 | 1.08 | 3/1312 (0.2%) |
| 37 | DR | 0.65 | 0/982 | 0.90 | 0/1312 |
| 38 | BS | 0.80 | 0/875 | 1.06 | 3/1168 (0.3%) |
| 38 | DS | 0.55 | 0/883 | 0.87 | 0/1176 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | BT | 0.89 | 0/1086 | 1.05 | 1/1455 (0.1%) |
| 39 | DT | 0.68 | 0/1072 | 0.81 | 0/1437 |
| 40 | BU | 1.10 | 1/977 (0.1%) | 1.09 | 5/1301 (0.4%) |
| 40 | DU | 0.70 | 0/977 | 0.87 | 0/1301 |
| 41 | BV | 1.02 | 0/777 | 1.10 | 1/1044 (0.1%) |
| 41 | DV | 0.67 | 0/781 | 0.86 | 1/1048 (0.1%) |
| 42 | BW | 1.05 | 1/901 (0.1%) | 1.10 | 3/1209 (0.2%) |
| 42 | DW | 0.77 | 0/887 | 0.90 | 2/1192 (0.2%) |
| 43 | BX | 0.99 | 0/756 | 1.06 | 2/1016 (0.2%) |
| 43 | DX | 0.75 | 0/746 | 0.88 | 1/1005 (0.1%) |
| 44 | BY | 0.85 | 0/798 | 1.03 | 2/1073 (0.2%) |
| 44 | DY | 0.64 | 0/794 | 0.87 | 0/1067 |
| 45 | BZ | 0.80 | 0/1486 | 0.94 | 2/2022 (0.1%) |
| 45 | DZ | 0.58 | 0/1483 | 0.80 | 0/2023 |
| 46 | B0 | 0.95 | 0/602 | 1.10 | 3/804 (0.4%) |
| 46 | D0 | 0.64 | 0/615 | 0.89 | 0/820 |
| 47 | B1 | 0.94 | 0/752 | 1.07 | 1/1003 (0.1%) |
| 47 | D1 | 0.70 | 0/752 | 0.92 | 2/1003 (0.2%) |
| 48 | B2 | 0.96 | 2/590 (0.3%) | 1.00 | 1/781 (0.1%) |
| 48 | D2 | 0.63 | 0/586 | 0.79 | 1/779 (0.1%) |
| 49 | B3 | 1.02 | 0/463 | 1.07 | 0/623 |
| 49 | D3 | 0.57 | 0/458 | 0.79 | 0/616 |
| 50 | B4 | 0.62 | 0/358 | 0.97 | 2/487 (0.4%) |
| 50 | D4 | 0.66 | 0/358 | 0.82 | 1/487 (0.2%) |
| 51 | B5 | 1.01 | 1/469 (0.2%) | 1.09 | 2/634 (0.3%) |
| 51 | D5 | 0.69 | 0/465 | 0.90 | 0/630 |
| 52 | B6 | 0.96 | 0/456 | 1.09 | 2/609 (0.3%) |
| 52 | D6 | 0.73 | 0/444 | 0.87 | 0/595 |
| 53 | B7 | 1.10 | 0/426 | 1.21 | 4/561 (0.7%) |
| 53 | D7 | 0.78 | 0/410 | 0.88 | 0/543 |
| 54 | B8 | 0.99 | 0/516 | 1.14 | 2/679 (0.3%) |
| 54 | D8 | 0.75 | 0/516 | 0.93 | 0/679 |
| 55 | B9 | 1.07 | 1/300 (0.3%) | 1.25 | 3/395 (0.8%) |
| 55 | D9 | 0.68 | 0/295 | 0.87 | 0/390 |
| All | All | 1.07 | 699/303213 (0.2%) | 1.58 | 7364/453838 (1.6%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | CA | 0 | 1 |
| 2 | AB | 0 | 4 |
| 2 | CB | 0 | 2 |
| 3 | AC | 0 | 2 |
| 4 | AD | 0 | 4 |
| 4 | CD | 0 | 5 |
| 5 | AE | 0 | 2 |
| 5 | CE | 0 | 1 |
| 7 | AG | 0 | 1 |
| 7 | CG | 0 | 1 |
| 9 | AI | 0 | 3 |
| 10 | AJ | 0 | 2 |
| 10 | CJ | 0 | 2 |
| 11 | AK | 0 | 1 |
| 12 | AL | 0 | 1 |
| 13 | AM | 0 | 3 |
| 13 | CM | 0 | 2 |
| 14 | CN | 0 | 1 |
| 16 | CP | 0 | 1 |
| 18 | AR | 0 | 1 |
| 20 | AT | 0 | 2 |
| 20 | CT | 0 | 2 |
| 21 | CU | 0 | 1 |
| 22 | AY | 0 | 1 |
| 27 | BD | 0 | 2 |
| 28 | BE | 0 | 2 |
| 28 | DE | 0 | 1 |
| 29 | BF | 0 | 2 |
| 29 | DF | 0 | 1 |
| 30 | DG | 0 | 3 |
| 31 | DH | 0 | 1 |
| 32 | BI | 0 | 3 |
| 34 | BO | 0 | 1 |
| 34 | DO | 0 | 1 |
| 35 | BP | 0 | 1 |
| 35 | DP | 0 | 1 |
| 36 | BQ | 0 | 2 |
| 36 | DQ | 0 | 1 |
| 38 | BS | 0 | 1 |
| 38 | DS | 0 | 1 |
| 39 | BT | 0 | 1 |
| 39 | DT | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 43 | BX | 0 | 1 |
| 45 | BZ | 0 | 1 |
| 47 | B1 | 0 | 1 |
| 47 | D1 | 0 | 1 |
| 48 | D2 | 0 | 1 |
| 50 | B4 | 0 | 1 |
| 50 | D4 | 0 | 1 |
| 51 | B5 | 0 | 1 |
| 52 | D6 | 0 | 1 |
| All | All | 0 | 82 |

The worst 5 of 699 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 25 | BA | 1142(A) | A | N9-C4 | -17.94 | 1.27 | 1.37 |
| 25 | BA | 528 | A | N9-C4 | -17.30 | 1.27 | 1.37 |
| 1 | CA | 189(D) | C | N3-C4 | -15.70 | 1.23 | 1.33 |
| 25 | BA | 676 | A | N9-C4 | -15.14 | 1.28 | 1.37 |
| 25 | BA | 1021 | A | N9-C4 | -14.78 | 1.28 | 1.37 |

The worst 5 of 7364 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|---------|-------------|----------|
| 1 | AA | 189(D) | C | N3-C4-N4 | -102.71 | 46.10 | 118.00 |
| 1 | CA | 189(D) | C | N1-C2-O2 | 44.80 | 145.78 | 118.90 |
| 1 | CA | 189(D) | C | N3-C4-N4 | -44.60 | 86.78 | 118.00 |
| 1 | AA | 189(D) | C | C2-N3-C4 | 43.68 | 141.74 | 119.90 |
| 1 | AA | 189(D) | C | C5-C4-N4 | 42.13 | 149.69 | 120.20 |

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|--------|------|-----------|
| 1 | AA | 189(D) | C | Sidechain |
| 2 | AB | 14 | GLY | Peptide |
| 2 | AB | 23 | ARG | Peptide |
| 2 | AB | 71 | VAL | Peptide |
| 2 | AB | 76 | GLN | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 31513 | 0 | 15906 | 882 | 0 |
| 1 | CA | 31406 | 0 | 15852 | 823 | 0 |
| 2 | AB | 1809 | 0 | 1781 | 104 | 0 |
| 2 | CB | 1817 | 0 | 1785 | 126 | 0 |
| 3 | AC | 1434 | 0 | 1299 | 59 | 0 |
| 3 | CC | 1453 | 0 | 1320 | 64 | 0 |
| 4 | AD | 1520 | 0 | 1407 | 80 | 0 |
| 4 | CD | 1537 | 0 | 1430 | 81 | 1 |
| 5 | AE | 1105 | 0 | 1130 | 50 | 0 |
| 5 | CE | 1115 | 0 | 1145 | 55 | 0 |
| 6 | AF | 781 | 0 | 741 | 36 | 1 |
| 6 | CF | 784 | 0 | 739 | 30 | 0 |
| 7 | AG | 1152 | 0 | 1098 | 58 | 0 |
| 7 | CG | 1149 | 0 | 1096 | 52 | 0 |
| 8 | AH | 1045 | 0 | 1033 | 52 | 0 |
| 8 | CH | 1049 | 0 | 1037 | 52 | 0 |
| 9 | AI | 863 | 0 | 760 | 54 | 0 |
| 9 | CI | 849 | 0 | 735 | 54 | 0 |
| 10 | AJ | 659 | 0 | 552 | 38 | 0 |
| 10 | CJ | 657 | 0 | 547 | 40 | 0 |
| 11 | AK | 843 | 0 | 841 | 34 | 0 |
| 11 | CK | 828 | 0 | 822 | 31 | 0 |
| 12 | AL | 909 | 0 | 927 | 50 | 0 |
| 12 | CL | 905 | 0 | 916 | 30 | 0 |
| 13 | AM | 814 | 0 | 765 | 47 | 0 |
| 13 | CM | 784 | 0 | 730 | 51 | 0 |
| 14 | AN | 473 | 0 | 491 | 39 | 0 |
| 14 | CN | 469 | 0 | 482 | 37 | 0 |
| 15 | AO | 724 | 0 | 749 | 34 | 0 |
| 15 | CO | 724 | 0 | 749 | 30 | 0 |
| 16 | AP | 646 | 0 | 636 | 42 | 0 |
| 16 | CP | 661 | 0 | 653 | 45 | 0 |
| 17 | AQ | 823 | 0 | 891 | 52 | 0 |
| 17 | CQ | 819 | 0 | 880 | 38 | 0 |
| 18 | AR | 514 | 0 | 530 | 27 | 0 |
| 18 | CR | 514 | 0 | 530 | 21 | 0 |
| 19 | AS | 560 | 0 | 466 | 24 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | CS | 529 | 0 | 443 | 22 | 0 |
| 20 | AT | 714 | 0 | 775 | 41 | 0 |
| 20 | CT | 773 | 0 | 836 | 32 | 0 |
| 21 | AU | 217 | 0 | 234 | 7 | 0 |
| 21 | CU | 180 | 0 | 173 | 4 | 0 |
| 22 | AY | 1031 | 0 | 1087 | 85 | 0 |
| 23 | AV | 1644 | 0 | 836 | 23 | 0 |
| 23 | CV | 1644 | 0 | 836 | 38 | 0 |
| 24 | AX | 131 | 0 | 66 | 4 | 0 |
| 24 | CX | 131 | 0 | 66 | 2 | 0 |
| 25 | BA | 59281 | 0 | 29884 | 1053 | 0 |
| 25 | DA | 58627 | 0 | 29570 | 1197 | 0 |
| 26 | BB | 2573 | 0 | 1306 | 47 | 0 |
| 26 | DB | 2573 | 0 | 1306 | 83 | 0 |
| 27 | BD | 2131 | 0 | 2207 | 97 | 0 |
| 27 | DD | 2136 | 0 | 2218 | 104 | 0 |
| 28 | BE | 1555 | 0 | 1607 | 65 | 0 |
| 28 | DE | 1555 | 0 | 1607 | 72 | 0 |
| 29 | BF | 1576 | 0 | 1616 | 71 | 0 |
| 29 | DF | 1578 | 0 | 1623 | 96 | 0 |
| 30 | BG | 1368 | 0 | 1324 | 52 | 0 |
| 30 | DG | 1361 | 0 | 1316 | 76 | 0 |
| 31 | BH | 1317 | 0 | 1376 | 52 | 0 |
| 31 | DH | 1317 | 0 | 1376 | 59 | 0 |
| 32 | BI | 1066 | 0 | 1095 | 47 | 0 |
| 32 | DI | 1057 | 0 | 1087 | 56 | 0 |
| 33 | BN | 1112 | 0 | 1180 | 49 | 0 |
| 33 | DN | 1112 | 0 | 1180 | 64 | 0 |
| 34 | BO | 923 | 0 | 981 | 37 | 0 |
| 34 | DO | 923 | 0 | 981 | 38 | 0 |
| 35 | BP | 1131 | 0 | 1201 | 61 | 0 |
| 35 | DP | 1131 | 0 | 1201 | 66 | 0 |
| 36 | BQ | 1122 | 0 | 1179 | 46 | 0 |
| 36 | DQ | 1122 | 0 | 1179 | 66 | 0 |
| 37 | BR | 968 | 0 | 1033 | 42 | 0 |
| 37 | DR | 968 | 0 | 1033 | 56 | 0 |
| 38 | BS | 865 | 0 | 905 | 53 | 0 |
| 38 | DS | 873 | 0 | 927 | 64 | 0 |
| 39 | BT | 1072 | 0 | 1116 | 31 | 0 |
| 39 | DT | 1058 | 0 | 1098 | 35 | 0 |
| 40 | BU | 959 | 0 | 1019 | 35 | 0 |
| 40 | DU | 959 | 0 | 1019 | 49 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41 | BV | 766 | 0 | 827 | 24 | 0 |
| 41 | DV | 770 | 0 | 838 | 40 | 0 |
| 42 | BW | 890 | 0 | 951 | 33 | 0 |
| 42 | DW | 877 | 0 | 932 | 32 | 0 |
| 43 | BX | 742 | 0 | 799 | 36 | 0 |
| 43 | DX | 732 | 0 | 777 | 17 | 0 |
| 44 | BY | 785 | 0 | 828 | 25 | 0 |
| 44 | DY | 781 | 0 | 829 | 42 | 0 |
| 45 | BZ | 1454 | 0 | 1452 | 66 | 0 |
| 45 | DZ | 1451 | 0 | 1421 | 72 | 0 |
| 46 | B0 | 594 | 0 | 604 | 30 | 0 |
| 46 | D0 | 607 | 0 | 622 | 39 | 0 |
| 47 | B1 | 745 | 0 | 804 | 33 | 0 |
| 47 | D1 | 745 | 0 | 804 | 37 | 0 |
| 48 | B2 | 588 | 0 | 643 | 28 | 0 |
| 48 | D2 | 584 | 0 | 623 | 26 | 0 |
| 49 | B3 | 458 | 0 | 503 | 16 | 0 |
| 49 | D3 | 453 | 0 | 501 | 28 | 0 |
| 50 | B4 | 349 | 0 | 336 | 22 | 0 |
| 50 | D4 | 349 | 0 | 336 | 19 | 0 |
| 51 | B5 | 455 | 0 | 472 | 20 | 0 |
| 51 | D5 | 451 | 0 | 461 | 25 | 0 |
| 52 | B6 | 449 | 0 | 462 | 25 | 0 |
| 52 | D6 | 437 | 0 | 440 | 16 | 0 |
| 53 | B7 | 418 | 0 | 467 | 22 | 0 |
| 53 | D7 | 402 | 0 | 434 | 11 | 0 |
| 54 | B8 | 509 | 0 | 565 | 24 | 0 |
| 54 | D8 | 509 | 0 | 565 | 26 | 0 |
| 55 | B9 | 297 | 0 | 316 | 16 | 0 |
| 55 | D9 | 292 | 0 | 313 | 14 | 0 |
| 56 | AA | 348 | 0 | 0 | 0 | 0 |
| 56 | AD | 2 | 0 | 0 | 0 | 0 |
| 56 | AE | 1 | 0 | 0 | 0 | 0 |
| 56 | AF | 1 | 0 | 0 | 0 | 0 |
| 56 | AI | 2 | 0 | 0 | 0 | 0 |
| 56 | AK | 1 | 0 | 0 | 0 | 0 |
| 56 | AT | 1 | 0 | 0 | 0 | 0 |
| 56 | AV | 18 | 0 | 0 | 0 | 0 |
| 56 | AY | 1 | 0 | 0 | 0 | 0 |
| 56 | B0 | 5 | 0 | 0 | 0 | 0 |
| 56 | B1 | 3 | 0 | 0 | 0 | 0 |
| 56 | B2 | 2 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | B3 | 2 | 0 | 0 | 0 | 0 |
| 56 | B5 | 3 | 0 | 0 | 0 | 0 |
| 56 | B6 | 1 | 0 | 0 | 0 | 0 |
| 56 | B7 | 1 | 0 | 0 | 0 | 0 |
| 56 | B8 | 2 | 0 | 0 | 0 | 0 |
| 56 | B9 | 1 | 0 | 0 | 0 | 0 |
| 56 | BA | 896 | 0 | 0 | 0 | 0 |
| 56 | BB | 30 | 0 | 0 | 0 | 0 |
| 56 | BD | 5 | 0 | 0 | 0 | 0 |
| 56 | BE | 5 | 0 | 0 | 0 | 0 |
| 56 | BF | 7 | 0 | 0 | 0 | 0 |
| 56 | BG | 2 | 0 | 0 | 0 | 0 |
| 56 | BO | 2 | 0 | 0 | 0 | 0 |
| 56 | BP | 2 | 0 | 0 | 0 | 0 |
| 56 | BQ | 4 | 0 | 0 | 0 | 0 |
| 56 | BR | 2 | 0 | 0 | 0 | 0 |
| 56 | BT | 1 | 0 | 0 | 0 | 0 |
| 56 | BU | 1 | 0 | 0 | 0 | 0 |
| 56 | BV | 2 | 0 | 0 | 0 | 0 |
| 56 | BX | 1 | 0 | 0 | 0 | 0 |
| 56 | BY | 2 | 0 | 0 | 0 | 0 |
| 56 | BZ | 2 | 0 | 0 | 0 | 0 |
| 56 | CA | 219 | 0 | 0 | 0 | 0 |
| 56 | CD | 1 | 0 | 0 | 0 | 0 |
| 56 | CT | 1 | 0 | 0 | 0 | 0 |
| 56 | CV | 10 | 0 | 0 | 0 | 0 |
| 56 | CX | 1 | 0 | 0 | 0 | 0 |
| 56 | D0 | 4 | 0 | 0 | 0 | 0 |
| 56 | D1 | 1 | 0 | 0 | 0 | 0 |
| 56 | D5 | 1 | 0 | 0 | 0 | 0 |
| 56 | D6 | 2 | 0 | 0 | 0 | 0 |
| 56 | D7 | 1 | 0 | 0 | 0 | 0 |
| 56 | D8 | 1 | 0 | 0 | 0 | 0 |
| 56 | DA | 696 | 0 | 0 | 0 | 0 |
| 56 | DB | 16 | 0 | 0 | 0 | 0 |
| 56 | DD | 4 | 0 | 0 | 0 | 0 |
| 56 | DE | 4 | 0 | 0 | 0 | 0 |
| 56 | DF | 3 | 0 | 0 | 0 | 0 |
| 56 | DO | 3 | 0 | 0 | 0 | 0 |
| 56 | DQ | 2 | 0 | 0 | 0 | 0 |
| 56 | DR | 1 | 0 | 0 | 0 | 0 |
| 56 | DT | 3 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | DU | 1 | 0 | 0 | 0 | 0 |
| 56 | DV | 1 | 0 | 0 | 0 | 0 |
| 56 | DX | 1 | 0 | 0 | 0 | 0 |
| 57 | AD | 1 | 0 | 0 | 0 | 0 |
| 57 | AN | 1 | 0 | 0 | 0 | 0 |
| 57 | B4 | 1 | 0 | 0 | 0 | 0 |
| 57 | B5 | 1 | 0 | 0 | 0 | 0 |
| 57 | B6 | 1 | 0 | 0 | 0 | 0 |
| 57 | B9 | 1 | 0 | 0 | 0 | 0 |
| 57 | BY | 1 | 0 | 0 | 0 | 0 |
| 57 | CD | 1 | 0 | 0 | 0 | 0 |
| 57 | CN | 1 | 0 | 0 | 0 | 0 |
| 57 | D4 | 1 | 0 | 0 | 0 | 0 |
| 57 | D5 | 1 | 0 | 0 | 0 | 0 |
| 57 | D6 | 1 | 0 | 0 | 0 | 0 |
| 57 | D9 | 1 | 0 | 0 | 0 | 0 |
| 57 | DY | 1 | 0 | 0 | 0 | 0 |
| 58 | AA | 372 | 0 | 0 | 22 | 0 |
| 58 | AD | 2 | 0 | 0 | 0 | 0 |
| 58 | AE | 3 | 0 | 0 | 0 | 0 |
| 58 | AI | 1 | 0 | 0 | 1 | 0 |
| 58 | AK | 2 | 0 | 0 | 0 | 0 |
| 58 | AL | 2 | 0 | 0 | 0 | 0 |
| 58 | AN | 1 | 0 | 0 | 0 | 0 |
| 58 | AT | 5 | 0 | 0 | 1 | 0 |
| 58 | AV | 16 | 0 | 0 | 1 | 0 |
| 58 | AX | 1 | 0 | 0 | 0 | 0 |
| 58 | AY | 2 | 0 | 0 | 1 | 0 |
| 58 | B0 | 4 | 0 | 0 | 0 | 0 |
| 58 | B1 | 1 | 0 | 0 | 0 | 0 |
| 58 | B3 | 1 | 0 | 0 | 0 | 0 |
| 58 | B6 | 4 | 0 | 0 | 0 | 0 |
| 58 | B7 | 2 | 0 | 0 | 0 | 0 |
| 58 | B8 | 4 | 0 | 0 | 1 | 0 |
| 58 | B9 | 1 | 0 | 0 | 0 | 0 |
| 58 | BA | 1491 | 0 | 0 | 71 | 0 |
| 58 | BB | 46 | 0 | 0 | 1 | 0 |
| 58 | BD | 10 | 0 | 0 | 0 | 0 |
| 58 | BE | 5 | 0 | 0 | 0 | 0 |
| 58 | BF | 5 | 0 | 0 | 0 | 0 |
| 58 | BG | 5 | 0 | 0 | 1 | 0 |
| 58 | BH | 1 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58 | BN | 3 | 0 | 0 | 0 | 0 |
| 58 | BO | 3 | 0 | 0 | 0 | 0 |
| 58 | BP | 9 | 0 | 0 | 2 | 0 |
| 58 | BQ | 4 | 0 | 0 | 0 | 0 |
| 58 | BR | 7 | 0 | 0 | 0 | 0 |
| 58 | BT | 1 | 0 | 0 | 0 | 0 |
| 58 | BU | 7 | 0 | 0 | 1 | 0 |
| 58 | BV | 1 | 0 | 0 | 0 | 0 |
| 58 | BW | 2 | 0 | 0 | 0 | 0 |
| 58 | BX | 2 | 0 | 0 | 0 | 0 |
| 58 | BY | 1 | 0 | 0 | 0 | 0 |
| 58 | CA | 330 | 0 | 0 | 17 | 0 |
| 58 | CB | 1 | 0 | 0 | 1 | 0 |
| 58 | CC | 1 | 0 | 0 | 0 | 0 |
| 58 | CD | 3 | 0 | 0 | 0 | 0 |
| 58 | CE | 1 | 0 | 0 | 0 | 0 |
| 58 | CK | 2 | 0 | 0 | 0 | 0 |
| 58 | CL | 3 | 0 | 0 | 1 | 0 |
| 58 | CN | 2 | 0 | 0 | 0 | 0 |
| 58 | CO | 2 | 0 | 0 | 1 | 0 |
| 58 | CQ | 2 | 0 | 0 | 1 | 0 |
| 58 | CT | 2 | 0 | 0 | 0 | 0 |
| 58 | CV | 13 | 0 | 0 | 0 | 0 |
| 58 | CX | 1 | 0 | 0 | 0 | 0 |
| 58 | D1 | 3 | 0 | 0 | 1 | 0 |
| 58 | D3 | 1 | 0 | 0 | 0 | 0 |
| 58 | D6 | 2 | 0 | 0 | 0 | 0 |
| 58 | D7 | 2 | 0 | 0 | 0 | 0 |
| 58 | D8 | 4 | 0 | 0 | 1 | 0 |
| 58 | DA | 1028 | 0 | 0 | 63 | 0 |
| 58 | DB | 40 | 0 | 0 | 2 | 0 |
| 58 | DD | 8 | 0 | 0 | 0 | 0 |
| 58 | DE | 11 | 0 | 0 | 1 | 0 |
| 58 | DF | 4 | 0 | 0 | 0 | 0 |
| 58 | DG | 1 | 0 | 0 | 0 | 0 |
| 58 | DN | 3 | 0 | 0 | 0 | 0 |
| 58 | DO | 5 | 0 | 0 | 1 | 0 |
| 58 | DP | 4 | 0 | 0 | 0 | 0 |
| 58 | DR | 5 | 0 | 0 | 1 | 0 |
| 58 | DT | 3 | 0 | 0 | 0 | 0 |
| 58 | DV | 1 | 0 | 0 | 0 | 0 |
| 58 | DW | 1 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58 | DY | 2 | 0 | 0 | 0 | 0 |
| All | All | 284877 | 0 | 186478 | 7600 | 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 17.

The worst 5 of 7600 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) |
|-----------------|-------------------|--------------------------|-------------------|
| 55:D9:11:CYS:SG | 55:D9:32:HIS:HE1 | 1.40 | 1.43 |
| 25:DA:885:C:N4 | 25:DA:890:A:N6 | 1.81 | 1.27 |
| 25:BA:885:C:N4 | 25:BA:890:A:N6 | 1.88 | 1.22 |
| 1:CA:1358:U:H3 | 1:CA:1363(A):A:N6 | 1.35 | 1.22 |
| 1:AA:1358:U:H3 | 1:AA:1363(A):A:N6 | 1.41 | 1.16 |

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) |
|---------------|-----------------------|--------------------------|-------------------|
| 6:AF:14:LEU:O | 4:CD:20:TYR:OH[3_654] | 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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | AB | 231/256 (90%) | 179 (78%) | 50 (22%) | 2 (1%) | 21 | 67 |
| 2 | CB | 233/256 (91%) | 182 (78%) | 45 (19%) | 6 (3%) | 7 | 40 |
| 3 | AC | 202/239 (84%) | 165 (82%) | 33 (16%) | 4 (2%) | 9 | 48 |
| 3 | CC | 204/239 (85%) | 168 (82%) | 36 (18%) | 0 | 100 | 100 |
| 4 | AD | 206/209 (99%) | 166 (81%) | 35 (17%) | 5 (2%) | 7 | 43 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4 | CD | 206/209 (99%) | 178 (86%) | 23 (11%) | 5 (2%) | 7 | 43 |
| 5 | AE | 146/162 (90%) | 120 (82%) | 26 (18%) | 0 | 100 | 100 |
| 5 | CE | 147/162 (91%) | 129 (88%) | 13 (9%) | 5 (3%) | 5 | 31 |
| 6 | AF | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 6 | CF | 98/101 (97%) | 89 (91%) | 9 (9%) | 0 | 100 | 100 |
| 7 | AG | 152/156 (97%) | 134 (88%) | 17 (11%) | 1 (1%) | 26 | 72 |
| 7 | CG | 152/156 (97%) | 131 (86%) | 20 (13%) | 1 (1%) | 26 | 72 |
| 8 | AH | 136/138 (99%) | 122 (90%) | 13 (10%) | 1 (1%) | 26 | 72 |
| 8 | CH | 136/138 (99%) | 126 (93%) | 10 (7%) | 0 | 100 | 100 |
| 9 | AI | 123/128 (96%) | 105 (85%) | 15 (12%) | 3 (2%) | 7 | 43 |
| 9 | CI | 123/128 (96%) | 106 (86%) | 13 (11%) | 4 (3%) | 5 | 32 |
| 10 | AJ | 94/105 (90%) | 81 (86%) | 9 (10%) | 4 (4%) | 3 | 25 |
| 10 | CJ | 94/105 (90%) | 74 (79%) | 17 (18%) | 3 (3%) | 5 | 33 |
| 11 | AK | 113/129 (88%) | 101 (89%) | 11 (10%) | 1 (1%) | 21 | 67 |
| 11 | CK | 112/129 (87%) | 98 (88%) | 14 (12%) | 0 | 100 | 100 |
| 12 | AL | 120/132 (91%) | 108 (90%) | 10 (8%) | 2 (2%) | 11 | 52 |
| 12 | CL | 120/132 (91%) | 111 (92%) | 7 (6%) | 2 (2%) | 11 | 52 |
| 13 | AM | 113/126 (90%) | 89 (79%) | 20 (18%) | 4 (4%) | 4 | 31 |
| 13 | CM | 110/126 (87%) | 82 (74%) | 21 (19%) | 7 (6%) | 2 | 13 |
| 14 | AN | 57/61 (93%) | 44 (77%) | 13 (23%) | 0 | 100 | 100 |
| 14 | CN | 57/61 (93%) | 48 (84%) | 8 (14%) | 1 (2%) | 11 | 51 |
| 15 | AO | 86/89 (97%) | 74 (86%) | 12 (14%) | 0 | 100 | 100 |
| 15 | CO | 86/89 (97%) | 75 (87%) | 11 (13%) | 0 | 100 | 100 |
| 16 | AP | 79/88 (90%) | 62 (78%) | 14 (18%) | 3 (4%) | 4 | 28 |
| 16 | CP | 80/88 (91%) | 66 (82%) | 10 (12%) | 4 (5%) | 3 | 21 |
| 17 | AQ | 97/105 (92%) | 83 (86%) | 13 (13%) | 1 (1%) | 19 | 65 |
| 17 | CQ | 97/105 (92%) | 83 (86%) | 13 (13%) | 1 (1%) | 19 | 65 |
| 18 | AR | 66/88 (75%) | 56 (85%) | 10 (15%) | 0 | 100 | 100 |
| 18 | CR | 66/88 (75%) | 58 (88%) | 8 (12%) | 0 | 100 | 100 |
| 19 | AS | 79/93 (85%) | 63 (80%) | 15 (19%) | 1 (1%) | 15 | 59 |
| 19 | CS | 73/93 (78%) | 60 (82%) | 13 (18%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 20 | AT | 94/106 (89%) | 73 (78%) | 19 (20%) | 2 (2%) | 9 | 46 |
| 20 | CT | 102/106 (96%) | 73 (72%) | 26 (26%) | 3 (3%) | 6 | 36 |
| 21 | AU | 23/27 (85%) | 21 (91%) | 2 (9%) | 0 | 100 | 100 |
| 21 | CU | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 22 | AY | 130/140 (93%) | 107 (82%) | 21 (16%) | 2 (2%) | 13 | 55 |
| 27 | BD | 273/276 (99%) | 254 (93%) | 19 (7%) | 0 | 100 | 100 |
| 27 | DD | 273/276 (99%) | 255 (93%) | 16 (6%) | 2 (1%) | 26 | 72 |
| 28 | BE | 202/206 (98%) | 189 (94%) | 9 (4%) | 4 (2%) | 9 | 48 |
| 28 | DE | 202/206 (98%) | 187 (93%) | 12 (6%) | 3 (2%) | 13 | 55 |
| 29 | BF | 198/210 (94%) | 183 (92%) | 15 (8%) | 0 | 100 | 100 |
| 29 | DF | 198/210 (94%) | 175 (88%) | 23 (12%) | 0 | 100 | 100 |
| 30 | BG | 179/182 (98%) | 158 (88%) | 17 (10%) | 4 (2%) | 8 | 45 |
| 30 | DG | 178/182 (98%) | 150 (84%) | 28 (16%) | 0 | 100 | 100 |
| 31 | BH | 172/180 (96%) | 160 (93%) | 12 (7%) | 0 | 100 | 100 |
| 31 | DH | 172/180 (96%) | 153 (89%) | 17 (10%) | 2 (1%) | 16 | 60 |
| 32 | BI | 145/148 (98%) | 116 (80%) | 25 (17%) | 4 (3%) | 6 | 37 |
| 32 | DI | 144/148 (97%) | 119 (83%) | 23 (16%) | 2 (1%) | 14 | 57 |
| 33 | BN | 138/140 (99%) | 124 (90%) | 11 (8%) | 3 (2%) | 8 | 45 |
| 33 | DN | 138/140 (99%) | 117 (85%) | 19 (14%) | 2 (1%) | 14 | 57 |
| 34 | BO | 120/122 (98%) | 113 (94%) | 6 (5%) | 1 (1%) | 24 | 69 |
| 34 | DO | 120/122 (98%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |
| 35 | BP | 147/150 (98%) | 128 (87%) | 17 (12%) | 2 (1%) | 14 | 57 |
| 35 | DP | 147/150 (98%) | 130 (88%) | 15 (10%) | 2 (1%) | 14 | 57 |
| 36 | BQ | 139/141 (99%) | 127 (91%) | 10 (7%) | 2 (1%) | 14 | 57 |
| 36 | DQ | 139/141 (99%) | 121 (87%) | 18 (13%) | 0 | 100 | 100 |
| 37 | BR | 116/118 (98%) | 107 (92%) | 9 (8%) | 0 | 100 | 100 |
| 37 | DR | 116/118 (98%) | 102 (88%) | 14 (12%) | 0 | 100 | 100 |
| 38 | BS | 108/112 (96%) | 93 (86%) | 12 (11%) | 3 (3%) | 6 | 37 |
| 38 | DS | 108/112 (96%) | 88 (82%) | 18 (17%) | 2 (2%) | 10 | 50 |
| 39 | BT | 130/146 (89%) | 124 (95%) | 6 (5%) | 0 | 100 | 100 |
| 39 | DT | 128/146 (88%) | 119 (93%) | 9 (7%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 40 | BU | 114/118 (97%) | 111 (97%) | 3 (3%) | 0 | 100 | 100 |
| 40 | DU | 114/118 (97%) | 107 (94%) | 7 (6%) | 0 | 100 | 100 |
| 41 | BV | 98/101 (97%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 41 | DV | 98/101 (97%) | 89 (91%) | 9 (9%) | 0 | 100 | 100 |
| 42 | BW | 110/113 (97%) | 104 (94%) | 6 (6%) | 0 | 100 | 100 |
| 42 | DW | 109/113 (96%) | 97 (89%) | 12 (11%) | 0 | 100 | 100 |
| 43 | BX | 93/96 (97%) | 87 (94%) | 6 (6%) | 0 | 100 | 100 |
| 43 | DX | 93/96 (97%) | 84 (90%) | 9 (10%) | 0 | 100 | 100 |
| 44 | BY | 105/110 (96%) | 94 (90%) | 10 (10%) | 1 (1%) | 19 | 65 |
| 44 | DY | 105/110 (96%) | 96 (91%) | 8 (8%) | 1 (1%) | 19 | 65 |
| 45 | BZ | 184/206 (89%) | 161 (88%) | 21 (11%) | 2 (1%) | 17 | 62 |
| 45 | DZ | 187/206 (91%) | 163 (87%) | 21 (11%) | 3 (2%) | 12 | 54 |
| 46 | B0 | 74/85 (87%) | 69 (93%) | 5 (7%) | 0 | 100 | 100 |
| 46 | D0 | 75/85 (88%) | 67 (89%) | 8 (11%) | 0 | 100 | 100 |
| 47 | B1 | 95/98 (97%) | 90 (95%) | 4 (4%) | 1 (1%) | 17 | 62 |
| 47 | D1 | 95/98 (97%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 48 | B2 | 68/72 (94%) | 62 (91%) | 5 (7%) | 1 (2%) | 13 | 55 |
| 48 | D2 | 69/72 (96%) | 60 (87%) | 9 (13%) | 0 | 100 | 100 |
| 49 | B3 | 57/60 (95%) | 54 (95%) | 2 (4%) | 1 (2%) | 11 | 51 |
| 49 | D3 | 56/60 (93%) | 52 (93%) | 4 (7%) | 0 | 100 | 100 |
| 50 | B4 | 44/71 (62%) | 36 (82%) | 8 (18%) | 0 | 100 | 100 |
| 50 | D4 | 44/71 (62%) | 34 (77%) | 9 (20%) | 1 (2%) | 8 | 44 |
| 51 | B5 | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 51 | D5 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 52 | B6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 52 | D6 | 51/54 (94%) | 45 (88%) | 6 (12%) | 0 | 100 | 100 |
| 53 | B7 | 46/49 (94%) | 43 (94%) | 1 (2%) | 2 (4%) | 3 | 25 |
| 53 | D7 | 46/49 (94%) | 41 (89%) | 4 (9%) | 1 (2%) | 8 | 45 |
| 54 | B8 | 62/65 (95%) | 58 (94%) | 4 (6%) | 0 | 100 | 100 |
| 54 | D8 | 62/65 (95%) | 57 (92%) | 5 (8%) | 0 | 100 | 100 |
| 55 | B9 | 34/37 (92%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 55 | D9 | 33/37 (89%) | 32 (97%) | 1 (3%) | 0 | 100 | 100 |
| All | All | 11478/12268 (94%) | 10072 (88%) | 1276 (11%) | 130 (1%) | 17 | 62 |

5 of 130 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 77 | ALA |
| 3 | AC | 99 | VAL |
| 3 | AC | 100 | ALA |
| 3 | AC | 157 | ILE |
| 4 | AD | 110 | PHE |

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 | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | AB | 180/220 (82%) | 127 (71%) | 53 (29%) | 0 | 1 |
| 2 | CB | 181/220 (82%) | 132 (73%) | 49 (27%) | 0 | 2 |
| 3 | AC | 112/188 (60%) | 89 (80%) | 23 (20%) | 1 | 7 |
| 3 | CC | 114/188 (61%) | 96 (84%) | 18 (16%) | 3 | 15 |
| 4 | AD | 139/181 (77%) | 112 (81%) | 27 (19%) | 2 | 9 |
| 4 | CD | 142/181 (78%) | 112 (79%) | 30 (21%) | 1 | 7 |
| 5 | AE | 108/123 (88%) | 77 (71%) | 31 (29%) | 0 | 1 |
| 5 | CE | 109/123 (89%) | 84 (77%) | 25 (23%) | 1 | 4 |
| 6 | AF | 77/90 (86%) | 64 (83%) | 13 (17%) | 2 | 13 |
| 6 | CF | 76/90 (84%) | 61 (80%) | 15 (20%) | 1 | 8 |
| 7 | AG | 103/127 (81%) | 83 (81%) | 20 (19%) | 2 | 9 |
| 7 | CG | 102/127 (80%) | 78 (76%) | 24 (24%) | 1 | 4 |
| 8 | AH | 103/119 (87%) | 85 (82%) | 18 (18%) | 2 | 12 |
| 8 | CH | 104/119 (87%) | 89 (86%) | 15 (14%) | 4 | 19 |
| 9 | AI | 64/99 (65%) | 55 (86%) | 9 (14%) | 4 | 20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 9 | CI | 62/99 (63%) | 52 (84%) | 10 (16%) | 3 | 14 |
| 10 | AJ | 52/92 (56%) | 38 (73%) | 14 (27%) | 0 | 2 |
| 10 | CJ | 52/92 (56%) | 36 (69%) | 16 (31%) | 0 | 1 |
| 11 | AK | 83/99 (84%) | 60 (72%) | 23 (28%) | 0 | 1 |
| 11 | CK | 81/99 (82%) | 61 (75%) | 20 (25%) | 1 | 3 |
| 12 | AL | 92/109 (84%) | 73 (79%) | 19 (21%) | 1 | 7 |
| 12 | CL | 91/109 (84%) | 71 (78%) | 20 (22%) | 1 | 6 |
| 13 | AM | 66/101 (65%) | 44 (67%) | 22 (33%) | 0 | 0 |
| 13 | CM | 62/101 (61%) | 39 (63%) | 23 (37%) | 0 | 0 |
| 14 | AN | 46/50 (92%) | 40 (87%) | 6 (13%) | 5 | 24 |
| 14 | CN | 45/50 (90%) | 30 (67%) | 15 (33%) | 0 | 0 |
| 15 | AO | 77/80 (96%) | 61 (79%) | 16 (21%) | 1 | 7 |
| 15 | CO | 77/80 (96%) | 64 (83%) | 13 (17%) | 2 | 13 |
| 16 | AP | 63/74 (85%) | 44 (70%) | 19 (30%) | 0 | 1 |
| 16 | CP | 65/74 (88%) | 49 (75%) | 16 (25%) | 1 | 3 |
| 17 | AQ | 94/97 (97%) | 79 (84%) | 15 (16%) | 3 | 14 |
| 17 | CQ | 93/97 (96%) | 77 (83%) | 16 (17%) | 2 | 12 |
| 18 | AR | 49/77 (64%) | 41 (84%) | 8 (16%) | 3 | 14 |
| 18 | CR | 49/77 (64%) | 36 (74%) | 13 (26%) | 0 | 2 |
| 19 | AS | 43/80 (54%) | 34 (79%) | 9 (21%) | 1 | 7 |
| 19 | CS | 42/80 (52%) | 28 (67%) | 14 (33%) | 0 | 0 |
| 20 | AT | 66/82 (80%) | 47 (71%) | 19 (29%) | 0 | 1 |
| 20 | CT | 72/82 (88%) | 56 (78%) | 16 (22%) | 1 | 5 |
| 21 | AU | 20/22 (91%) | 14 (70%) | 6 (30%) | 0 | 1 |
| 21 | CU | 14/22 (64%) | 13 (93%) | 1 (7%) | 18 | 57 |
| 22 | AY | 108/115 (94%) | 74 (68%) | 34 (32%) | 0 | 1 |
| 27 | BD | 214/218 (98%) | 169 (79%) | 45 (21%) | 1 | 7 |
| 27 | DD | 215/218 (99%) | 167 (78%) | 48 (22%) | 1 | 5 |
| 28 | BE | 163/166 (98%) | 126 (77%) | 37 (23%) | 1 | 5 |
| 28 | DE | 163/166 (98%) | 128 (78%) | 35 (22%) | 1 | 6 |
| 29 | BF | 158/166 (95%) | 123 (78%) | 35 (22%) | 1 | 5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 29 | DF | 159/166 (96%) | 128 (80%) | 31 (20%) | 2 | 9 |
| 30 | BG | 128/156 (82%) | 103 (80%) | 25 (20%) | 2 | 9 |
| 30 | DG | 127/156 (81%) | 95 (75%) | 32 (25%) | 1 | 2 |
| 31 | BH | 141/148 (95%) | 113 (80%) | 28 (20%) | 1 | 8 |
| 31 | DH | 141/148 (95%) | 111 (79%) | 30 (21%) | 1 | 7 |
| 32 | BI | 105/124 (85%) | 75 (71%) | 30 (29%) | 0 | 1 |
| 32 | DI | 104/124 (84%) | 76 (73%) | 28 (27%) | 0 | 2 |
| 33 | BN | 117/119 (98%) | 93 (80%) | 24 (20%) | 1 | 7 |
| 33 | DN | 117/119 (98%) | 90 (77%) | 27 (23%) | 1 | 4 |
| 34 | BO | 98/100 (98%) | 73 (74%) | 25 (26%) | 1 | 2 |
| 34 | DO | 98/100 (98%) | 70 (71%) | 28 (29%) | 0 | 1 |
| 35 | BP | 114/116 (98%) | 87 (76%) | 27 (24%) | 1 | 4 |
| 35 | DP | 114/116 (98%) | 90 (79%) | 24 (21%) | 1 | 7 |
| 36 | BQ | 111/111 (100%) | 91 (82%) | 20 (18%) | 2 | 11 |
| 36 | DQ | 111/111 (100%) | 93 (84%) | 18 (16%) | 3 | 14 |
| 37 | BR | 101/101 (100%) | 79 (78%) | 22 (22%) | 1 | 6 |
| 37 | DR | 101/101 (100%) | 79 (78%) | 22 (22%) | 1 | 6 |
| 38 | BS | 84/88 (96%) | 66 (79%) | 18 (21%) | 1 | 6 |
| 38 | DS | 86/88 (98%) | 68 (79%) | 18 (21%) | 1 | 7 |
| 39 | BT | 111/127 (87%) | 90 (81%) | 21 (19%) | 2 | 10 |
| 39 | DT | 110/127 (87%) | 82 (74%) | 28 (26%) | 1 | 2 |
| 40 | BU | 93/94 (99%) | 77 (83%) | 16 (17%) | 2 | 12 |
| 40 | DU | 93/94 (99%) | 77 (83%) | 16 (17%) | 2 | 12 |
| 41 | BV | 80/82 (98%) | 66 (82%) | 14 (18%) | 2 | 12 |
| 41 | DV | 81/82 (99%) | 56 (69%) | 25 (31%) | 0 | 1 |
| 42 | BW | 91/92 (99%) | 71 (78%) | 20 (22%) | 1 | 6 |
| 42 | DW | 89/92 (97%) | 74 (83%) | 15 (17%) | 2 | 13 |
| 43 | BX | 75/78 (96%) | 63 (84%) | 12 (16%) | 3 | 14 |
| 43 | DX | 73/78 (94%) | 61 (84%) | 12 (16%) | 3 | 13 |
| 44 | BY | 80/91 (88%) | 63 (79%) | 17 (21%) | 1 | 7 |
| 44 | DY | 79/91 (87%) | 59 (75%) | 20 (25%) | 1 | 2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 45 | BZ | 156/179 (87%) | 128 (82%) | 28 (18%) | 2 | 11 |
| 45 | DZ | 152/179 (85%) | 119 (78%) | 33 (22%) | 1 | 6 |
| 46 | B0 | 59/67 (88%) | 47 (80%) | 12 (20%) | 1 | 7 |
| 46 | D0 | 61/67 (91%) | 47 (77%) | 14 (23%) | 1 | 4 |
| 47 | B1 | 78/83 (94%) | 61 (78%) | 17 (22%) | 1 | 6 |
| 47 | D1 | 78/83 (94%) | 58 (74%) | 20 (26%) | 0 | 2 |
| 48 | B2 | 65/67 (97%) | 49 (75%) | 16 (25%) | 1 | 3 |
| 48 | D2 | 63/67 (94%) | 50 (79%) | 13 (21%) | 1 | 7 |
| 49 | B3 | 49/52 (94%) | 44 (90%) | 5 (10%) | 9 | 36 |
| 49 | D3 | 49/52 (94%) | 40 (82%) | 9 (18%) | 2 | 10 |
| 50 | B4 | 39/63 (62%) | 28 (72%) | 11 (28%) | 0 | 1 |
| 50 | D4 | 39/63 (62%) | 25 (64%) | 14 (36%) | 0 | 0 |
| 51 | B5 | 50/52 (96%) | 41 (82%) | 9 (18%) | 2 | 11 |
| 51 | D5 | 49/52 (94%) | 39 (80%) | 10 (20%) | 1 | 7 |
| 52 | B6 | 50/52 (96%) | 34 (68%) | 16 (32%) | 0 | 0 |
| 52 | D6 | 48/52 (92%) | 38 (79%) | 10 (21%) | 1 | 7 |
| 53 | B7 | 41/42 (98%) | 32 (78%) | 9 (22%) | 1 | 6 |
| 53 | D7 | 38/42 (90%) | 30 (79%) | 8 (21%) | 1 | 7 |
| 54 | B8 | 52/55 (94%) | 45 (86%) | 7 (14%) | 5 | 22 |
| 54 | D8 | 52/55 (94%) | 43 (83%) | 9 (17%) | 2 | 12 |
| 55 | B9 | 32/34 (94%) | 26 (81%) | 6 (19%) | 2 | 10 |
| 55 | D9 | 32/34 (94%) | 25 (78%) | 7 (22%) | 1 | 6 |
| All | All | 8835/10181 (87%) | 6886 (78%) | 1949 (22%) | 1 | 5 |

5 of 1949 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | B1 | 26 | ARG |
| 5 | CE | 112 | LEU |
| 44 | DY | 107 | ASP |
| 48 | B2 | 51 | ARG |
| 2 | CB | 80 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | BZ | 54 | HIS |
| 6 | CF | 73 | ASN |
| 46 | D0 | 12 | ASN |
| 52 | B6 | 20 | ASN |
| 2 | CB | 16 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1462/1522 (96%) | 386 (26%) | 33 (2%) |
| 1 | CA | 1457/1522 (95%) | 367 (25%) | 33 (2%) |
| 23 | AV | 76/77 (98%) | 20 (26%) | 1 (1%) |
| 23 | CV | 76/77 (98%) | 21 (27%) | 0 |
| 24 | AX | 5/16 (31%) | 1 (20%) | 0 |
| 24 | CX | 5/16 (31%) | 0 | 0 |
| 25 | BA | 2744/2915 (94%) | 642 (23%) | 64 (2%) |
| 25 | DA | 2711/2915 (93%) | 632 (23%) | 55 (2%) |
| 26 | BB | 119/122 (97%) | 24 (20%) | 0 |
| 26 | DB | 119/122 (97%) | 26 (21%) | 2 (1%) |
| All | All | 8774/9304 (94%) | 2119 (24%) | 188 (2%) |

5 of 2119 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 13 | U |
| 1 | AA | 22 | G |
| 1 | AA | 28 | G |

5 of 188 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2318 | G |
| 1 | CA | 428 | G |
| 25 | DA | 2282 | G |
| 25 | BA | 2335 | A |
| 25 | BA | 2778 | A |

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 2350 ligands modelled in this entry, 2350 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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 | AA | 1466/1522 (96%) | -0.12 | 23 (1%) 74 62 | 43, 93, 137, 172 | 0 |
| 1 | CA | 1461/1522 (95%) | -0.00 | 32 (2%) 65 50 | 55, 104, 145, 167 | 0 |
| 2 | AB | 233/256 (91%) | -0.23 | 3 (1%) 79 67 | 72, 113, 134, 153 | 0 |
| 2 | CB | 235/256 (91%) | 0.03 | 9 (3%) 44 29 | 100, 125, 139, 147 | 0 |
| 3 | AC | 204/239 (85%) | -0.15 | 3 (1%) 76 63 | 97, 112, 125, 133 | 0 |
| 3 | CC | 206/239 (86%) | 0.13 | 10 (4%) 33 20 | 110, 125, 136, 142 | 0 |
| 4 | AD | 208/209 (99%) | -0.29 | 2 (0%) 84 75 | 76, 103, 118, 125 | 0 |
| 4 | CD | 208/209 (99%) | -0.33 | 0 100 100 | 85, 98, 114, 120 | 0 |
| 5 | AE | 148/162 (91%) | -0.36 | 1 (0%) 89 83 | 67, 89, 108, 134 | 0 |
| 5 | CE | 149/162 (91%) | -0.26 | 1 (0%) 89 83 | 83, 99, 110, 131 | 0 |
| 6 | AF | 100/101 (99%) | -0.45 | 0 100 100 | 68, 88, 104, 110 | 0 |
| 6 | CF | 100/101 (99%) | -0.40 | 0 100 100 | 78, 96, 110, 117 | 0 |
| 7 | AG | 154/156 (98%) | -0.15 | 5 (3%) 51 36 | 87, 102, 120, 133 | 0 |
| 7 | CG | 154/156 (98%) | 0.14 | 13 (8%) 14 7 | 107, 119, 133, 144 | 0 |
| 8 | AH | 138/138 (100%) | -0.37 | 0 100 100 | 73, 91, 100, 111 | 0 |
| 8 | CH | 138/138 (100%) | -0.34 | 1 (0%) 89 83 | 82, 100, 111, 116 | 0 |
| 9 | AI | 125/128 (97%) | 0.05 | 3 (2%) 62 47 | 71, 114, 126, 137 | 0 |
| 9 | CI | 125/128 (97%) | 0.43 | 13 (10%) 8 5 | 101, 130, 138, 142 | 0 |
| 10 | AJ | 96/105 (91%) | 0.40 | 9 (9%) 11 6 | 88, 119, 136, 140 | 0 |
| 10 | CJ | 96/105 (91%) | 0.95 | 17 (17%) 2 1 | 111, 133, 141, 143 | 0 |
| 11 | AK | 115/129 (89%) | -0.35 | 0 100 100 | 53, 87, 104, 113 | 0 |
| 11 | CK | 114/129 (88%) | -0.24 | 1 (0%) 85 78 | 78, 103, 118, 127 | 0 |
| 12 | AL | 122/132 (92%) | -0.47 | 0 100 100 | 61, 84, 100, 111 | 0 |
| 12 | CL | 122/132 (92%) | -0.35 | 1 (0%) 87 80 | 72, 90, 105, 114 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AM | 115/126 (91%) | -0.31 | 0 100 100 | 66, 100, 113, 118 | 0 |
| 13 | CM | 112/126 (88%) | 0.12 | 2 (1%) 71 58 | 102, 127, 135, 139 | 0 |
| 14 | AN | 59/61 (96%) | -0.05 | 1 (1%) 73 60 | 94, 106, 114, 121 | 0 |
| 14 | CN | 59/61 (96%) | 0.51 | 5 (8%) 13 7 | 116, 125, 133, 135 | 0 |
| 15 | AO | 88/89 (98%) | -0.35 | 0 100 100 | 65, 86, 106, 117 | 0 |
| 15 | CO | 88/89 (98%) | -0.29 | 0 100 100 | 74, 96, 114, 118 | 0 |
| 16 | AP | 81/88 (92%) | -0.22 | 0 100 100 | 83, 100, 122, 127 | 0 |
| 16 | CP | 82/88 (93%) | -0.25 | 1 (1%) 81 69 | 84, 94, 112, 122 | 0 |
| 17 | AQ | 99/105 (94%) | -0.22 | 1 (1%) 84 75 | 68, 89, 104, 113 | 0 |
| 17 | CQ | 99/105 (94%) | -0.34 | 0 100 100 | 77, 95, 110, 113 | 0 |
| 18 | AR | 68/88 (77%) | -0.44 | 1 (1%) 76 63 | 69, 84, 102, 106 | 0 |
| 18 | CR | 68/88 (77%) | -0.25 | 0 100 100 | 82, 92, 111, 115 | 0 |
| 19 | AS | 81/93 (87%) | 0.01 | 2 (2%) 61 47 | 96, 110, 130, 141 | 0 |
| 19 | CS | 75/93 (80%) | 0.66 | 5 (6%) 21 12 | 107, 131, 142, 146 | 0 |
| 20 | AT | 96/106 (90%) | -0.32 | 0 100 100 | 77, 97, 113, 118 | 0 |
| 20 | CT | 104/106 (98%) | -0.15 | 3 (2%) 55 41 | 81, 101, 123, 139 | 0 |
| 21 | AU | 25/27 (92%) | 0.42 | 0 100 100 | 80, 98, 105, 107 | 0 |
| 21 | CU | 23/27 (85%) | 1.50 | 4 (17%) 2 1 | 115, 126, 132, 134 | 0 |
| 22 | AY | 132/140 (94%) | 1.59 | 37 (28%) 1 0 | 69, 110, 138, 152 | 0 |
| 23 | AV | 77/77 (100%) | -0.05 | 1 (1%) 79 67 | 55, 82, 112, 134 | 0 |
| 23 | CV | 77/77 (100%) | 0.05 | 1 (1%) 79 67 | 73, 109, 133, 156 | 0 |
| 24 | AX | 6/16 (37%) | 1.06 | 1 (16%) 2 1 | 67, 73, 127, 128 | 0 |
| 24 | CX | 6/16 (37%) | 1.05 | 2 (33%) 0 0 | 89, 96, 142, 147 | 0 |
| 25 | BA | 2752/2915 (94%) | -0.42 | 30 (1%) 82 72 | 23, 43, 115, 170 | 0 |
| 25 | DA | 2722/2915 (93%) | -0.25 | 50 (1%) 71 58 | 44, 74, 127, 170 | 0 |
| 26 | BB | 120/122 (98%) | -0.46 | 0 100 100 | 36, 64, 90, 125 | 0 |
| 26 | DB | 120/122 (98%) | 0.07 | 1 (0%) 87 80 | 73, 114, 129, 146 | 0 |
| 27 | BD | 275/276 (99%) | -0.69 | 1 (0%) 93 90 | 27, 43, 62, 110 | 0 |
| 27 | DD | 275/276 (99%) | -0.45 | 2 (0%) 89 83 | 41, 62, 82, 100 | 0 |
| 28 | BE | 204/206 (99%) | -0.69 | 0 100 100 | 22, 45, 71, 94 | 0 |
| 28 | DE | 204/206 (99%) | -0.45 | 1 (0%) 91 87 | 43, 74, 100, 113 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 29 | BF | 203/210 (96%) | -0.61 | 0 100 100 | 26, 49, 87, 115 | 0 |
| 29 | DF | 203/210 (96%) | -0.41 | 0 100 100 | 47, 88, 114, 127 | 0 |
| 30 | BG | 181/182 (99%) | -0.46 | 0 100 100 | 58, 77, 105, 116 | 0 |
| 30 | DG | 180/182 (98%) | -0.16 | 1 (0%) 90 84 | 101, 117, 127, 136 | 0 |
| 31 | BH | 174/180 (96%) | -0.52 | 0 100 100 | 38, 65, 84, 98 | 0 |
| 31 | DH | 174/180 (96%) | 0.33 | 8 (4%) 36 23 | 96, 116, 130, 140 | 0 |
| 32 | BI | 147/148 (99%) | -0.38 | 0 100 100 | 50, 95, 112, 128 | 0 |
| 32 | DI | 146/148 (98%) | -0.11 | 2 (1%) 78 65 | 68, 108, 126, 131 | 0 |
| 33 | BN | 140/140 (100%) | -0.70 | 0 100 100 | 30, 42, 69, 83 | 0 |
| 33 | DN | 140/140 (100%) | -0.34 | 0 100 100 | 64, 86, 107, 117 | 0 |
| 34 | BO | 122/122 (100%) | -0.69 | 0 100 100 | 33, 52, 71, 82 | 0 |
| 34 | DO | 122/122 (100%) | -0.58 | 0 100 100 | 57, 73, 88, 96 | 0 |
| 35 | BP | 149/150 (99%) | -0.60 | 0 100 100 | 25, 55, 86, 108 | 0 |
| 35 | DP | 149/150 (99%) | -0.30 | 0 100 100 | 52, 91, 116, 127 | 0 |
| 36 | BQ | 141/141 (100%) | -0.64 | 0 100 100 | 33, 50, 70, 90 | 0 |
| 36 | DQ | 141/141 (100%) | -0.33 | 2 (1%) 78 65 | 67, 90, 106, 114 | 0 |
| 37 | BR | 118/118 (100%) | -0.74 | 0 100 100 | 27, 41, 59, 67 | 0 |
| 37 | DR | 118/118 (100%) | -0.55 | 0 100 100 | 49, 65, 86, 95 | 0 |
| 38 | BS | 110/112 (98%) | -0.61 | 0 100 100 | 44, 62, 86, 97 | 0 |
| 38 | DS | 110/112 (98%) | -0.18 | 0 100 100 | 90, 109, 119, 127 | 0 |
| 39 | BT | 132/146 (90%) | -0.73 | 0 100 100 | 41, 55, 94, 127 | 0 |
| 39 | DT | 130/146 (89%) | -0.51 | 0 100 100 | 62, 77, 108, 123 | 0 |
| 40 | BU | 116/118 (98%) | -0.77 | 1 (0%) 85 78 | 25, 36, 55, 71 | 0 |
| 40 | DU | 116/118 (98%) | -0.39 | 1 (0%) 85 78 | 54, 82, 103, 108 | 0 |
| 41 | BV | 100/101 (99%) | -0.77 | 0 100 100 | 28, 46, 73, 90 | 0 |
| 41 | DV | 100/101 (99%) | -0.18 | 0 100 100 | 56, 98, 119, 123 | 0 |
| 42 | BW | 112/113 (99%) | -0.64 | 0 100 100 | 28, 37, 63, 89 | 0 |
| 42 | DW | 111/113 (98%) | -0.41 | 1 (0%) 85 78 | 49, 63, 89, 114 | 0 |
| 43 | BX | 95/96 (98%) | -0.65 | 0 100 100 | 34, 46, 77, 92 | 0 |
| 43 | DX | 95/96 (98%) | -0.43 | 0 100 100 | 61, 77, 100, 107 | 0 |
| 44 | BY | 107/110 (97%) | -0.48 | 0 100 100 | 41, 60, 91, 109 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | DY | 107/110 (97%) | -0.02 | 7 (6%) 22 12 | 77, 96, 112, 124 | 0 |
| 45 | BZ | 186/206 (90%) | -0.51 | 0 100 100 | 49, 76, 104, 126 | 0 |
| 45 | DZ | 189/206 (91%) | 0.07 | 5 (2%) 59 45 | 98, 114, 131, 139 | 0 |
| 46 | B0 | 76/85 (89%) | -0.64 | 0 100 100 | 32, 42, 59, 83 | 0 |
| 46 | D0 | 77/85 (90%) | -0.09 | 0 100 100 | 73, 85, 101, 124 | 0 |
| 47 | B1 | 97/98 (98%) | -0.48 | 0 100 100 | 32, 51, 90, 104 | 0 |
| 47 | D1 | 97/98 (98%) | -0.24 | 2 (2%) 67 52 | 50, 72, 105, 115 | 0 |
| 48 | B2 | 70/72 (97%) | -0.53 | 0 100 100 | 41, 60, 78, 103 | 0 |
| 48 | D2 | 71/72 (98%) | -0.28 | 1 (1%) 78 65 | 78, 94, 106, 110 | 0 |
| 49 | B3 | 59/60 (98%) | -0.71 | 0 100 100 | 33, 41, 76, 93 | 0 |
| 49 | D3 | 58/60 (96%) | -0.03 | 0 100 100 | 71, 84, 114, 128 | 0 |
| 50 | B4 | 46/71 (64%) | -0.57 | 0 100 100 | 78, 96, 112, 114 | 0 |
| 50 | D4 | 46/71 (64%) | -0.10 | 0 100 100 | 118, 126, 136, 138 | 0 |
| 51 | B5 | 59/60 (98%) | -0.78 | 0 100 100 | 25, 41, 62, 74 | 0 |
| 51 | D5 | 59/60 (98%) | -0.56 | 0 100 100 | 47, 66, 85, 106 | 0 |
| 52 | B6 | 53/54 (98%) | -0.67 | 0 100 100 | 42, 49, 66, 76 | 0 |
| 52 | D6 | 53/54 (98%) | -0.36 | 0 100 100 | 67, 81, 93, 101 | 0 |
| 53 | B7 | 48/49 (97%) | -0.45 | 1 (2%) 67 52 | 25, 33, 68, 89 | 0 |
| 53 | D7 | 48/49 (97%) | -0.34 | 0 100 100 | 41, 53, 82, 105 | 0 |
| 54 | B8 | 64/65 (98%) | -0.60 | 0 100 100 | 35, 41, 49, 72 | 0 |
| 54 | D8 | 64/65 (98%) | -0.28 | 1 (1%) 74 62 | 60, 71, 83, 94 | 0 |
| 55 | B9 | 36/37 (97%) | -0.36 | 0 100 100 | 33, 46, 58, 72 | 0 |
| 55 | D9 | 35/37 (94%) | 0.47 | 3 (8%) 13 7 | 73, 88, 103, 115 | 0 |
| All | All | 20489/21572 (94%) | -0.27 | 335 (1%) 74 62 | 22, 83, 131, 172 | 0 |

The worst 5 of 335 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 25 | BA | 1509 | C | 9.1 |
| 22 | AY | 34 | SER | 7.2 |
| 25 | BA | 2801(A) | A | 5.9 |
| 1 | CA | 1286 | A | 5.8 |
| 25 | BA | 1508 | A | 5.7 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | BA | 3367 | 1/1 | 0.85 | 0.81 | 93.45 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3043 | 1/1 | 0.92 | 0.95 | 77.49 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1735 | 1/1 | 0.92 | 0.72 | 55.22 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3156 | 1/1 | 0.90 | 0.76 | 54.38 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3153 | 1/1 | 0.90 | 0.79 | 47.18 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3274 | 1/1 | 0.85 | 0.75 | 45.59 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3076 | 1/1 | 0.93 | 0.51 | 42.66 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3284 | 1/1 | 0.92 | 0.43 | 38.83 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3250 | 1/1 | 0.92 | 0.41 | 38.06 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3124 | 1/1 | 0.95 | 0.51 | 37.41 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3614 | 1/1 | 0.94 | 0.44 | 36.40 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3243 | 1/1 | 0.95 | 0.42 | 35.70 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3488 | 1/1 | 0.85 | 0.69 | 32.53 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3321 | 1/1 | 0.95 | 0.64 | 30.79 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3227 | 1/1 | 0.94 | 0.36 | 30.71 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3166 | 1/1 | 0.97 | 0.46 | 30.42 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3252 | 1/1 | 0.97 | 0.49 | 30.08 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3455 | 1/1 | 0.92 | 0.48 | 30.00 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3537 | 1/1 | 0.96 | 0.51 | 28.37 | 68,68,68,68 | 0 |
| 56 | MG | DD | 302 | 1/1 | 0.97 | 0.52 | 28.19 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3200 | 1/1 | 0.93 | 0.45 | 28.16 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3347 | 1/1 | 0.71 | 0.57 | 27.29 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1650 | 1/1 | 0.78 | 0.50 | 26.66 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3853 | 1/1 | 0.79 | 0.30 | 26.52 | 76,76,76,76 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | BA | 3199 | 1/1 | 0.94 | 0.34 | 25.63 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3192 | 1/1 | 0.80 | 0.59 | 25.21 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3165 | 1/1 | 0.96 | 0.47 | 24.89 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3220 | 1/1 | 0.96 | 0.37 | 24.50 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3341 | 1/1 | 0.80 | 0.53 | 24.19 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3366 | 1/1 | 0.90 | 0.37 | 23.82 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3437 | 1/1 | 0.88 | 0.52 | 23.61 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3317 | 1/1 | 0.80 | 0.37 | 23.30 | 61,61,61,61 | 0 |
| 56 | MG | D6 | 102 | 1/1 | 0.80 | 0.95 | 23.21 | 82,82,82,82 | 0 |
| 56 | MG | CA | 1682 | 1/1 | 0.94 | 0.49 | 22.60 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3030 | 1/1 | 0.87 | 0.52 | 22.30 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3782 | 1/1 | 0.91 | 0.44 | 22.01 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3059 | 1/1 | 0.89 | 0.38 | 21.94 | 67,67,67,67 | 0 |
| 56 | MG | CA | 1605 | 1/1 | 0.83 | 0.52 | 21.93 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3273 | 1/1 | 0.89 | 0.37 | 21.18 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3453 | 1/1 | 0.95 | 0.59 | 21.17 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3325 | 1/1 | 0.75 | 0.38 | 21.02 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3051 | 1/1 | 0.94 | 0.37 | 20.24 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3169 | 1/1 | 0.97 | 0.44 | 20.21 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3156 | 1/1 | 0.88 | 0.48 | 19.31 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3080 | 1/1 | 0.96 | 0.35 | 19.14 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1728 | 1/1 | 0.95 | 0.50 | 18.99 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3403 | 1/1 | 0.97 | 0.43 | 18.03 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3059 | 1/1 | 0.98 | 0.34 | 17.59 | 25,25,25,25 | 0 |
| 56 | MG | AA | 1842 | 1/1 | 0.89 | 0.64 | 17.30 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3183 | 1/1 | 0.98 | 0.40 | 17.13 | 22,22,22,22 | 0 |
| 56 | MG | AA | 1645 | 1/1 | 0.92 | 0.30 | 16.96 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3041 | 1/1 | 0.96 | 0.48 | 16.96 | 54,54,54,54 | 0 |
| 56 | MG | BD | 303 | 1/1 | 0.95 | 0.40 | 16.78 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3178 | 1/1 | 0.88 | 0.41 | 16.67 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3536 | 1/1 | 0.97 | 0.33 | 16.42 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3459 | 1/1 | 0.98 | 0.37 | 16.04 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3188 | 1/1 | 0.87 | 0.33 | 15.06 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3069 | 1/1 | 0.95 | 0.33 | 15.05 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3172 | 1/1 | 0.91 | 0.44 | 15.05 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3353 | 1/1 | 0.96 | 0.62 | 15.01 | 80,80,80,80 | 0 |
| 56 | MG | AA | 1607 | 1/1 | 0.91 | 0.29 | 14.90 | 44,44,44,44 | 0 |
| 56 | MG | AA | 1687 | 1/1 | 0.78 | 0.55 | 14.85 | 105,105,105,105 | 0 |
| 56 | MG | BA | 3875 | 1/1 | 0.94 | 0.38 | 14.60 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3024 | 1/1 | 0.78 | 0.40 | 14.48 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3087 | 1/1 | 0.82 | 0.36 | 14.44 | 40,40,40,40 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | BE | 301 | 1/1 | 0.96 | 0.42 | 14.43 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3887 | 1/1 | 0.98 | 0.27 | 14.39 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3450 | 1/1 | 0.96 | 0.26 | 13.85 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3700 | 1/1 | 0.95 | 0.28 | 13.72 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3419 | 1/1 | 0.94 | 0.25 | 13.69 | 35,35,35,35 | 0 |
| 56 | MG | CA | 1625 | 1/1 | 0.94 | 0.42 | 13.67 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3477 | 1/1 | 0.94 | 0.31 | 13.61 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3098 | 1/1 | 0.85 | 0.28 | 13.60 | 51,51,51,51 | 0 |
| 56 | MG | BV | 201 | 1/1 | 0.96 | 0.38 | 13.55 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3123 | 1/1 | 0.84 | 0.43 | 13.27 | 61,61,61,61 | 0 |
| 56 | MG | AA | 1619 | 1/1 | 0.90 | 0.41 | 13.24 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3054 | 1/1 | 0.98 | 0.30 | 13.22 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3340 | 1/1 | 0.91 | 0.31 | 13.16 | 55,55,55,55 | 0 |
| 56 | MG | BP | 201 | 1/1 | 0.94 | 0.34 | 13.14 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1644 | 1/1 | 0.98 | 0.29 | 13.09 | 48,48,48,48 | 0 |
| 56 | MG | AA | 1636 | 1/1 | 0.94 | 0.42 | 12.99 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3484 | 1/1 | 0.91 | 0.32 | 12.94 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3084 | 1/1 | 0.95 | 0.26 | 12.88 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1692 | 1/1 | 0.89 | 0.69 | 12.80 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1628 | 1/1 | 0.91 | 0.38 | 12.70 | 51,51,51,51 | 0 |
| 56 | MG | B3 | 101 | 1/1 | 0.91 | 0.51 | 12.70 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3285 | 1/1 | 0.90 | 0.42 | 12.66 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3154 | 1/1 | 0.84 | 0.33 | 12.58 | 53,53,53,53 | 0 |
| 56 | MG | CA | 1697 | 1/1 | 0.95 | 0.57 | 12.42 | 117,117,117,117 | 0 |
| 56 | MG | DA | 3097 | 1/1 | 0.98 | 0.46 | 12.37 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3254 | 1/1 | 0.97 | 0.39 | 12.30 | 21,21,21,21 | 0 |
| 56 | MG | AA | 1822 | 1/1 | 0.80 | 0.41 | 12.15 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3417 | 1/1 | 0.99 | 0.37 | 12.08 | 46,46,46,46 | 0 |
| 56 | MG | DE | 303 | 1/1 | 0.96 | 0.45 | 11.91 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1737 | 1/1 | 0.82 | 0.29 | 11.88 | 90,90,90,90 | 0 |
| 56 | MG | BA | 3221 | 1/1 | 0.98 | 0.33 | 11.85 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3218 | 1/1 | 0.97 | 0.23 | 11.79 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3092 | 1/1 | 0.95 | 0.27 | 11.62 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3017 | 1/1 | 0.83 | 0.32 | 11.32 | 69,69,69,69 | 0 |
| 56 | MG | AA | 1800 | 1/1 | 0.87 | 0.73 | 11.19 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3452 | 1/1 | 0.95 | 0.35 | 11.18 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3687 | 1/1 | 0.98 | 0.21 | 11.14 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3048 | 1/1 | 0.77 | 0.35 | 11.01 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3666 | 1/1 | 0.86 | 0.42 | 10.96 | 100,100,100,100 | 0 |
| 56 | MG | DA | 3045 | 1/1 | 0.97 | 0.23 | 10.83 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1685 | 1/1 | 0.72 | 0.62 | 10.79 | 91,91,91,91 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | DA | 3244 | 1/1 | 0.94 | 0.33 | 10.58 | 64,64,64,64 | 0 |
| 56 | MG | AA | 1659 | 1/1 | 0.92 | 0.46 | 10.50 | 97,97,97,97 | 0 |
| 56 | MG | CA | 1743 | 1/1 | 0.94 | 0.59 | 10.37 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3218 | 1/1 | 0.85 | 0.55 | 10.29 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3399 | 1/1 | 0.96 | 0.38 | 10.29 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3548 | 1/1 | 0.96 | 0.25 | 10.27 | 39,39,39,39 | 0 |
| 56 | MG | BB | 201 | 1/1 | 0.94 | 0.38 | 10.06 | 57,57,57,57 | 0 |
| 56 | MG | CA | 1679 | 1/1 | 0.92 | 0.26 | 9.87 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3250 | 1/1 | 0.92 | 0.41 | 9.79 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3374 | 1/1 | 0.98 | 0.37 | 9.79 | 24,24,24,24 | 0 |
| 56 | MG | BU | 201 | 1/1 | 0.91 | 0.35 | 9.77 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3073 | 1/1 | 0.95 | 0.66 | 9.76 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3408 | 1/1 | 0.81 | 0.28 | 9.62 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3393 | 1/1 | 0.97 | 0.31 | 9.59 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3410 | 1/1 | 0.95 | 0.50 | 9.52 | 54,54,54,54 | 0 |
| 56 | MG | D7 | 101 | 1/1 | 0.87 | 0.69 | 9.50 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3419 | 1/1 | 0.93 | 0.25 | 9.50 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3029 | 1/1 | 0.80 | 0.78 | 9.48 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3068 | 1/1 | 0.97 | 0.33 | 9.43 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3198 | 1/1 | 0.91 | 0.33 | 9.38 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3210 | 1/1 | 0.92 | 0.28 | 9.36 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3450 | 1/1 | 0.97 | 0.32 | 9.26 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3552 | 1/1 | 0.98 | 0.28 | 9.14 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1628 | 1/1 | 0.99 | 0.28 | 9.11 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3598 | 1/1 | 0.96 | 0.34 | 9.01 | 69,69,69,69 | 0 |
| 56 | MG | CA | 1706 | 1/1 | 0.89 | 0.88 | 9.01 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3277 | 1/1 | 0.86 | 0.26 | 8.88 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3124 | 1/1 | 0.91 | 0.23 | 8.80 | 34,34,34,34 | 0 |
| 56 | MG | AA | 1782 | 1/1 | 0.96 | 0.23 | 8.68 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3209 | 1/1 | 0.92 | 0.28 | 8.67 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3123 | 1/1 | 0.87 | 0.25 | 8.65 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3211 | 1/1 | 0.98 | 0.29 | 8.51 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3759 | 1/1 | 0.95 | 0.22 | 8.46 | 40,40,40,40 | 0 |
| 56 | MG | BB | 213 | 1/1 | 0.93 | 0.39 | 8.38 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3791 | 1/1 | 0.97 | 0.24 | 8.30 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3079 | 1/1 | 0.94 | 0.39 | 8.23 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3045 | 1/1 | 0.82 | 0.30 | 8.21 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3286 | 1/1 | 0.83 | 0.35 | 8.21 | 69,69,69,69 | 0 |
| 56 | MG | AA | 1845 | 1/1 | 0.99 | 0.55 | 8.06 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3515 | 1/1 | 0.98 | 0.23 | 8.04 | 51,51,51,51 | 0 |
| 56 | MG | AA | 1806 | 1/1 | 0.92 | 0.39 | 7.93 | 59,59,59,59 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3051 | 1/1 | 0.93 | 0.40 | 7.91 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3753 | 1/1 | 0.97 | 0.26 | 7.80 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3375 | 1/1 | 0.94 | 0.27 | 7.74 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3550 | 1/1 | 0.99 | 0.42 | 7.74 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3576 | 1/1 | 0.90 | 0.31 | 7.71 | 75,75,75,75 | 0 |
| 56 | MG | CA | 1778 | 1/1 | 0.97 | 0.35 | 7.64 | 81,81,81,81 | 0 |
| 56 | MG | BA | 3014 | 1/1 | 0.87 | 0.43 | 7.59 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3433 | 1/1 | 0.97 | 0.26 | 7.59 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3602 | 1/1 | 0.93 | 0.22 | 7.57 | 22,22,22,22 | 0 |
| 56 | MG | DE | 302 | 1/1 | 0.96 | 0.52 | 7.54 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3121 | 1/1 | 0.95 | 0.32 | 7.43 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1771 | 1/1 | 0.85 | 0.27 | 7.42 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3146 | 1/1 | 0.89 | 0.25 | 7.36 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3018 | 1/1 | 0.89 | 0.29 | 7.35 | 51,51,51,51 | 0 |
| 56 | MG | DQ | 202 | 1/1 | 0.92 | 0.38 | 7.34 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3145 | 1/1 | 0.98 | 0.26 | 7.15 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3601 | 1/1 | 0.95 | 0.31 | 7.09 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3224 | 1/1 | 0.94 | 0.22 | 7.04 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3142 | 1/1 | 0.93 | 0.26 | 7.00 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3127 | 1/1 | 0.98 | 0.29 | 6.95 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1739 | 1/1 | 0.82 | 0.54 | 6.92 | 99,99,99,99 | 0 |
| 56 | MG | BA | 3383 | 1/1 | 0.88 | 0.21 | 6.92 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3550 | 1/1 | 0.99 | 0.26 | 6.88 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3021 | 1/1 | 0.88 | 0.24 | 6.87 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3572 | 1/1 | 0.98 | 0.26 | 6.80 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3100 | 1/1 | 0.95 | 0.28 | 6.77 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3582 | 1/1 | 0.93 | 0.20 | 6.70 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3369 | 1/1 | 0.82 | 0.21 | 6.70 | 94,94,94,94 | 0 |
| 56 | MG | AA | 1663 | 1/1 | 0.94 | 0.22 | 6.69 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3632 | 1/1 | 0.97 | 0.31 | 6.59 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3625 | 1/1 | 0.77 | 0.27 | 6.58 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3248 | 1/1 | 0.95 | 0.24 | 6.54 | 24,24,24,24 | 0 |
| 56 | MG | AA | 1711 | 1/1 | 0.75 | 0.42 | 6.45 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3732 | 1/1 | 0.96 | 0.18 | 6.43 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3101 | 1/1 | 0.94 | 0.33 | 6.30 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3056 | 1/1 | 0.96 | 0.28 | 6.24 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3052 | 1/1 | 0.94 | 0.28 | 6.24 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3553 | 1/1 | 0.99 | 0.22 | 6.19 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3427 | 1/1 | 0.98 | 0.29 | 6.14 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3451 | 1/1 | 0.95 | 0.28 | 6.08 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3460 | 1/1 | 0.92 | 0.28 | 6.07 | 67,67,67,67 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 1691 | 1/1 | 0.95 | 0.45 | 5.90 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3510 | 1/1 | 0.80 | 0.23 | 5.89 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1626 | 1/1 | 0.91 | 0.43 | 5.89 | 62,62,62,62 | 0 |
| 56 | MG | CA | 1656 | 1/1 | 0.90 | 0.28 | 5.85 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3390 | 1/1 | 0.98 | 0.19 | 5.78 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1786 | 1/1 | 0.86 | 0.31 | 5.66 | 69,69,69,69 | 0 |
| 56 | MG | CA | 1693 | 1/1 | 0.89 | 0.35 | 5.59 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3530 | 1/1 | 0.94 | 0.31 | 5.56 | 72,72,72,72 | 0 |
| 56 | MG | DB | 201 | 1/1 | 0.96 | 0.20 | 5.55 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3486 | 1/1 | 0.99 | 0.24 | 5.45 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1608 | 1/1 | 0.86 | 0.51 | 5.45 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3624 | 1/1 | 0.86 | 0.24 | 5.44 | 82,82,82,82 | 0 |
| 56 | MG | CA | 1606 | 1/1 | 0.86 | 0.26 | 5.38 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3251 | 1/1 | 0.91 | 0.27 | 5.20 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3134 | 1/1 | 0.95 | 0.22 | 5.17 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3461 | 1/1 | 0.96 | 0.28 | 5.14 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1604 | 1/1 | 0.99 | 0.23 | 5.11 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1690 | 1/1 | 0.97 | 0.30 | 5.07 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3386 | 1/1 | 0.94 | 0.30 | 5.02 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3225 | 1/1 | 0.90 | 0.23 | 5.01 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3197 | 1/1 | 0.82 | 0.27 | 4.95 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3581 | 1/1 | 0.96 | 0.18 | 4.92 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3168 | 1/1 | 0.94 | 0.31 | 4.85 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3193 | 1/1 | 0.93 | 0.25 | 4.76 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3038 | 1/1 | 0.95 | 0.20 | 4.75 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3467 | 1/1 | 0.92 | 0.32 | 4.73 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3540 | 1/1 | 0.99 | 0.26 | 4.59 | 57,57,57,57 | 0 |
| 56 | MG | CA | 1726 | 1/1 | 0.93 | 0.26 | 4.56 | 70,70,70,70 | 0 |
| 56 | MG | DT | 203 | 1/1 | 0.91 | 0.19 | 4.55 | 73,73,73,73 | 0 |
| 56 | MG | CA | 1637 | 1/1 | 0.87 | 0.26 | 4.44 | 80,80,80,80 | 0 |
| 56 | MG | AA | 1797 | 1/1 | 0.93 | 0.34 | 4.34 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3539 | 1/1 | 0.70 | 0.26 | 4.31 | 102,102,102,102 | 0 |
| 56 | MG | BD | 301 | 1/1 | 0.86 | 0.27 | 4.24 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1776 | 1/1 | 0.96 | 0.22 | 4.24 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3766 | 1/1 | 0.96 | 0.19 | 4.23 | 38,38,38,38 | 0 |
| 56 | MG | DD | 303 | 1/1 | 0.90 | 0.28 | 4.18 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3615 | 1/1 | 0.91 | 0.20 | 4.17 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3654 | 1/1 | 0.97 | 0.19 | 4.15 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3868 | 1/1 | 0.92 | 0.20 | 4.13 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3411 | 1/1 | 0.84 | 0.22 | 4.11 | 55,55,55,55 | 0 |
| 56 | MG | BD | 302 | 1/1 | 0.84 | 0.39 | 4.11 | 51,51,51,51 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3175 | 1/1 | 0.90 | 0.22 | 4.08 | 75,75,75,75 | 0 |
| 56 | MG | AA | 1631 | 1/1 | 0.97 | 0.31 | 4.01 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3677 | 1/1 | 0.98 | 0.26 | 3.99 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3233 | 1/1 | 0.95 | 0.24 | 3.94 | 22,22,22,22 | 0 |
| 56 | MG | CA | 1788 | 1/1 | 0.73 | 0.28 | 3.94 | 118,118,118,118 | 0 |
| 56 | MG | BA | 3376 | 1/1 | 0.96 | 0.35 | 3.92 | 43,43,43,43 | 0 |
| 56 | MG | AD | 302 | 1/1 | 0.96 | 0.39 | 3.92 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3264 | 1/1 | 0.93 | 0.21 | 3.90 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3075 | 1/1 | 0.94 | 0.42 | 3.88 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3077 | 1/1 | 0.95 | 0.34 | 3.85 | 45,45,45,45 | 0 |
| 56 | MG | AA | 1635 | 1/1 | 0.90 | 0.20 | 3.83 | 65,65,65,65 | 0 |
| 56 | MG | D6 | 103 | 1/1 | 0.96 | 0.32 | 3.83 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3682 | 1/1 | 0.98 | 0.20 | 3.81 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3702 | 1/1 | 0.97 | 0.22 | 3.79 | 49,49,49,49 | 0 |
| 56 | MG | B2 | 102 | 1/1 | 0.77 | 0.35 | 3.74 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3627 | 1/1 | 0.92 | 0.21 | 3.73 | 81,81,81,81 | 0 |
| 56 | MG | CA | 1761 | 1/1 | 0.96 | 0.29 | 3.70 | 68,68,68,68 | 0 |
| 56 | MG | BG | 201 | 1/1 | 0.82 | 0.32 | 3.70 | 54,54,54,54 | 0 |
| 56 | MG | CA | 1722 | 1/1 | 0.75 | 0.33 | 3.66 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3558 | 1/1 | 0.96 | 0.25 | 3.66 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3249 | 1/1 | 0.92 | 0.26 | 3.66 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3567 | 1/1 | 0.86 | 0.29 | 3.64 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3317 | 1/1 | 0.88 | 0.21 | 3.64 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3692 | 1/1 | 0.91 | 0.24 | 3.58 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3447 | 1/1 | 0.97 | 0.19 | 3.58 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3141 | 1/1 | 0.91 | 0.24 | 3.57 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3586 | 1/1 | 0.94 | 0.28 | 3.57 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3203 | 1/1 | 0.94 | 0.19 | 3.55 | 44,44,44,44 | 0 |
| 56 | MG | BF | 305 | 1/1 | 0.93 | 0.22 | 3.43 | 52,52,52,52 | 0 |
| 56 | MG | AA | 1726 | 1/1 | 0.83 | 0.24 | 3.42 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3357 | 1/1 | 0.92 | 0.24 | 3.38 | 51,51,51,51 | 0 |
| 56 | MG | CA | 1753 | 1/1 | 0.96 | 0.22 | 3.33 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3312 | 1/1 | 0.84 | 0.29 | 3.30 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3854 | 1/1 | 0.98 | 0.18 | 3.30 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3585 | 1/1 | 0.92 | 0.23 | 3.30 | 104,104,104,104 | 0 |
| 56 | MG | BA | 3837 | 1/1 | 0.94 | 0.24 | 3.26 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3872 | 1/1 | 0.92 | 0.19 | 3.25 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3770 | 1/1 | 0.89 | 0.18 | 3.24 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3599 | 1/1 | 0.98 | 0.26 | 3.23 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1683 | 1/1 | 0.95 | 0.28 | 3.21 | 106,106,106,106 | 0 |
| 56 | MG | CA | 1602 | 1/1 | 0.96 | 0.25 | 3.21 | 72,72,72,72 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3629 | 1/1 | 0.77 | 0.37 | 3.09 | 104,104,104,104 | 0 |
| 56 | MG | CA | 1647 | 1/1 | 0.84 | 0.24 | 3.07 | 71,71,71,71 | 0 |
| 56 | MG | DF | 302 | 1/1 | 0.96 | 0.34 | 3.06 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3047 | 1/1 | 0.94 | 0.27 | 3.01 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3030 | 1/1 | 0.95 | 0.18 | 2.97 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1630 | 1/1 | 0.96 | 0.21 | 2.97 | 98,98,98,98 | 0 |
| 56 | MG | D0 | 101 | 1/1 | 0.91 | 0.21 | 2.96 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3204 | 1/1 | 0.97 | 0.20 | 2.94 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3029 | 1/1 | 0.94 | 0.21 | 2.89 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3074 | 1/1 | 0.94 | 0.30 | 2.84 | 69,69,69,69 | 0 |
| 56 | MG | BR | 201 | 1/1 | 0.99 | 0.24 | 2.81 | 19,19,19,19 | 0 |
| 56 | MG | CA | 1621 | 1/1 | 0.95 | 0.20 | 2.81 | 100,100,100,100 | 0 |
| 56 | MG | BA | 3064 | 1/1 | 0.98 | 0.16 | 2.77 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3044 | 1/1 | 0.96 | 0.21 | 2.75 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3061 | 1/1 | 0.90 | 0.27 | 2.73 | 45,45,45,45 | 0 |
| 56 | MG | DB | 203 | 1/1 | 0.85 | 0.27 | 2.73 | 105,105,105,105 | 0 |
| 56 | MG | BA | 3805 | 1/1 | 0.93 | 0.19 | 2.65 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3648 | 1/1 | 0.96 | 0.17 | 2.60 | 49,49,49,49 | 0 |
| 56 | MG | D1 | 101 | 1/1 | 0.94 | 0.30 | 2.58 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3809 | 1/1 | 0.97 | 0.17 | 2.54 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1754 | 1/1 | 0.83 | 0.35 | 2.54 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3646 | 1/1 | 0.94 | 0.17 | 2.43 | 62,62,62,62 | 0 |
| 56 | MG | CA | 1705 | 1/1 | 0.92 | 0.44 | 2.42 | 112,112,112,112 | 0 |
| 56 | MG | AA | 1648 | 1/1 | 0.91 | 0.21 | 2.40 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1809 | 1/1 | 0.81 | 0.20 | 2.36 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3109 | 1/1 | 0.92 | 0.20 | 2.36 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1897 | 1/1 | 0.90 | 0.22 | 2.36 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3354 | 1/1 | 0.97 | 0.22 | 2.36 | 43,43,43,43 | 0 |
| 56 | MG | B1 | 101 | 1/1 | 0.85 | 0.29 | 2.33 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3676 | 1/1 | 0.97 | 0.17 | 2.33 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1874 | 1/1 | 0.92 | 0.24 | 2.32 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3675 | 1/1 | 0.96 | 0.19 | 2.30 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1838 | 1/1 | 0.80 | 0.20 | 2.30 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3571 | 1/1 | 0.80 | 0.17 | 2.27 | 31,31,31,31 | 0 |
| 56 | MG | DV | 201 | 1/1 | 0.91 | 0.25 | 2.26 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3679 | 1/1 | 0.95 | 0.21 | 2.26 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3894 | 1/1 | 0.95 | 0.19 | 2.25 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3525 | 1/1 | 0.93 | 0.18 | 2.22 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1919 | 1/1 | 0.93 | 0.22 | 2.22 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1745 | 1/1 | 0.65 | 0.23 | 2.17 | 99,99,99,99 | 0 |
| 56 | MG | CA | 1612 | 1/1 | 0.73 | 0.24 | 2.10 | 84,84,84,84 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AV | 101 | 1/1 | 0.98 | 0.34 | 2.09 | 48,48,48,48 | 0 |
| 56 | MG | CA | 1732 | 1/1 | 0.89 | 0.23 | 2.09 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3600 | 1/1 | 0.97 | 0.21 | 2.08 | 57,57,57,57 | 0 |
| 56 | MG | AA | 1872 | 1/1 | 0.97 | 0.18 | 2.06 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3035 | 1/1 | 0.56 | 0.24 | 2.05 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1642 | 1/1 | 0.84 | 0.31 | 2.03 | 73,73,73,73 | 0 |
| 56 | MG | BF | 307 | 1/1 | 0.97 | 0.22 | 1.98 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1758 | 1/1 | 0.99 | 0.21 | 1.95 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3094 | 1/1 | 0.94 | 0.17 | 1.93 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3596 | 1/1 | 0.94 | 0.19 | 1.93 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1706 | 1/1 | 0.84 | 0.23 | 1.91 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3611 | 1/1 | 0.95 | 0.14 | 1.85 | 43,43,43,43 | 0 |
| 56 | MG | B2 | 101 | 1/1 | 0.88 | 0.21 | 1.84 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3064 | 1/1 | 0.85 | 0.26 | 1.84 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3518 | 1/1 | 0.98 | 0.23 | 1.84 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3247 | 1/1 | 0.99 | 0.19 | 1.81 | 20,20,20,20 | 0 |
| 56 | MG | CA | 1615 | 1/1 | 0.91 | 0.23 | 1.78 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3817 | 1/1 | 0.98 | 0.18 | 1.76 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3106 | 1/1 | 0.95 | 0.17 | 1.74 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3015 | 1/1 | 0.96 | 0.15 | 1.74 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1660 | 1/1 | 0.98 | 0.22 | 1.73 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3532 | 1/1 | 0.69 | 0.21 | 1.71 | 90,90,90,90 | 0 |
| 56 | MG | AA | 1652 | 1/1 | 0.97 | 0.28 | 1.71 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3798 | 1/1 | 0.94 | 0.20 | 1.68 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3441 | 1/1 | 0.89 | 0.18 | 1.68 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1640 | 1/1 | 0.96 | 0.19 | 1.65 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3413 | 1/1 | 0.92 | 0.19 | 1.65 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3496 | 1/1 | 0.97 | 0.19 | 1.64 | 47,47,47,47 | 0 |
| 56 | MG | AD | 303 | 1/1 | 0.90 | 0.19 | 1.62 | 93,93,93,93 | 0 |
| 56 | MG | CA | 1701 | 1/1 | 0.72 | 0.20 | 1.62 | 109,109,109,109 | 0 |
| 56 | MG | BA | 3063 | 1/1 | 0.88 | 0.14 | 1.62 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3784 | 1/1 | 0.97 | 0.21 | 1.60 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3012 | 1/1 | 0.89 | 0.52 | 1.58 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3425 | 1/1 | 0.93 | 0.18 | 1.56 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3283 | 1/1 | 0.87 | 0.23 | 1.55 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3127 | 1/1 | 0.92 | 0.17 | 1.55 | 41,41,41,41 | 0 |
| 56 | MG | AI | 201 | 1/1 | 0.93 | 0.26 | 1.54 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3475 | 1/1 | 0.97 | 0.20 | 1.51 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3531 | 1/1 | 0.99 | 0.23 | 1.46 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1935 | 1/1 | 0.98 | 0.18 | 1.39 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3594 | 1/1 | 0.96 | 0.22 | 1.38 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3673 | 1/1 | 0.98 | 0.17 | 1.36 | 43,43,43,43 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3384 | 1/1 | 0.96 | 0.20 | 1.35 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3749 | 1/1 | 0.91 | 0.18 | 1.32 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3540 | 1/1 | 0.97 | 0.16 | 1.26 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3121 | 1/1 | 0.92 | 0.15 | 1.20 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3836 | 1/1 | 0.97 | 0.20 | 1.19 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3120 | 1/1 | 0.87 | 0.26 | 1.14 | 51,51,51,51 | 0 |
| 56 | MG | AA | 1810 | 1/1 | 0.93 | 0.28 | 1.13 | 84,84,84,84 | 0 |
| 56 | MG | BF | 301 | 1/1 | 0.96 | 0.21 | 1.06 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1601 | 1/1 | 0.93 | 0.21 | 1.02 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1759 | 1/1 | 0.94 | 0.18 | 1.00 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3879 | 1/1 | 0.89 | 0.18 | 0.99 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3391 | 1/1 | 0.93 | 0.17 | 0.94 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3011 | 1/1 | 0.90 | 0.34 | 0.94 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3432 | 1/1 | 0.97 | 0.17 | 0.93 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3859 | 1/1 | 0.97 | 0.15 | 0.88 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3434 | 1/1 | 0.96 | 0.20 | 0.85 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3385 | 1/1 | 0.97 | 0.18 | 0.85 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3711 | 1/1 | 0.99 | 0.16 | 0.84 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3132 | 1/1 | 0.97 | 0.14 | 0.84 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3493 | 1/1 | 0.90 | 0.21 | 0.83 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3042 | 1/1 | 0.92 | 0.16 | 0.76 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3757 | 1/1 | 0.96 | 0.15 | 0.69 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1821 | 1/1 | 0.85 | 0.22 | 0.69 | 78,78,78,78 | 0 |
| 57 | ZN | AD | 301 | 1/1 | 0.97 | 0.29 | 0.67 | 93,93,93,93 | 0 |
| 56 | MG | DA | 3308 | 1/1 | 0.97 | 0.16 | 0.65 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3032 | 1/1 | 0.92 | 0.16 | 0.64 | 51,51,51,51 | 0 |
| 56 | MG | CA | 1618 | 1/1 | 0.89 | 0.15 | 0.60 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3043 | 1/1 | 0.87 | 0.18 | 0.57 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3748 | 1/1 | 0.89 | 0.15 | 0.53 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3747 | 1/1 | 0.99 | 0.15 | 0.49 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3067 | 1/1 | 0.95 | 0.17 | 0.44 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3537 | 1/1 | 0.98 | 0.15 | 0.43 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3503 | 1/1 | 0.95 | 0.15 | 0.40 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3437 | 1/1 | 0.97 | 0.17 | 0.39 | 70,70,70,70 | 0 |
| 56 | MG | DB | 215 | 1/1 | 0.90 | 0.17 | 0.37 | 94,94,94,94 | 0 |
| 56 | MG | CV | 101 | 1/1 | 0.93 | 0.19 | 0.36 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3100 | 1/1 | 0.96 | 0.16 | 0.33 | 48,48,48,48 | 0 |
| 56 | MG | BB | 205 | 1/1 | 0.99 | 0.13 | 0.33 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3893 | 1/1 | 0.89 | 0.15 | 0.32 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3513 | 1/1 | 0.93 | 0.17 | 0.31 | 59,59,59,59 | 0 |
| 56 | MG | DE | 304 | 1/1 | 0.92 | 0.22 | 0.30 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1895 | 1/1 | 0.97 | 0.18 | 0.30 | 87,87,87,87 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | BA | 3845 | 1/1 | 0.99 | 0.14 | 0.25 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3624 | 1/1 | 0.96 | 0.15 | 0.22 | 57,57,57,57 | 0 |
| 56 | MG | CA | 1773 | 1/1 | 0.41 | 0.15 | 0.18 | 124,124,124,124 | 0 |
| 56 | MG | BA | 3734 | 1/1 | 0.97 | 0.12 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | CA | 1607 | 1/1 | 0.90 | 0.16 | 0.11 | 73,73,73,73 | 0 |
| 57 | ZN | CD | 301 | 1/1 | 0.96 | 0.28 | 0.11 | 90,90,90,90 | 0 |
| 56 | MG | BA | 3044 | 1/1 | 0.94 | 0.13 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3446 | 1/1 | 0.97 | 0.14 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | CA | 1644 | 1/1 | 0.86 | 0.17 | 0.09 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3672 | 1/1 | 0.94 | 0.15 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3431 | 1/1 | 0.98 | 0.14 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3019 | 1/1 | 0.97 | 0.22 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3865 | 1/1 | 0.94 | 0.14 | 0.05 | 97,97,97,97 | 0 |
| 56 | MG | B0 | 103 | 1/1 | 0.94 | 0.17 | 0.05 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3001 | 1/1 | 0.96 | 0.14 | 0.05 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3506 | 1/1 | 0.99 | 0.14 | 0.05 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3066 | 1/1 | 0.94 | 0.17 | 0.01 | 35,35,35,35 | 0 |
| 56 | MG | CA | 1678 | 1/1 | 0.93 | 0.19 | 0.01 | 84,84,84,84 | 0 |
| 56 | MG | AA | 1614 | 1/1 | 0.89 | 0.15 | -0.03 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3065 | 1/1 | 0.97 | 0.12 | -0.07 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3168 | 1/1 | 0.98 | 0.16 | -0.11 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3443 | 1/1 | 0.98 | 0.15 | -0.14 | 41,41,41,41 | 0 |
| 56 | MG | CA | 1813 | 1/1 | 0.92 | 0.20 | -0.14 | 113,113,113,113 | 0 |
| 56 | MG | DA | 3040 | 1/1 | 0.80 | 0.17 | -0.17 | 78,78,78,78 | 0 |
| 56 | MG | CA | 1728 | 1/1 | 0.83 | 0.16 | -0.18 | 83,83,83,83 | 0 |
| 56 | MG | CA | 1710 | 1/1 | 0.93 | 0.17 | -0.22 | 95,95,95,95 | 0 |
| 56 | MG | AA | 1611 | 1/1 | 0.76 | 0.16 | -0.24 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3754 | 1/1 | 0.94 | 0.15 | -0.26 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3731 | 1/1 | 0.95 | 0.14 | -0.29 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3593 | 1/1 | 0.91 | 0.12 | -0.29 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3804 | 1/1 | 0.96 | 0.14 | -0.31 | 59,59,59,59 | 0 |
| 56 | MG | DT | 201 | 1/1 | 0.80 | 0.20 | -0.34 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3472 | 1/1 | 0.85 | 0.14 | -0.37 | 78,78,78,78 | 0 |
| 56 | MG | CA | 1658 | 1/1 | 0.89 | 0.18 | -0.40 | 91,91,91,91 | 0 |
| 56 | MG | AA | 1864 | 1/1 | 0.96 | 0.14 | -0.40 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3561 | 1/1 | 0.99 | 0.17 | -0.43 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1608 | 1/1 | 0.92 | 0.17 | -0.44 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3831 | 1/1 | 0.97 | 0.14 | -0.44 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3062 | 1/1 | 0.97 | 0.14 | -0.46 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3856 | 1/1 | 0.96 | 0.14 | -0.52 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3630 | 1/1 | 0.98 | 0.13 | -0.53 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3576 | 1/1 | 0.97 | 0.13 | -0.53 | 66,66,66,66 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | AA | 1873 | 1/1 | 0.92 | 0.15 | -0.60 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3601 | 1/1 | 0.98 | 0.15 | -0.62 | 24,24,24,24 | 0 |
| 56 | MG | BQ | 204 | 1/1 | 0.97 | 0.15 | -0.66 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3387 | 1/1 | 0.99 | 0.16 | -0.66 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3037 | 1/1 | 0.96 | 0.14 | -0.77 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3707 | 1/1 | 0.96 | 0.14 | -0.79 | 25,25,25,25 | 0 |
| 57 | ZN | D4 | 101 | 1/1 | 0.95 | 0.13 | -0.80 | 178,178,178,178 | 0 |
| 56 | MG | CA | 1620 | 1/1 | 0.96 | 0.14 | -0.84 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3678 | 1/1 | 0.99 | 0.14 | -0.85 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3643 | 1/1 | 0.94 | 0.14 | -0.88 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3851 | 1/1 | 0.94 | 0.14 | -0.89 | 35,35,35,35 | 0 |
| 56 | MG | AA | 1732 | 1/1 | 0.95 | 0.10 | -0.90 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1852 | 1/1 | 0.94 | 0.13 | -0.96 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3819 | 1/1 | 0.83 | 0.13 | -0.97 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3396 | 1/1 | 0.88 | 0.15 | -0.98 | 95,95,95,95 | 0 |
| 56 | MG | DA | 3033 | 1/1 | 0.81 | 0.12 | -1.00 | 74,74,74,74 | 0 |
| 56 | MG | DF | 303 | 1/1 | 0.95 | 0.12 | -1.01 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3664 | 1/1 | 0.98 | 0.14 | -1.03 | 31,31,31,31 | 0 |
| 56 | MG | CV | 105 | 1/1 | 0.86 | 0.15 | -1.03 | 106,106,106,106 | 0 |
| 57 | ZN | B6 | 101 | 1/1 | 0.98 | 0.11 | -1.11 | 48,48,48,48 | 0 |
| 57 | ZN | AN | 101 | 1/1 | 0.97 | 0.15 | -1.13 | 164,164,164,164 | 0 |
| 56 | MG | DA | 3046 | 1/1 | 0.84 | 0.12 | -1.16 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3672 | 1/1 | 0.94 | 0.10 | -1.19 | 87,87,87,87 | 0 |
| 57 | ZN | B5 | 104 | 1/1 | 0.98 | 0.09 | -1.20 | 75,75,75,75 | 0 |
| 56 | MG | AA | 1876 | 1/1 | 0.96 | 0.07 | -1.21 | 89,89,89,89 | 0 |
| 57 | ZN | D9 | 101 | 1/1 | 0.93 | 0.16 | -1.27 | 117,117,117,117 | 0 |
| 57 | ZN | DY | 201 | 1/1 | 0.97 | 0.07 | -1.28 | 123,123,123,123 | 0 |
| 57 | ZN | D5 | 102 | 1/1 | 0.98 | 0.08 | -1.29 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1933 | 1/1 | 0.96 | 0.13 | -1.29 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3013 | 1/1 | 0.83 | 0.13 | -1.32 | 97,97,97,97 | 0 |
| 56 | MG | DA | 3421 | 1/1 | 0.87 | 0.12 | -1.36 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3484 | 1/1 | 0.97 | 0.12 | -1.37 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3688 | 1/1 | 0.98 | 0.12 | -1.44 | 25,25,25,25 | 0 |
| 56 | MG | BG | 202 | 1/1 | 0.91 | 0.07 | -1.46 | 82,82,82,82 | 0 |
| 57 | ZN | D6 | 101 | 1/1 | 0.97 | 0.09 | -1.47 | 106,106,106,106 | 0 |
| 56 | MG | DA | 3022 | 1/1 | 0.97 | 0.10 | -1.48 | 46,46,46,46 | 0 |
| 57 | ZN | B4 | 101 | 1/1 | 0.97 | 0.05 | -1.51 | 137,137,137,137 | 0 |
| 56 | MG | AA | 1943 | 1/1 | 0.80 | 0.14 | -1.54 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3563 | 1/1 | 0.88 | 0.11 | -1.55 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3767 | 1/1 | 0.94 | 0.12 | -1.56 | 51,51,51,51 | 0 |
| 57 | ZN | B9 | 101 | 1/1 | 0.99 | 0.08 | -1.57 | 51,51,51,51 | 0 |
| 56 | MG | B5 | 103 | 1/1 | 0.96 | 0.12 | -1.60 | 61,61,61,61 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | AA | 1908 | 1/1 | 0.97 | 0.11 | -1.63 | 97,97,97,97 | 0 |
| 56 | MG | AA | 1799 | 1/1 | 0.96 | 0.13 | -1.68 | 95,95,95,95 | 0 |
| 56 | MG | AA | 1637 | 1/1 | 0.78 | 0.12 | -1.74 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3019 | 1/1 | 0.91 | 0.10 | -1.74 | 65,65,65,65 | 0 |
| 56 | MG | BE | 305 | 1/1 | 0.92 | 0.11 | -1.77 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3638 | 1/1 | 0.98 | 0.11 | -1.81 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3041 | 1/1 | 0.95 | 0.10 | -1.86 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1649 | 1/1 | 0.90 | 0.13 | -1.87 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3301 | 1/1 | 0.97 | 0.11 | -1.88 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3667 | 1/1 | 0.99 | 0.10 | -1.90 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3389 | 1/1 | 0.99 | 0.09 | -1.93 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3634 | 1/1 | 0.89 | 0.13 | -1.95 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3523 | 1/1 | 0.96 | 0.09 | -1.96 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3553 | 1/1 | 0.95 | 0.11 | -2.01 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3485 | 1/1 | 0.96 | 0.12 | -2.03 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3501 | 1/1 | 0.96 | 0.12 | -2.10 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3397 | 1/1 | 0.89 | 0.11 | -2.13 | 35,35,35,35 | 0 |
| 57 | ZN | CN | 101 | 1/1 | 0.93 | 0.10 | -2.13 | 165,165,165,165 | 0 |
| 57 | ZN | BY | 201 | 1/1 | 0.98 | 0.06 | -2.15 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3686 | 1/1 | 0.96 | 0.13 | -2.26 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3555 | 1/1 | 0.97 | 0.10 | -2.29 | 47,47,47,47 | 0 |
| 56 | MG | BB | 222 | 1/1 | 0.91 | 0.11 | -2.29 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3038 | 1/1 | 0.92 | 0.11 | -2.30 | 50,50,50,50 | 0 |
| 56 | MG | CA | 1748 | 1/1 | 0.81 | 0.15 | -2.32 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3398 | 1/1 | 0.79 | 0.12 | -2.35 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3680 | 1/1 | 0.96 | 0.08 | -2.41 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3597 | 1/1 | 0.98 | 0.10 | -2.42 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3665 | 1/1 | 0.92 | 0.09 | -2.42 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3489 | 1/1 | 0.90 | 0.10 | -2.45 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1878 | 1/1 | 0.89 | 0.14 | -2.48 | 46,46,46,46 | 0 |
| 56 | MG | BB | 228 | 1/1 | 0.94 | 0.09 | -2.49 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3640 | 1/1 | 0.93 | 0.11 | -2.55 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3040 | 1/1 | 0.88 | 0.09 | -2.55 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3007 | 1/1 | 0.96 | 0.10 | -2.56 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3692 | 1/1 | 0.98 | 0.11 | -2.59 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3525 | 1/1 | 0.96 | 0.10 | -2.61 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3691 | 1/1 | 0.98 | 0.10 | -2.62 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3694 | 1/1 | 0.96 | 0.13 | -2.66 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3428 | 1/1 | 0.94 | 0.14 | -2.68 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3477 | 1/1 | 0.98 | 0.09 | -2.69 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1921 | 1/1 | 0.90 | 0.12 | -2.77 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3646 | 1/1 | 0.98 | 0.13 | -2.88 | 44,44,44,44 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | BA | 3698 | 1/1 | 0.97 | 0.08 | -2.88 | 44,44,44,44 | 0 |
| 56 | MG | AA | 1892 | 1/1 | 0.97 | 0.08 | -2.90 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1736 | 1/1 | 0.85 | 0.09 | -2.92 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3690 | 1/1 | 0.96 | 0.10 | -3.00 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3660 | 1/1 | 0.98 | 0.08 | -3.02 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3420 | 1/1 | 0.98 | 0.10 | -3.02 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3416 | 1/1 | 0.97 | 0.11 | -3.09 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3455 | 1/1 | 0.98 | 0.14 | -3.12 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3252 | 1/1 | 0.92 | 0.11 | -3.15 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3584 | 1/1 | 0.96 | 0.10 | -3.16 | 76,76,76,76 | 0 |
| 56 | MG | AA | 1938 | 1/1 | 0.96 | 0.10 | -3.17 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3544 | 1/1 | 0.97 | 0.11 | -3.18 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3402 | 1/1 | 0.98 | 0.11 | -3.20 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3539 | 1/1 | 0.97 | 0.10 | -3.21 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3810 | 1/1 | 0.93 | 0.12 | -3.21 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3669 | 1/1 | 0.99 | 0.09 | -3.28 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3087 | 1/1 | 0.83 | 0.10 | -3.32 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3444 | 1/1 | 0.93 | 0.08 | -3.43 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3466 | 1/1 | 0.84 | 0.07 | -3.53 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3643 | 1/1 | 0.98 | 0.05 | -3.56 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3723 | 1/1 | 0.94 | 0.09 | -3.61 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3556 | 1/1 | 0.95 | 0.07 | -3.94 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3439 | 1/1 | 0.93 | 0.08 | -4.02 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3585 | 1/1 | 0.98 | 0.06 | -4.06 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3463 | 1/1 | 0.96 | 0.10 | -4.07 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3021 | 1/1 | 0.96 | 0.11 | -4.13 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3495 | 1/1 | 0.93 | 0.10 | -4.13 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3407 | 1/1 | 0.99 | 0.11 | -4.16 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3504 | 1/1 | 0.93 | 0.08 | -4.17 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3406 | 1/1 | 0.97 | 0.11 | -4.19 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3671 | 1/1 | 0.97 | 0.06 | -4.58 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3547 | 1/1 | 0.98 | 0.04 | -4.73 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3631 | 1/1 | 0.99 | 0.08 | -4.79 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3689 | 1/1 | 0.98 | 0.09 | -5.51 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3666 | 1/1 | 0.97 | 0.06 | -5.62 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3575 | 1/1 | 0.95 | 0.11 | -5.74 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3552 | 1/1 | 0.97 | 0.06 | -6.31 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3559 | 1/1 | 0.99 | 0.09 | -6.67 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3408 | 1/1 | 0.99 | 0.07 | -7.54 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3555 | 1/1 | 0.96 | 0.05 | -7.60 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3695 | 1/1 | 0.99 | 0.07 | -7.91 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3487 | 1/1 | 0.94 | 0.05 | -8.38 | 70,70,70,70 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 56 | MG | BA | 3534 | 1/1 | 0.99 | 0.06 | -9.24 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3590 | 1/1 | 0.98 | 0.07 | -11.63 | 56,56,56,56 | 0 |
| 56 | MG | B6 | 102 | 1/1 | 0.97 | 0.07 | -13.49 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3670 | 1/1 | 0.96 | 0.07 | -14.40 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3554 | 1/1 | 0.96 | 0.30 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3709 | 1/1 | 0.98 | 0.13 | - | 49,49,49,49 | 0 |
| 56 | MG | DA | 3573 | 1/1 | 0.95 | 0.17 | - | 42,42,42,42 | 0 |
| 56 | MG | DB | 207 | 1/1 | 0.88 | 0.12 | - | 79,79,79,79 | 0 |
| 56 | MG | CD | 302 | 1/1 | 0.93 | 0.38 | - | 53,53,53,53 | 0 |
| 56 | MG | CA | 1782 | 1/1 | 0.78 | 0.38 | - | 96,96,96,96 | 0 |
| 56 | MG | BA | 3185 | 1/1 | 0.95 | 0.11 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3618 | 1/1 | 0.97 | 0.10 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3768 | 1/1 | 0.97 | 0.04 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3411 | 1/1 | 0.95 | 0.37 | - | 55,55,55,55 | 0 |
| 56 | MG | AA | 1811 | 1/1 | 0.85 | 0.27 | - | 120,120,120,120 | 0 |
| 56 | MG | DA | 3326 | 1/1 | 0.71 | 0.42 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3293 | 1/1 | 0.90 | 0.32 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3105 | 1/1 | 0.86 | 0.45 | - | 52,52,52,52 | 0 |
| 56 | MG | BA | 3806 | 1/1 | 0.94 | 0.21 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3758 | 1/1 | 0.96 | 0.09 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3331 | 1/1 | 0.82 | 0.50 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3507 | 1/1 | 0.92 | 0.32 | - | 53,53,53,53 | 0 |
| 56 | MG | CA | 1764 | 1/1 | 0.92 | 0.11 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3012 | 1/1 | 0.93 | 0.10 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3882 | 1/1 | 0.79 | 0.09 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3764 | 1/1 | 0.82 | 0.07 | - | 85,85,85,85 | 0 |
| 56 | MG | CA | 1657 | 1/1 | 0.84 | 0.14 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3824 | 1/1 | 0.90 | 0.27 | - | 90,90,90,90 | 0 |
| 56 | MG | AA | 1778 | 1/1 | 0.74 | 0.60 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3439 | 1/1 | 0.85 | 0.30 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3225 | 1/1 | 0.98 | 0.38 | - | 43,43,43,43 | 0 |
| 56 | MG | BA | 3627 | 1/1 | 0.97 | 0.07 | - | 56,56,56,56 | 0 |
| 56 | MG | BQ | 201 | 1/1 | 0.95 | 0.17 | - | 18,18,18,18 | 0 |
| 56 | MG | CA | 1720 | 1/1 | 0.96 | 0.24 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 3258 | 1/1 | 0.68 | 0.40 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3459 | 1/1 | 0.93 | 0.20 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3463 | 1/1 | 0.73 | 0.34 | - | 57,57,57,57 | 0 |
| 56 | MG | CA | 1652 | 1/1 | 0.89 | 0.40 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3117 | 1/1 | 0.92 | 0.34 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3192 | 1/1 | 0.78 | 0.33 | - | 53,53,53,53 | 0 |
| 56 | MG | AA | 1796 | 1/1 | 0.77 | 0.33 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3237 | 1/1 | 0.63 | 0.36 | - | 59,59,59,59 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3685 | 1/1 | 0.98 | 0.07 | - | 40,40,40,40 | 0 |
| 56 | MG | DA | 3287 | 1/1 | 0.88 | 0.40 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3401 | 1/1 | 0.97 | 0.29 | - | 36,36,36,36 | 0 |
| 56 | MG | AA | 1830 | 1/1 | 0.85 | 0.40 | - | 57,57,57,57 | 0 |
| 56 | MG | CA | 1683 | 1/1 | 0.74 | 0.32 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3281 | 1/1 | 0.87 | 0.52 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3246 | 1/1 | 0.96 | 0.17 | - | 48,48,48,48 | 0 |
| 56 | MG | BA | 3832 | 1/1 | 0.97 | 0.15 | - | 40,40,40,40 | 0 |
| 56 | MG | AA | 1753 | 1/1 | 0.90 | 0.34 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3422 | 1/1 | 0.99 | 0.10 | - | 47,47,47,47 | 0 |
| 56 | MG | BA | 3403 | 1/1 | 0.90 | 0.47 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3885 | 1/1 | 0.68 | 0.28 | - | 91,91,91,91 | 0 |
| 56 | MG | BF | 303 | 1/1 | 0.94 | 0.11 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3191 | 1/1 | 0.84 | 0.39 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3781 | 1/1 | 0.90 | 0.12 | - | 84,84,84,84 | 0 |
| 56 | MG | AA | 1904 | 1/1 | 0.86 | 0.07 | - | 118,118,118,118 | 0 |
| 56 | MG | DA | 3304 | 1/1 | 0.71 | 0.44 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3728 | 1/1 | 0.72 | 0.24 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3608 | 1/1 | 0.94 | 0.07 | - | 82,82,82,82 | 0 |
| 56 | MG | CA | 1707 | 1/1 | 0.94 | 1.37 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3570 | 1/1 | 0.96 | 0.12 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3840 | 1/1 | 0.97 | 0.06 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3278 | 1/1 | 0.96 | 0.10 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3548 | 1/1 | 0.93 | 0.16 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3077 | 1/1 | 0.92 | 0.24 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3239 | 1/1 | 0.94 | 0.16 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3640 | 1/1 | 0.91 | 0.10 | - | 33,33,33,33 | 0 |
| 56 | MG | AA | 1941 | 1/1 | 0.94 | 0.17 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3417 | 1/1 | 0.95 | 0.43 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3061 | 1/1 | 0.87 | 0.76 | - | 78,78,78,78 | 0 |
| 56 | MG | BF | 304 | 1/1 | 0.94 | 0.39 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3111 | 1/1 | 0.92 | 0.26 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3594 | 1/1 | 0.97 | 0.15 | - | 44,44,44,44 | 0 |
| 56 | MG | AA | 1790 | 1/1 | 0.91 | 0.17 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3693 | 1/1 | 0.87 | 0.34 | - | 103,103,103,103 | 0 |
| 56 | MG | DA | 3159 | 1/1 | 0.90 | 0.26 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3586 | 1/1 | 0.98 | 0.12 | - | 52,52,52,52 | 0 |
| 56 | MG | BA | 3226 | 1/1 | 0.87 | 0.22 | - | 36,36,36,36 | 0 |
| 56 | MG | AA | 1824 | 1/1 | 0.98 | 0.28 | - | 33,33,33,33 | 0 |
| 56 | MG | AA | 1670 | 1/1 | 0.88 | 0.29 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3511 | 1/1 | 0.92 | 0.22 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3371 | 1/1 | 0.93 | 0.20 | - | 65,65,65,65 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3241 | 1/1 | 0.94 | 0.31 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3645 | 1/1 | 0.95 | 0.06 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3883 | 1/1 | 0.90 | 0.29 | - | 43,43,43,43 | 0 |
| 56 | MG | BA | 3877 | 1/1 | 0.98 | 0.21 | - | 21,21,21,21 | 0 |
| 56 | MG | BA | 3090 | 1/1 | 0.89 | 0.40 | - | 46,46,46,46 | 0 |
| 56 | MG | CV | 109 | 1/1 | 0.86 | 0.09 | - | 102,102,102,102 | 0 |
| 56 | MG | DA | 3143 | 1/1 | 0.95 | 0.22 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3281 | 1/1 | 0.93 | 0.26 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3351 | 1/1 | 0.90 | 0.37 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3135 | 1/1 | 0.77 | 0.39 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3565 | 1/1 | 0.99 | 0.13 | - | 34,34,34,34 | 0 |
| 56 | MG | BA | 3713 | 1/1 | 0.88 | 0.11 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3442 | 1/1 | 0.95 | 0.30 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3155 | 1/1 | 0.89 | 0.29 | - | 56,56,56,56 | 0 |
| 56 | MG | DA | 3227 | 1/1 | 0.83 | 0.32 | - | 79,79,79,79 | 0 |
| 56 | MG | AA | 1879 | 1/1 | 0.92 | 0.22 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3658 | 1/1 | 0.96 | 0.26 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3828 | 1/1 | 0.86 | 0.16 | - | 99,99,99,99 | 0 |
| 56 | MG | DA | 3258 | 1/1 | 0.44 | 0.43 | - | 91,91,91,91 | 0 |
| 56 | MG | BA | 3028 | 1/1 | 0.93 | 0.16 | - | 33,33,33,33 | 0 |
| 56 | MG | DA | 3473 | 1/1 | 0.96 | 0.14 | - | 81,81,81,81 | 0 |
| 56 | MG | AA | 1632 | 1/1 | 0.95 | 0.50 | - | 51,51,51,51 | 0 |
| 56 | MG | DA | 3367 | 1/1 | 0.92 | 0.11 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3137 | 1/1 | 0.95 | 0.33 | - | 55,55,55,55 | 0 |
| 56 | MG | CA | 1751 | 1/1 | 0.83 | 0.10 | - | 86,86,86,86 | 0 |
| 56 | MG | BA | 3235 | 1/1 | 0.94 | 0.06 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3800 | 1/1 | 0.71 | 0.14 | - | 111,111,111,111 | 0 |
| 56 | MG | BB | 217 | 1/1 | 0.93 | 0.10 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3270 | 1/1 | 0.94 | 0.22 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3128 | 1/1 | 0.95 | 0.35 | - | 60,60,60,60 | 0 |
| 56 | MG | CA | 1696 | 1/1 | 0.97 | 0.11 | - | 99,99,99,99 | 0 |
| 56 | MG | BA | 3635 | 1/1 | 0.97 | 0.14 | - | 75,75,75,75 | 0 |
| 56 | MG | CA | 1695 | 1/1 | 0.92 | 0.13 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3771 | 1/1 | 0.92 | 0.17 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3179 | 1/1 | 0.94 | 0.26 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3131 | 1/1 | 0.98 | 0.16 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 3315 | 1/1 | 0.94 | 0.52 | - | 47,47,47,47 | 0 |
| 56 | MG | DA | 3257 | 1/1 | 0.92 | 0.73 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3873 | 1/1 | 0.85 | 0.08 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3200 | 1/1 | 0.94 | 0.64 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3155 | 1/1 | 0.87 | 0.44 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1613 | 1/1 | 0.89 | 0.55 | - | 68,68,68,68 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1694 | 1/1 | 0.82 | 0.32 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1875 | 1/1 | 0.97 | 0.22 | - | 59,59,59,59 | 0 |
| 56 | MG | B0 | 101 | 1/1 | 0.96 | 0.35 | - | 43,43,43,43 | 0 |
| 56 | MG | DA | 3230 | 1/1 | 0.89 | 0.13 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3129 | 1/1 | 0.96 | 0.29 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3816 | 1/1 | 0.96 | 0.14 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3144 | 1/1 | 0.92 | 0.11 | - | 34,34,34,34 | 0 |
| 56 | MG | BA | 3506 | 1/1 | 0.93 | 0.29 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3017 | 1/1 | 0.89 | 0.21 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3588 | 1/1 | 0.55 | 0.11 | - | 109,109,109,109 | 0 |
| 56 | MG | AA | 1629 | 1/1 | 0.86 | 0.38 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3658 | 1/1 | 0.94 | 0.18 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3113 | 1/1 | 0.92 | 0.18 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3057 | 1/1 | 0.89 | 0.23 | - | 30,30,30,30 | 0 |
| 56 | MG | CA | 1631 | 1/1 | 0.83 | 0.59 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3404 | 1/1 | 0.89 | 0.17 | - | 52,52,52,52 | 0 |
| 56 | MG | B1 | 102 | 1/1 | 0.95 | 0.15 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3342 | 1/1 | 0.74 | 0.46 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3801 | 1/1 | 0.79 | 0.38 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3591 | 1/1 | 0.90 | 0.28 | - | 64,64,64,64 | 0 |
| 56 | MG | AA | 1680 | 1/1 | 0.86 | 0.12 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3508 | 1/1 | 0.96 | 0.17 | - | 87,87,87,87 | 0 |
| 56 | MG | AA | 1795 | 1/1 | 0.84 | 0.54 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 1642 | 1/1 | 0.70 | 0.54 | - | 84,84,84,84 | 0 |
| 56 | MG | AA | 1649 | 1/1 | 0.94 | 0.15 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3652 | 1/1 | 0.92 | 0.14 | - | 53,53,53,53 | 0 |
| 56 | MG | CA | 1704 | 1/1 | 0.57 | 0.23 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3360 | 1/1 | 0.96 | 0.21 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3841 | 1/1 | 0.89 | 0.28 | - | 91,91,91,91 | 0 |
| 56 | MG | BA | 3163 | 1/1 | 0.98 | 0.16 | - | 40,40,40,40 | 0 |
| 56 | MG | CA | 1806 | 1/1 | 0.89 | 0.06 | - | 102,102,102,102 | 0 |
| 56 | MG | DA | 3593 | 1/1 | 0.97 | 0.07 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3058 | 1/1 | 0.72 | 0.43 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3583 | 1/1 | 0.92 | 0.18 | - | 96,96,96,96 | 0 |
| 56 | MG | DA | 3276 | 1/1 | 0.87 | 0.22 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3502 | 1/1 | 0.95 | 0.17 | - | 68,68,68,68 | 0 |
| 56 | MG | DB | 211 | 1/1 | 0.93 | 0.07 | - | 83,83,83,83 | 0 |
| 56 | MG | AA | 1911 | 1/1 | 0.58 | 0.30 | - | 106,106,106,106 | 0 |
| 56 | MG | AA | 1913 | 1/1 | 0.82 | 0.14 | - | 109,109,109,109 | 0 |
| 56 | MG | DA | 3687 | 1/1 | 0.96 | 0.08 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 1769 | 1/1 | 0.95 | 0.20 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3864 | 1/1 | 0.88 | 0.10 | - | 79,79,79,79 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1762 | 1/1 | 0.70 | 0.31 | - | 74,74,74,74 | 0 |
| 56 | MG | BB | 227 | 1/1 | 0.76 | 0.06 | - | 81,81,81,81 | 0 |
| 56 | MG | AA | 1622 | 1/1 | 0.94 | 0.70 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3834 | 1/1 | 0.96 | 0.19 | - | 27,27,27,27 | 0 |
| 56 | MG | AA | 1720 | 1/1 | 0.73 | 0.42 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3304 | 1/1 | 0.95 | 0.22 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3465 | 1/1 | 0.94 | 0.14 | - | 104,104,104,104 | 0 |
| 56 | MG | CA | 1712 | 1/1 | 0.89 | 0.25 | - | 83,83,83,83 | 0 |
| 56 | MG | BB | 230 | 1/1 | 0.96 | 0.18 | - | 56,56,56,56 | 0 |
| 56 | MG | DA | 3306 | 1/1 | 0.94 | 0.07 | - | 106,106,106,106 | 0 |
| 56 | MG | BA | 3406 | 1/1 | 0.77 | 0.21 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3340 | 1/1 | 0.96 | 0.46 | - | 55,55,55,55 | 0 |
| 56 | MG | AA | 1787 | 1/1 | 0.85 | 0.27 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3368 | 1/1 | 0.89 | 0.24 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3122 | 1/1 | 0.91 | 0.31 | - | 56,56,56,56 | 0 |
| 56 | MG | DB | 205 | 1/1 | 0.80 | 0.22 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3632 | 1/1 | 0.94 | 0.12 | - | 59,59,59,59 | 0 |
| 56 | MG | AA | 1785 | 1/1 | 0.81 | 0.31 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3461 | 1/1 | 0.94 | 0.16 | - | 58,58,58,58 | 0 |
| 56 | MG | CA | 1765 | 1/1 | 0.92 | 0.34 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3228 | 1/1 | 0.92 | 0.23 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3436 | 1/1 | 0.98 | 0.29 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3231 | 1/1 | 0.93 | 0.25 | - | 74,74,74,74 | 0 |
| 56 | MG | BQ | 203 | 1/1 | 0.98 | 0.24 | - | 62,62,62,62 | 0 |
| 56 | MG | CA | 1791 | 1/1 | 0.87 | 0.24 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3184 | 1/1 | 0.97 | 0.43 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3675 | 1/1 | 0.96 | 0.11 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1917 | 1/1 | 0.84 | 0.17 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3434 | 1/1 | 0.99 | 0.48 | - | 22,22,22,22 | 0 |
| 56 | MG | AA | 1755 | 1/1 | 0.90 | 0.30 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3433 | 1/1 | 0.91 | 0.27 | - | 30,30,30,30 | 0 |
| 56 | MG | BA | 3615 | 1/1 | 0.97 | 0.23 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3568 | 1/1 | 0.95 | 0.17 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3316 | 1/1 | 0.94 | 0.21 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3527 | 1/1 | 0.86 | 0.27 | - | 81,81,81,81 | 0 |
| 56 | MG | BA | 3844 | 1/1 | 0.85 | 0.17 | - | 99,99,99,99 | 0 |
| 56 | MG | AA | 1679 | 1/1 | 0.64 | 0.28 | - | 84,84,84,84 | 0 |
| 56 | MG | CV | 107 | 1/1 | 0.81 | 0.30 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3498 | 1/1 | 0.98 | 0.07 | - | 51,51,51,51 | 0 |
| 56 | MG | AA | 1804 | 1/1 | 0.94 | 0.19 | - | 115,115,115,115 | 0 |
| 56 | MG | BA | 3067 | 1/1 | 0.96 | 0.11 | - | 40,40,40,40 | 0 |
| 56 | MG | AA | 1885 | 1/1 | 0.91 | 0.24 | - | 90,90,90,90 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3080 | 1/1 | 0.95 | 0.19 | - | 44,44,44,44 | 0 |
| 56 | MG | AA | 1808 | 1/1 | 0.89 | 0.38 | - | 75,75,75,75 | 0 |
| 56 | MG | CA | 1626 | 1/1 | 0.93 | 0.31 | - | 50,50,50,50 | 0 |
| 56 | MG | CA | 1804 | 1/1 | 0.87 | 0.23 | - | 103,103,103,103 | 0 |
| 56 | MG | BA | 3704 | 1/1 | 0.95 | 0.15 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3112 | 1/1 | 0.92 | 0.31 | - | 61,61,61,61 | 0 |
| 56 | MG | CA | 1717 | 1/1 | 0.86 | 0.50 | - | 77,77,77,77 | 0 |
| 56 | MG | AA | 1690 | 1/1 | 0.86 | 0.35 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3368 | 1/1 | 0.87 | 0.13 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3491 | 1/1 | 0.84 | 0.32 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3182 | 1/1 | 0.96 | 0.41 | - | 25,25,25,25 | 0 |
| 56 | MG | AA | 1763 | 1/1 | 0.91 | 0.24 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3655 | 1/1 | 0.90 | 0.23 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1843 | 1/1 | 0.83 | 0.12 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3637 | 1/1 | 0.95 | 0.09 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3160 | 1/1 | 0.84 | 0.31 | - | 69,69,69,69 | 0 |
| 56 | MG | AA | 1859 | 1/1 | 0.96 | 0.11 | - | 91,91,91,91 | 0 |
| 56 | MG | AA | 1834 | 1/1 | 0.81 | 0.39 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3173 | 1/1 | 0.98 | 0.18 | - | 31,31,31,31 | 0 |
| 56 | MG | BA | 3216 | 1/1 | 0.94 | 0.14 | - | 28,28,28,28 | 0 |
| 56 | MG | DA | 3390 | 1/1 | 0.94 | 0.14 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3026 | 1/1 | 0.91 | 0.31 | - | 92,92,92,92 | 0 |
| 56 | MG | BB | 204 | 1/1 | 0.94 | 0.36 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3426 | 1/1 | 0.94 | 0.14 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3229 | 1/1 | 0.93 | 0.17 | - | 41,41,41,41 | 0 |
| 56 | MG | DA | 3199 | 1/1 | 0.76 | 1.06 | - | 81,81,81,81 | 0 |
| 56 | MG | AA | 1641 | 1/1 | 0.84 | 0.49 | - | 44,44,44,44 | 0 |
| 56 | MG | CA | 1686 | 1/1 | 0.96 | 0.14 | - | 72,72,72,72 | 0 |
| 56 | MG | DO | 203 | 1/1 | 0.98 | 0.17 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3324 | 1/1 | 0.90 | 0.59 | - | 62,62,62,62 | 0 |
| 56 | MG | CA | 1673 | 1/1 | 0.87 | 0.27 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3470 | 1/1 | 0.97 | 0.27 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 1738 | 1/1 | 0.91 | 0.19 | - | 98,98,98,98 | 0 |
| 56 | MG | BA | 3365 | 1/1 | 0.91 | 0.20 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3270 | 1/1 | 0.97 | 0.40 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3529 | 1/1 | 0.92 | 0.13 | - | 82,82,82,82 | 0 |
| 56 | MG | AA | 1923 | 1/1 | 0.75 | 0.15 | - | 115,115,115,115 | 0 |
| 56 | MG | CA | 1650 | 1/1 | 0.91 | 0.38 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3240 | 1/1 | 0.91 | 0.20 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3002 | 1/1 | 0.79 | 0.31 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3661 | 1/1 | 0.97 | 0.17 | - | 61,61,61,61 | 0 |
| 56 | MG | BQ | 202 | 1/1 | 0.95 | 0.18 | - | 46,46,46,46 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 1724 | 1/1 | 0.93 | 0.29 | - | 88,88,88,88 | 0 |
| 56 | MG | BA | 3850 | 1/1 | 0.93 | 0.27 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3284 | 1/1 | 0.90 | 0.22 | - | 41,41,41,41 | 0 |
| 56 | MG | DA | 3405 | 1/1 | 0.95 | 0.24 | - | 43,43,43,43 | 0 |
| 56 | MG | AA | 1713 | 1/1 | 0.96 | 0.31 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3789 | 1/1 | 0.97 | 0.12 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3337 | 1/1 | 0.92 | 0.20 | - | 51,51,51,51 | 0 |
| 56 | MG | DA | 3482 | 1/1 | 0.85 | 0.20 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1686 | 1/1 | 0.68 | 0.43 | - | 112,112,112,112 | 0 |
| 56 | MG | BA | 3563 | 1/1 | 0.96 | 0.12 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3377 | 1/1 | 0.72 | 0.44 | - | 89,89,89,89 | 0 |
| 56 | MG | CA | 1783 | 1/1 | 0.83 | 0.06 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3086 | 1/1 | 0.94 | 0.33 | - | 32,32,32,32 | 0 |
| 56 | MG | DA | 3288 | 1/1 | 0.76 | 0.31 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3620 | 1/1 | 0.93 | 0.06 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3110 | 1/1 | 0.93 | 0.29 | - | 51,51,51,51 | 0 |
| 56 | MG | BB | 225 | 1/1 | 0.98 | 0.14 | - | 56,56,56,56 | 0 |
| 56 | MG | DA | 3547 | 1/1 | 0.96 | 0.10 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3637 | 1/1 | 0.95 | 0.09 | - | 62,62,62,62 | 0 |
| 56 | MG | AF | 201 | 1/1 | 0.80 | 0.36 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3454 | 1/1 | 0.95 | 0.14 | - | 91,91,91,91 | 0 |
| 56 | MG | DA | 3375 | 1/1 | 0.71 | 0.14 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 3839 | 1/1 | 0.97 | 0.12 | - | 33,33,33,33 | 0 |
| 56 | MG | CA | 1616 | 1/1 | 0.97 | 0.67 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3004 | 1/1 | 0.89 | 0.25 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3299 | 1/1 | 0.74 | 0.69 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3524 | 1/1 | 0.90 | 0.19 | - | 99,99,99,99 | 0 |
| 56 | MG | BA | 3256 | 1/1 | 0.49 | 0.21 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3820 | 1/1 | 0.84 | 0.41 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3531 | 1/1 | 0.96 | 0.04 | - | 59,59,59,59 | 0 |
| 56 | MG | D0 | 102 | 1/1 | 0.56 | 0.37 | - | 99,99,99,99 | 0 |
| 56 | MG | DA | 3641 | 1/1 | 0.98 | 0.15 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3788 | 1/1 | 0.94 | 0.15 | - | 48,48,48,48 | 0 |
| 56 | MG | BA | 3078 | 1/1 | 0.89 | 0.53 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1721 | 1/1 | 0.87 | 0.27 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3630 | 1/1 | 0.97 | 0.21 | - | 47,47,47,47 | 0 |
| 56 | MG | BA | 3393 | 1/1 | 0.97 | 0.14 | - | 28,28,28,28 | 0 |
| 56 | MG | AV | 116 | 1/1 | 0.97 | 0.15 | - | 84,84,84,84 | 0 |
| 56 | MG | CA | 1808 | 1/1 | 0.59 | 0.29 | - | 102,102,102,102 | 0 |
| 56 | MG | DA | 3262 | 1/1 | 0.90 | 0.66 | - | 67,67,67,67 | 0 |
| 56 | MG | AV | 111 | 1/1 | 0.94 | 0.26 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3691 | 1/1 | 0.72 | 0.10 | - | 91,91,91,91 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3410 | 1/1 | 0.98 | 0.24 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3352 | 1/1 | 0.89 | 0.31 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3266 | 1/1 | 0.91 | 0.22 | - | 62,62,62,62 | 0 |
| 56 | MG | DO | 201 | 1/1 | 0.85 | 0.30 | - | 80,80,80,80 | 0 |
| 56 | MG | D0 | 103 | 1/1 | 0.93 | 0.17 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3161 | 1/1 | 0.89 | 0.31 | - | 49,49,49,49 | 0 |
| 56 | MG | DA | 3642 | 1/1 | 0.97 | 0.10 | - | 71,71,71,71 | 0 |
| 56 | MG | DB | 208 | 1/1 | 0.87 | 0.12 | - | 98,98,98,98 | 0 |
| 56 | MG | BA | 3752 | 1/1 | 0.98 | 0.23 | - | 28,28,28,28 | 0 |
| 56 | MG | BA | 3265 | 1/1 | 0.87 | 0.24 | - | 67,67,67,67 | 0 |
| 56 | MG | CA | 1801 | 1/1 | 0.89 | 0.13 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3148 | 1/1 | 0.91 | 0.21 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3448 | 1/1 | 0.77 | 0.36 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3310 | 1/1 | 0.84 | 0.90 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3060 | 1/1 | 0.93 | 0.19 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3501 | 1/1 | 0.81 | 0.36 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3715 | 1/1 | 0.97 | 0.14 | - | 21,21,21,21 | 0 |
| 56 | MG | DA | 3349 | 1/1 | 0.88 | 0.44 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3520 | 1/1 | 0.96 | 0.36 | - | 38,38,38,38 | 0 |
| 56 | MG | BA | 3339 | 1/1 | 0.78 | 0.36 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3619 | 1/1 | 0.96 | 0.06 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3157 | 1/1 | 0.86 | 0.32 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3321 | 1/1 | 0.91 | 0.33 | - | 52,52,52,52 | 0 |
| 56 | MG | BA | 3414 | 1/1 | 0.93 | 0.15 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3426 | 1/1 | 0.92 | 0.16 | - | 42,42,42,42 | 0 |
| 56 | MG | BA | 3033 | 1/1 | 0.92 | 0.34 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3855 | 1/1 | 0.76 | 0.48 | - | 103,103,103,103 | 0 |
| 56 | MG | BA | 3290 | 1/1 | 0.86 | 0.26 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3318 | 1/1 | 0.85 | 0.19 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3395 | 1/1 | 0.81 | 0.17 | - | 100,100,100,100 | 0 |
| 56 | MG | DA | 3081 | 1/1 | 0.76 | 0.41 | - | 65,65,65,65 | 0 |
| 56 | MG | AA | 1714 | 1/1 | 0.90 | 0.23 | - | 74,74,74,74 | 0 |
| 56 | MG | AV | 118 | 1/1 | 0.87 | 0.09 | - | 83,83,83,83 | 0 |
| 56 | MG | CA | 1757 | 1/1 | 0.77 | 0.29 | - | 94,94,94,94 | 0 |
| 56 | MG | CA | 1718 | 1/1 | 0.92 | 0.37 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3128 | 1/1 | 0.83 | 0.48 | - | 59,59,59,59 | 0 |
| 56 | MG | BB | 206 | 1/1 | 0.81 | 0.17 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3007 | 1/1 | 0.83 | 0.14 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3874 | 1/1 | 0.82 | 0.30 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3896 | 1/1 | 0.89 | 0.16 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3372 | 1/1 | 0.94 | 0.16 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3823 | 1/1 | 0.90 | 0.17 | - | 78,78,78,78 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3863 | 1/1 | 0.95 | 0.09 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3299 | 1/1 | 0.94 | 0.24 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3180 | 1/1 | 0.95 | 0.36 | - | 41,41,41,41 | 0 |
| 56 | MG | CA | 1723 | 1/1 | 0.92 | 0.08 | - | 96,96,96,96 | 0 |
| 56 | MG | BA | 3359 | 1/1 | 0.75 | 0.47 | - | 72,72,72,72 | 0 |
| 56 | MG | CA | 1645 | 1/1 | 0.83 | 0.40 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3331 | 1/1 | 0.86 | 0.26 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3005 | 1/1 | 0.95 | 0.13 | - | 59,59,59,59 | 0 |
| 56 | MG | CA | 1603 | 1/1 | 0.83 | 0.68 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3189 | 1/1 | 0.91 | 0.28 | - | 49,49,49,49 | 0 |
| 56 | MG | CA | 1708 | 1/1 | 0.76 | 1.02 | - | 91,91,91,91 | 0 |
| 56 | MG | AA | 1717 | 1/1 | 0.87 | 0.18 | - | 76,76,76,76 | 0 |
| 56 | MG | CA | 1796 | 1/1 | 0.56 | 0.16 | - | 102,102,102,102 | 0 |
| 56 | MG | DA | 3613 | 1/1 | 0.97 | 0.11 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3436 | 1/1 | 0.94 | 0.08 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3490 | 1/1 | 0.98 | 0.25 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3302 | 1/1 | 0.81 | 0.32 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3476 | 1/1 | 0.96 | 0.12 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3603 | 1/1 | 0.96 | 0.12 | - | 32,32,32,32 | 0 |
| 56 | MG | BA | 3638 | 1/1 | 0.94 | 0.25 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3107 | 1/1 | 0.96 | 0.14 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3336 | 1/1 | 0.92 | 0.41 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3078 | 1/1 | 0.90 | 0.42 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3545 | 1/1 | 0.75 | 0.11 | - | 83,83,83,83 | 0 |
| 56 | MG | BT | 201 | 1/1 | 0.90 | 0.14 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3847 | 1/1 | 0.93 | 0.30 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3102 | 1/1 | 0.87 | 0.24 | - | 60,60,60,60 | 0 |
| 56 | MG | B0 | 105 | 1/1 | 0.98 | 0.15 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3526 | 1/1 | 0.94 | 0.09 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3469 | 1/1 | 0.86 | 0.09 | - | 84,84,84,84 | 0 |
| 56 | MG | DB | 209 | 1/1 | 0.72 | 0.40 | - | 86,86,86,86 | 0 |
| 56 | MG | AA | 1846 | 1/1 | 0.84 | 0.34 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3639 | 1/1 | 0.95 | 0.09 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1664 | 1/1 | 0.95 | 0.13 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3112 | 1/1 | 0.87 | 0.24 | - | 56,56,56,56 | 0 |
| 56 | MG | CA | 1636 | 1/1 | 0.90 | 0.45 | - | 50,50,50,50 | 0 |
| 56 | MG | CA | 1785 | 1/1 | 0.88 | 0.10 | - | 87,87,87,87 | 0 |
| 56 | MG | DA | 3660 | 1/1 | 0.95 | 0.11 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3678 | 1/1 | 0.59 | 0.27 | - | 89,89,89,89 | 0 |
| 56 | MG | BA | 3807 | 1/1 | 0.92 | 0.17 | - | 64,64,64,64 | 0 |
| 56 | MG | AA | 1924 | 1/1 | 0.98 | 0.10 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3799 | 1/1 | 0.72 | 0.10 | - | 72,72,72,72 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3812 | 1/1 | 0.82 | 0.10 | - | 87,87,87,87 | 0 |
| 56 | MG | AA | 1868 | 1/1 | 0.94 | 0.28 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3667 | 1/1 | 0.88 | 0.13 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3465 | 1/1 | 0.93 | 0.28 | - | 40,40,40,40 | 0 |
| 56 | MG | BA | 3114 | 1/1 | 0.95 | 0.40 | - | 37,37,37,37 | 0 |
| 56 | MG | AA | 1934 | 1/1 | 0.97 | 0.08 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3541 | 1/1 | 0.88 | 0.11 | - | 106,106,106,106 | 0 |
| 56 | MG | DA | 3694 | 1/1 | 0.72 | 0.13 | - | 95,95,95,95 | 0 |
| 56 | MG | DB | 214 | 1/1 | 0.84 | 0.29 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3443 | 1/1 | 0.85 | 0.13 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3048 | 1/1 | 0.97 | 0.13 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1707 | 1/1 | 0.89 | 0.18 | - | 64,64,64,64 | 0 |
| 56 | MG | AA | 1634 | 1/1 | 0.95 | 0.34 | - | 47,47,47,47 | 0 |
| 56 | MG | CA | 1640 | 1/1 | 0.85 | 0.23 | - | 72,72,72,72 | 0 |
| 56 | MG | AA | 1775 | 1/1 | 0.83 | 0.11 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3236 | 1/1 | 0.93 | 0.15 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3351 | 1/1 | 0.93 | 0.12 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3458 | 1/1 | 0.94 | 0.31 | - | 44,44,44,44 | 0 |
| 56 | MG | AA | 1749 | 1/1 | 0.71 | 0.75 | - | 69,69,69,69 | 0 |
| 56 | MG | BE | 302 | 1/1 | 0.98 | 0.54 | - | 51,51,51,51 | 0 |
| 56 | MG | AA | 1733 | 1/1 | 0.78 | 0.15 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3610 | 1/1 | 0.99 | 0.10 | - | 41,41,41,41 | 0 |
| 56 | MG | AI | 202 | 1/1 | 0.81 | 0.40 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3519 | 1/1 | 0.97 | 0.40 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3651 | 1/1 | 0.90 | 0.16 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3370 | 1/1 | 0.90 | 0.15 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 1681 | 1/1 | 0.89 | 0.28 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 1733 | 1/1 | 0.94 | 0.08 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3260 | 1/1 | 0.87 | 0.22 | - | 71,71,71,71 | 0 |
| 56 | MG | AA | 1756 | 1/1 | 0.96 | 0.24 | - | 90,90,90,90 | 0 |
| 56 | MG | B0 | 102 | 1/1 | 0.91 | 0.17 | - | 50,50,50,50 | 0 |
| 56 | MG | AA | 1850 | 1/1 | 0.95 | 0.47 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3376 | 1/1 | 0.79 | 0.30 | - | 69,69,69,69 | 0 |
| 56 | MG | AA | 1877 | 1/1 | 0.95 | 0.08 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3779 | 1/1 | 0.92 | 0.39 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1931 | 1/1 | 0.81 | 0.25 | - | 103,103,103,103 | 0 |
| 56 | MG | DA | 3228 | 1/1 | 0.86 | 0.33 | - | 90,90,90,90 | 0 |
| 56 | MG | AA | 1831 | 1/1 | 0.92 | 0.17 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3325 | 1/1 | 0.81 | 0.23 | - | 83,83,83,83 | 0 |
| 56 | MG | AV | 107 | 1/1 | 0.90 | 0.33 | - | 87,87,87,87 | 0 |
| 56 | MG | BA | 3027 | 1/1 | 0.97 | 0.19 | - | 44,44,44,44 | 0 |
| 56 | MG | BB | 229 | 1/1 | 0.98 | 0.04 | - | 67,67,67,67 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3605 | 1/1 | 0.89 | 0.19 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1656 | 1/1 | 0.94 | 0.08 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3599 | 1/1 | 0.94 | 0.10 | - | 52,52,52,52 | 0 |
| 56 | MG | BA | 3769 | 1/1 | 0.96 | 0.17 | - | 55,55,55,55 | 0 |
| 56 | MG | DA | 3207 | 1/1 | 0.87 | 0.15 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3521 | 1/1 | 0.91 | 0.42 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3587 | 1/1 | 0.95 | 0.18 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3130 | 1/1 | 0.98 | 0.10 | - | 52,52,52,52 | 0 |
| 56 | MG | CA | 1731 | 1/1 | 0.92 | 0.43 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3517 | 1/1 | 0.99 | 0.17 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3826 | 1/1 | 0.90 | 0.47 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3573 | 1/1 | 0.97 | 0.07 | - | 54,54,54,54 | 0 |
| 56 | MG | CA | 1792 | 1/1 | 0.92 | 0.12 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3523 | 1/1 | 0.69 | 0.42 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3589 | 1/1 | 0.97 | 0.07 | - | 81,81,81,81 | 0 |
| 56 | MG | BA | 3478 | 1/1 | 0.87 | 0.25 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3609 | 1/1 | 0.96 | 0.07 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3211 | 1/1 | 0.81 | 0.34 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3710 | 1/1 | 0.98 | 0.17 | - | 58,58,58,58 | 0 |
| 56 | MG | DA | 3026 | 1/1 | 0.96 | 0.29 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3438 | 1/1 | 0.87 | 0.37 | - | 62,62,62,62 | 0 |
| 56 | MG | CA | 1663 | 1/1 | 0.91 | 0.47 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3445 | 1/1 | 0.96 | 0.14 | - | 68,68,68,68 | 0 |
| 56 | MG | AA | 1731 | 1/1 | 0.83 | 0.17 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 1700 | 1/1 | 0.78 | 0.74 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3054 | 1/1 | 0.82 | 0.25 | - | 58,58,58,58 | 0 |
| 56 | MG | CA | 1643 | 1/1 | 0.97 | 0.40 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3212 | 1/1 | 0.96 | 0.15 | - | 35,35,35,35 | 0 |
| 56 | MG | BA | 3745 | 1/1 | 0.94 | 0.13 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3813 | 1/1 | 0.89 | 0.08 | - | 66,66,66,66 | 0 |
| 56 | MG | CA | 1641 | 1/1 | 0.96 | 0.24 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3629 | 1/1 | 0.98 | 0.09 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3052 | 1/1 | 0.65 | 1.02 | - | 79,79,79,79 | 0 |
| 56 | MG | AA | 1605 | 1/1 | 0.92 | 0.28 | - | 81,81,81,81 | 0 |
| 56 | MG | BA | 3230 | 1/1 | 0.88 | 0.09 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3429 | 1/1 | 0.95 | 0.24 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3829 | 1/1 | 0.95 | 0.38 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3862 | 1/1 | 0.98 | 0.11 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3508 | 1/1 | 0.94 | 0.25 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3197 | 1/1 | 0.91 | 0.23 | - | 41,41,41,41 | 0 |
| 56 | MG | DA | 3621 | 1/1 | 0.98 | 0.07 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3183 | 1/1 | 0.94 | 0.17 | - | 106,106,106,106 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3544 | 1/1 | 0.87 | 0.11 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3628 | 1/1 | 0.96 | 0.11 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3137 | 1/1 | 0.92 | 0.21 | - | 39,39,39,39 | 0 |
| 56 | MG | DA | 3345 | 1/1 | 0.92 | 0.10 | - | 67,67,67,67 | 0 |
| 56 | MG | DA | 3129 | 1/1 | 0.87 | 0.17 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3303 | 1/1 | 0.93 | 0.61 | - | 51,51,51,51 | 0 |
| 56 | MG | DA | 3396 | 1/1 | 0.97 | 0.13 | - | 37,37,37,37 | 0 |
| 56 | MG | AA | 1841 | 1/1 | 0.98 | 0.11 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1912 | 1/1 | 0.87 | 0.14 | - | 106,106,106,106 | 0 |
| 56 | MG | DA | 3578 | 1/1 | 0.94 | 0.16 | - | 50,50,50,50 | 0 |
| 56 | MG | CA | 1639 | 1/1 | 0.87 | 0.77 | - | 96,96,96,96 | 0 |
| 56 | MG | AA | 1823 | 1/1 | 0.67 | 0.99 | - | 77,77,77,77 | 0 |
| 56 | MG | CA | 1684 | 1/1 | 0.86 | 0.16 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3256 | 1/1 | 0.83 | 0.36 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3423 | 1/1 | 0.87 | 0.18 | - | 85,85,85,85 | 0 |
| 56 | MG | AA | 1616 | 1/1 | 0.95 | 0.13 | - | 65,65,65,65 | 0 |
| 56 | MG | AA | 1803 | 1/1 | 0.76 | 0.91 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3298 | 1/1 | 0.88 | 0.24 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3108 | 1/1 | 0.95 | 0.28 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3251 | 1/1 | 0.94 | 0.47 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3760 | 1/1 | 0.93 | 0.08 | - | 68,68,68,68 | 0 |
| 56 | MG | AA | 1801 | 1/1 | 0.84 | 0.38 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3535 | 1/1 | 0.90 | 0.36 | - | 96,96,96,96 | 0 |
| 56 | MG | CA | 1613 | 1/1 | 0.85 | 0.42 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1857 | 1/1 | 0.95 | 0.22 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3560 | 1/1 | 0.97 | 0.18 | - | 39,39,39,39 | 0 |
| 56 | MG | BA | 3473 | 1/1 | 0.99 | 0.33 | - | 22,22,22,22 | 0 |
| 56 | MG | BA | 3282 | 1/1 | 0.95 | 0.17 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3389 | 1/1 | 0.89 | 0.60 | - | 38,38,38,38 | 0 |
| 56 | MG | AA | 1894 | 1/1 | 0.85 | 0.40 | - | 83,83,83,83 | 0 |
| 56 | MG | AA | 1747 | 1/1 | 0.93 | 0.31 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3871 | 1/1 | 0.84 | 0.12 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3334 | 1/1 | 0.86 | 0.42 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3207 | 1/1 | 0.92 | 0.30 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3232 | 1/1 | 0.95 | 0.16 | - | 40,40,40,40 | 0 |
| 56 | MG | BA | 3294 | 1/1 | 0.80 | 0.13 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3679 | 1/1 | 0.97 | 0.05 | - | 34,34,34,34 | 0 |
| 56 | MG | AA | 1945 | 1/1 | 0.90 | 0.08 | - | 107,107,107,107 | 0 |
| 56 | MG | BA | 3095 | 1/1 | 0.88 | 0.16 | - | 48,48,48,48 | 0 |
| 56 | MG | CA | 1800 | 1/1 | 0.92 | 0.05 | - | 105,105,105,105 | 0 |
| 56 | MG | AA | 1744 | 1/1 | 0.91 | 0.23 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3320 | 1/1 | 0.87 | 0.24 | - | 56,56,56,56 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3243 | 1/1 | 0.95 | 0.07 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3219 | 1/1 | 0.92 | 0.17 | - | 67,67,67,67 | 0 |
| 56 | MG | DA | 3167 | 1/1 | 0.97 | 0.36 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3341 | 1/1 | 0.85 | 0.25 | - | 53,53,53,53 | 0 |
| 56 | MG | DB | 213 | 1/1 | 0.79 | 0.35 | - | 115,115,115,115 | 0 |
| 56 | MG | BB | 220 | 1/1 | 0.92 | 0.11 | - | 44,44,44,44 | 0 |
| 56 | MG | AA | 1758 | 1/1 | 0.91 | 0.26 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3533 | 1/1 | 0.97 | 0.11 | - | 61,61,61,61 | 0 |
| 56 | MG | B0 | 104 | 1/1 | 0.99 | 0.19 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1839 | 1/1 | 0.98 | 0.06 | - | 69,69,69,69 | 0 |
| 56 | MG | CA | 1674 | 1/1 | 0.81 | 0.35 | - | 79,79,79,79 | 0 |
| 56 | MG | AA | 1942 | 1/1 | 0.92 | 0.26 | - | 93,93,93,93 | 0 |
| 56 | MG | DA | 3091 | 1/1 | 0.96 | 0.11 | - | 47,47,47,47 | 0 |
| 56 | MG | CA | 1750 | 1/1 | 0.92 | 0.18 | - | 56,56,56,56 | 0 |
| 56 | MG | AA | 1623 | 1/1 | 0.95 | 0.19 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3010 | 1/1 | 0.92 | 0.59 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3574 | 1/1 | 0.97 | 0.18 | - | 36,36,36,36 | 0 |
| 56 | MG | DA | 3110 | 1/1 | 0.91 | 0.31 | - | 60,60,60,60 | 0 |
| 56 | MG | AA | 1910 | 1/1 | 0.95 | 0.18 | - | 87,87,87,87 | 0 |
| 56 | MG | DA | 3220 | 1/1 | 0.94 | 0.17 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3697 | 1/1 | 0.95 | 0.15 | - | 51,51,51,51 | 0 |
| 56 | MG | CA | 1781 | 1/1 | 0.96 | 0.18 | - | 103,103,103,103 | 0 |
| 56 | MG | BA | 3706 | 1/1 | 0.95 | 0.21 | - | 29,29,29,29 | 0 |
| 56 | MG | DA | 3328 | 1/1 | 0.96 | 0.15 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3633 | 1/1 | 0.96 | 0.11 | - | 52,52,52,52 | 0 |
| 56 | MG | DQ | 201 | 1/1 | 0.87 | 0.47 | - | 43,43,43,43 | 0 |
| 56 | MG | BA | 3431 | 1/1 | 0.77 | 0.28 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3717 | 1/1 | 0.95 | 0.17 | - | 21,21,21,21 | 0 |
| 56 | MG | DA | 3072 | 1/1 | 0.68 | 0.38 | - | 65,65,65,65 | 0 |
| 56 | MG | CA | 1680 | 1/1 | 0.76 | 0.33 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3086 | 1/1 | 0.93 | 0.34 | - | 51,51,51,51 | 0 |
| 56 | MG | DA | 3065 | 1/1 | 0.92 | 1.02 | - | 59,59,59,59 | 0 |
| 56 | MG | CA | 1646 | 1/1 | 0.89 | 0.10 | - | 73,73,73,73 | 0 |
| 56 | MG | AA | 1676 | 1/1 | 0.94 | 0.58 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3154 | 1/1 | 0.90 | 0.34 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3796 | 1/1 | 0.92 | 0.38 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3543 | 1/1 | 0.99 | 0.05 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3358 | 1/1 | 0.93 | 0.22 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3094 | 1/1 | 0.92 | 0.21 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3657 | 1/1 | 0.95 | 0.26 | - | 51,51,51,51 | 0 |
| 56 | MG | CA | 1669 | 1/1 | 0.96 | 0.83 | - | 78,78,78,78 | 0 |
| 56 | MG | CA | 1775 | 1/1 | 0.71 | 0.14 | - | 99,99,99,99 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3335 | 1/1 | 0.97 | 0.32 | - | 47,47,47,47 | 0 |
| 56 | MG | DA | 3232 | 1/1 | 0.70 | 0.39 | - | 91,91,91,91 | 0 |
| 56 | MG | CA | 1799 | 1/1 | 0.90 | 0.13 | - | 94,94,94,94 | 0 |
| 56 | MG | DA | 3571 | 1/1 | 0.94 | 0.11 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3589 | 1/1 | 0.83 | 0.13 | - | 38,38,38,38 | 0 |
| 56 | MG | BA | 3878 | 1/1 | 0.98 | 0.12 | - | 81,81,81,81 | 0 |
| 56 | MG | BA | 3031 | 1/1 | 0.95 | 0.22 | - | 29,29,29,29 | 0 |
| 56 | MG | BA | 3146 | 1/1 | 0.97 | 0.30 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1643 | 1/1 | 0.87 | 0.56 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3179 | 1/1 | 0.91 | 0.25 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3811 | 1/1 | 0.94 | 0.12 | - | 85,85,85,85 | 0 |
| 56 | MG | AA | 1723 | 1/1 | 0.80 | 0.23 | - | 102,102,102,102 | 0 |
| 56 | MG | DA | 3271 | 1/1 | 0.70 | 0.45 | - | 68,68,68,68 | 0 |
| 56 | MG | AA | 1657 | 1/1 | 0.85 | 0.46 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3509 | 1/1 | 0.80 | 0.50 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3004 | 1/1 | 0.86 | 0.42 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3186 | 1/1 | 0.89 | 0.32 | - | 76,76,76,76 | 0 |
| 56 | MG | AA | 1928 | 1/1 | 0.90 | 0.10 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3139 | 1/1 | 0.76 | 0.42 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3072 | 1/1 | 0.97 | 0.64 | - | 48,48,48,48 | 0 |
| 56 | MG | BA | 3172 | 1/1 | 0.96 | 0.49 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3178 | 1/1 | 0.95 | 0.34 | - | 43,43,43,43 | 0 |
| 56 | MG | CA | 1689 | 1/1 | 0.88 | 0.85 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3435 | 1/1 | 0.88 | 0.09 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3674 | 1/1 | 0.67 | 0.24 | - | 105,105,105,105 | 0 |
| 56 | MG | BA | 3587 | 1/1 | 0.98 | 0.14 | - | 48,48,48,48 | 0 |
| 56 | MG | BA | 3532 | 1/1 | 0.95 | 0.23 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 3322 | 1/1 | 0.93 | 0.33 | - | 52,52,52,52 | 0 |
| 56 | MG | DA | 3296 | 1/1 | 0.69 | 0.31 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3695 | 1/1 | 0.80 | 0.14 | - | 107,107,107,107 | 0 |
| 56 | MG | DA | 3564 | 1/1 | 0.91 | 0.12 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3445 | 1/1 | 0.97 | 0.14 | - | 43,43,43,43 | 0 |
| 56 | MG | CA | 1665 | 1/1 | 0.82 | 0.64 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 1622 | 1/1 | 0.80 | 0.76 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3348 | 1/1 | 0.85 | 0.31 | - | 77,77,77,77 | 0 |
| 56 | MG | AA | 1646 | 1/1 | 0.85 | 0.45 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 1635 | 1/1 | 0.86 | 0.44 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3774 | 1/1 | 0.94 | 0.28 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3880 | 1/1 | 0.84 | 0.09 | - | 84,84,84,84 | 0 |
| 56 | MG | CV | 110 | 1/1 | 0.89 | 0.10 | - | 100,100,100,100 | 0 |
| 56 | MG | BA | 3756 | 1/1 | 0.92 | 0.12 | - | 56,56,56,56 | 0 |
| 56 | MG | AA | 1625 | 1/1 | 0.90 | 0.17 | - | 69,69,69,69 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3656 | 1/1 | 0.88 | 0.17 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1816 | 1/1 | 0.94 | 0.19 | - | 107,107,107,107 | 0 |
| 56 | MG | BA | 3273 | 1/1 | 0.93 | 0.29 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3412 | 1/1 | 0.96 | 0.12 | - | 52,52,52,52 | 0 |
| 56 | MG | CA | 1810 | 1/1 | 0.82 | 0.08 | - | 92,92,92,92 | 0 |
| 56 | MG | AA | 1697 | 1/1 | 0.84 | 0.30 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3703 | 1/1 | 0.95 | 0.08 | - | 65,65,65,65 | 0 |
| 56 | MG | AA | 1665 | 1/1 | 0.78 | 0.29 | - | 73,73,73,73 | 0 |
| 56 | MG | AT | 201 | 1/1 | 0.91 | 0.26 | - | 111,111,111,111 | 0 |
| 56 | MG | CA | 1784 | 1/1 | 0.92 | 0.15 | - | 96,96,96,96 | 0 |
| 56 | MG | BA | 3884 | 1/1 | 0.93 | 0.08 | - | 66,66,66,66 | 0 |
| 56 | MG | AA | 1888 | 1/1 | 0.87 | 0.20 | - | 97,97,97,97 | 0 |
| 56 | MG | BA | 3257 | 1/1 | 0.92 | 0.26 | - | 48,48,48,48 | 0 |
| 56 | MG | AA | 1906 | 1/1 | 0.91 | 0.22 | - | 89,89,89,89 | 0 |
| 56 | MG | AA | 1725 | 1/1 | 0.94 | 0.19 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3362 | 1/1 | 0.89 | 0.44 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3527 | 1/1 | 0.93 | 0.09 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3082 | 1/1 | 0.80 | 0.27 | - | 45,45,45,45 | 0 |
| 56 | MG | CA | 1802 | 1/1 | 0.57 | 0.10 | - | 115,115,115,115 | 0 |
| 56 | MG | DA | 3164 | 1/1 | 0.91 | 0.41 | - | 87,87,87,87 | 0 |
| 56 | MG | BA | 3157 | 1/1 | 0.91 | 0.43 | - | 42,42,42,42 | 0 |
| 56 | MG | AA | 1915 | 1/1 | 0.59 | 0.17 | - | 121,121,121,121 | 0 |
| 56 | MG | BA | 3486 | 1/1 | 0.93 | 0.33 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3515 | 1/1 | 0.92 | 0.46 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3398 | 1/1 | 0.93 | 0.22 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3342 | 1/1 | 0.84 | 0.31 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3185 | 1/1 | 0.85 | 0.29 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1621 | 1/1 | 0.92 | 0.15 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3293 | 1/1 | 0.36 | 0.16 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3418 | 1/1 | 0.96 | 0.25 | - | 59,59,59,59 | 0 |
| 56 | MG | AV | 106 | 1/1 | 0.80 | 0.24 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3595 | 1/1 | 0.95 | 0.12 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3309 | 1/1 | 0.73 | 0.41 | - | 88,88,88,88 | 0 |
| 56 | MG | AA | 1766 | 1/1 | 0.91 | 0.17 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3693 | 1/1 | 0.97 | 0.10 | - | 38,38,38,38 | 0 |
| 56 | MG | BA | 3009 | 1/1 | 0.89 | 0.18 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3085 | 1/1 | 0.88 | 0.31 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 1766 | 1/1 | 0.96 | 0.10 | - | 106,106,106,106 | 0 |
| 56 | MG | DB | 212 | 1/1 | 0.82 | 0.13 | - | 111,111,111,111 | 0 |
| 56 | MG | CA | 1604 | 1/1 | 0.81 | 0.45 | - | 114,114,114,114 | 0 |
| 56 | MG | DA | 3606 | 1/1 | 0.87 | 0.08 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3370 | 1/1 | 0.92 | 0.54 | - | 67,67,67,67 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3402 | 1/1 | 0.88 | 0.44 | - | 55,55,55,55 | 0 |
| 56 | MG | D0 | 104 | 1/1 | 0.87 | 0.26 | - | 86,86,86,86 | 0 |
| 56 | MG | BA | 3888 | 1/1 | 0.68 | 0.13 | - | 99,99,99,99 | 0 |
| 56 | MG | DO | 202 | 1/1 | 0.93 | 0.13 | - | 95,95,95,95 | 0 |
| 56 | MG | BA | 3777 | 1/1 | 0.90 | 0.33 | - | 65,65,65,65 | 0 |
| 56 | MG | CA | 1716 | 1/1 | 0.96 | 0.24 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3416 | 1/1 | 0.83 | 0.21 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3636 | 1/1 | 0.97 | 0.07 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3027 | 1/1 | 0.79 | 0.41 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3608 | 1/1 | 0.96 | 0.14 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3190 | 1/1 | 0.93 | 0.38 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3783 | 1/1 | 0.96 | 0.23 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3849 | 1/1 | 0.85 | 0.20 | - | 83,83,83,83 | 0 |
| 56 | MG | AA | 1862 | 1/1 | 0.97 | 0.08 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3175 | 1/1 | 0.94 | 0.38 | - | 34,34,34,34 | 0 |
| 56 | MG | CA | 1610 | 1/1 | 0.92 | 0.11 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1734 | 1/1 | 0.88 | 0.27 | - | 80,80,80,80 | 0 |
| 56 | MG | CA | 1744 | 1/1 | 0.94 | 0.06 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1698 | 1/1 | 0.88 | 0.19 | - | 97,97,97,97 | 0 |
| 56 | MG | BA | 3604 | 1/1 | 0.98 | 0.06 | - | 80,80,80,80 | 0 |
| 56 | MG | B9 | 102 | 1/1 | 0.95 | 0.28 | - | 43,43,43,43 | 0 |
| 56 | MG | AA | 1651 | 1/1 | 0.86 | 0.24 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3818 | 1/1 | 0.96 | 0.28 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3062 | 1/1 | 0.92 | 0.24 | - | 65,65,65,65 | 0 |
| 56 | MG | AV | 104 | 1/1 | 0.76 | 0.29 | - | 81,81,81,81 | 0 |
| 56 | MG | CV | 103 | 1/1 | 0.92 | 0.19 | - | 88,88,88,88 | 0 |
| 56 | MG | BA | 3384 | 1/1 | 0.61 | 0.77 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3543 | 1/1 | 0.96 | 0.11 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3259 | 1/1 | 0.87 | 0.32 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3483 | 1/1 | 0.81 | 0.30 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3468 | 1/1 | 0.95 | 0.21 | - | 54,54,54,54 | 0 |
| 56 | MG | AA | 1869 | 1/1 | 0.99 | 0.30 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3076 | 1/1 | 0.93 | 0.19 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3474 | 1/1 | 0.94 | 0.32 | - | 56,56,56,56 | 0 |
| 56 | MG | CT | 201 | 1/1 | 0.89 | 0.36 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3034 | 1/1 | 0.94 | 0.21 | - | 23,23,23,23 | 0 |
| 56 | MG | CA | 1735 | 1/1 | 0.98 | 0.07 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3528 | 1/1 | 0.84 | 0.22 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3557 | 1/1 | 0.83 | 0.54 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3262 | 1/1 | 0.92 | 0.28 | - | 57,57,57,57 | 0 |
| 56 | MG | CA | 1795 | 1/1 | 0.65 | 0.13 | - | 100,100,100,100 | 0 |
| 56 | MG | BA | 3665 | 1/1 | 0.92 | 0.14 | - | 44,44,44,44 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BB | 219 | 1/1 | 0.63 | 0.21 | - | 85,85,85,85 | 0 |
| 56 | MG | AA | 1722 | 1/1 | 0.82 | 0.39 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3296 | 1/1 | 0.90 | 0.30 | - | 43,43,43,43 | 0 |
| 56 | MG | BA | 3330 | 1/1 | 0.93 | 0.22 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3323 | 1/1 | 0.94 | 0.13 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3018 | 1/1 | 0.91 | 0.38 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3492 | 1/1 | 0.97 | 0.12 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3363 | 1/1 | 0.77 | 0.39 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3392 | 1/1 | 0.97 | 0.10 | - | 42,42,42,42 | 0 |
| 56 | MG | DA | 3343 | 1/1 | 0.87 | 0.65 | - | 70,70,70,70 | 0 |
| 56 | MG | AA | 1602 | 1/1 | 0.84 | 0.18 | - | 104,104,104,104 | 0 |
| 56 | MG | CA | 1714 | 1/1 | 0.87 | 0.14 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3400 | 1/1 | 0.87 | 0.06 | - | 122,122,122,122 | 0 |
| 56 | MG | DA | 3235 | 1/1 | 0.91 | 0.25 | - | 53,53,53,53 | 0 |
| 56 | MG | BB | 208 | 1/1 | 0.93 | 0.32 | - | 54,54,54,54 | 0 |
| 56 | MG | AA | 1832 | 1/1 | 0.98 | 0.40 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3664 | 1/1 | 0.86 | 0.22 | - | 97,97,97,97 | 0 |
| 56 | MG | AA | 1777 | 1/1 | 0.94 | 0.36 | - | 61,61,61,61 | 0 |
| 56 | MG | CA | 1756 | 1/1 | 0.93 | 0.85 | - | 84,84,84,84 | 0 |
| 56 | MG | AA | 1674 | 1/1 | 0.78 | 0.44 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3395 | 1/1 | 0.86 | 0.15 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3006 | 1/1 | 0.91 | 0.20 | - | 55,55,55,55 | 0 |
| 56 | MG | AA | 1692 | 1/1 | 0.92 | 0.29 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3516 | 1/1 | 0.97 | 0.33 | - | 56,56,56,56 | 0 |
| 56 | MG | AA | 1783 | 1/1 | 0.88 | 0.26 | - | 61,61,61,61 | 0 |
| 56 | MG | CA | 1817 | 1/1 | 0.57 | 0.24 | - | 111,111,111,111 | 0 |
| 56 | MG | BA | 3726 | 1/1 | 0.98 | 0.36 | - | 48,48,48,48 | 0 |
| 56 | MG | CA | 1611 | 1/1 | 0.96 | 0.14 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3264 | 1/1 | 0.88 | 0.25 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3169 | 1/1 | 0.98 | 0.20 | - | 51,51,51,51 | 0 |
| 56 | MG | DA | 3037 | 1/1 | 0.94 | 0.14 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3380 | 1/1 | 0.87 | 0.18 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3031 | 1/1 | 0.94 | 0.11 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1865 | 1/1 | 0.88 | 0.20 | - | 81,81,81,81 | 0 |
| 56 | MG | AV | 103 | 1/1 | 0.87 | 0.30 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3082 | 1/1 | 0.64 | 0.12 | - | 89,89,89,89 | 0 |
| 56 | MG | DA | 3311 | 1/1 | 0.92 | 0.36 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3500 | 1/1 | 0.92 | 0.19 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3269 | 1/1 | 0.91 | 0.20 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3032 | 1/1 | 0.90 | 0.13 | - | 45,45,45,45 | 0 |
| 56 | MG | DB | 202 | 1/1 | 0.90 | 0.43 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3079 | 1/1 | 0.93 | 0.51 | - | 54,54,54,54 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3205 | 1/1 | 0.88 | 0.39 | - | 43,43,43,43 | 0 |
| 56 | MG | DA | 3372 | 1/1 | 0.85 | 0.33 | - | 78,78,78,78 | 0 |
| 56 | MG | CA | 1815 | 1/1 | 0.92 | 0.14 | - | 119,119,119,119 | 0 |
| 56 | MG | BA | 3042 | 1/1 | 0.93 | 0.23 | - | 37,37,37,37 | 0 |
| 56 | MG | BB | 223 | 1/1 | 0.98 | 0.18 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3657 | 1/1 | 0.94 | 0.07 | - | 89,89,89,89 | 0 |
| 56 | MG | CA | 1667 | 1/1 | 0.91 | 0.32 | - | 66,66,66,66 | 0 |
| 56 | MG | AA | 1861 | 1/1 | 0.98 | 0.13 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3300 | 1/1 | 0.93 | 0.29 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3238 | 1/1 | 0.90 | 0.30 | - | 55,55,55,55 | 0 |
| 56 | MG | AA | 1738 | 1/1 | 0.94 | 0.14 | - | 84,84,84,84 | 0 |
| 56 | MG | AA | 1681 | 1/1 | 0.95 | 0.24 | - | 91,91,91,91 | 0 |
| 56 | MG | BA | 3721 | 1/1 | 0.95 | 0.23 | - | 23,23,23,23 | 0 |
| 56 | MG | DA | 3229 | 1/1 | 0.94 | 0.43 | - | 52,52,52,52 | 0 |
| 56 | MG | AA | 1647 | 1/1 | 0.92 | 0.30 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3075 | 1/1 | 0.94 | 0.18 | - | 47,47,47,47 | 0 |
| 56 | MG | BA | 3023 | 1/1 | 0.97 | 0.13 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3348 | 1/1 | 0.94 | 0.26 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3460 | 1/1 | 0.92 | 0.41 | - | 52,52,52,52 | 0 |
| 56 | MG | CA | 1789 | 1/1 | 0.94 | 0.23 | - | 66,66,66,66 | 0 |
| 56 | MG | AA | 1883 | 1/1 | 0.87 | 0.06 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3226 | 1/1 | 0.86 | 0.76 | - | 62,62,62,62 | 0 |
| 56 | MG | CA | 1819 | 1/1 | 0.81 | 0.25 | - | 96,96,96,96 | 0 |
| 56 | MG | BA | 3424 | 1/1 | 0.84 | 0.21 | - | 42,42,42,42 | 0 |
| 56 | MG | CA | 1617 | 1/1 | 0.93 | 0.47 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3464 | 1/1 | 0.88 | 0.17 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3274 | 1/1 | 0.89 | 0.21 | - | 35,35,35,35 | 0 |
| 56 | MG | DA | 3681 | 1/1 | 0.90 | 0.12 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3388 | 1/1 | 0.95 | 0.09 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1609 | 1/1 | 0.96 | 0.69 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3377 | 1/1 | 0.82 | 0.45 | - | 50,50,50,50 | 0 |
| 56 | MG | AA | 1682 | 1/1 | 0.91 | 0.31 | - | 118,118,118,118 | 0 |
| 56 | MG | AA | 1700 | 1/1 | 0.94 | 0.22 | - | 116,116,116,116 | 0 |
| 56 | MG | DA | 3162 | 1/1 | 0.85 | 0.77 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3584 | 1/1 | 0.95 | 0.14 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3724 | 1/1 | 0.89 | 0.19 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3424 | 1/1 | 0.96 | 0.15 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3356 | 1/1 | 0.93 | 0.17 | - | 66,66,66,66 | 0 |
| 56 | MG | BB | 202 | 1/1 | 0.94 | 0.15 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3891 | 1/1 | 0.93 | 0.20 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3130 | 1/1 | 0.95 | 0.08 | - | 30,30,30,30 | 0 |
| 56 | MG | CA | 1675 | 1/1 | 0.77 | 0.46 | - | 77,77,77,77 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3674 | 1/1 | 0.97 | 0.12 | - | 27,27,27,27 | 0 |
| 56 | MG | BA | 3118 | 1/1 | 0.93 | 0.58 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3472 | 1/1 | 0.82 | 0.68 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1930 | 1/1 | 0.82 | 0.13 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3315 | 1/1 | 0.85 | 0.41 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3008 | 1/1 | 0.91 | 0.28 | - | 108,108,108,108 | 0 |
| 56 | MG | BA | 3579 | 1/1 | 0.95 | 0.17 | - | 64,64,64,64 | 0 |
| 56 | MG | AA | 1617 | 1/1 | 0.91 | 0.06 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3181 | 1/1 | 0.89 | 0.33 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3023 | 1/1 | 0.91 | 0.20 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3015 | 1/1 | 0.93 | 0.53 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3202 | 1/1 | 0.96 | 0.16 | - | 42,42,42,42 | 0 |
| 56 | MG | BA | 3696 | 1/1 | 0.97 | 0.07 | - | 30,30,30,30 | 0 |
| 56 | MG | AA | 1940 | 1/1 | 0.95 | 0.14 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3790 | 1/1 | 0.89 | 0.20 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1818 | 1/1 | 0.93 | 0.19 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3645 | 1/1 | 0.95 | 0.14 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3481 | 1/1 | 0.91 | 0.15 | - | 87,87,87,87 | 0 |
| 56 | MG | DA | 3119 | 1/1 | 0.91 | 0.44 | - | 39,39,39,39 | 0 |
| 56 | MG | BB | 218 | 1/1 | 0.95 | 0.12 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3248 | 1/1 | 0.95 | 0.22 | - | 53,53,53,53 | 0 |
| 56 | MG | CV | 102 | 1/1 | 0.88 | 0.21 | - | 85,85,85,85 | 0 |
| 56 | MG | CA | 1760 | 1/1 | 0.93 | 0.75 | - | 103,103,103,103 | 0 |
| 56 | MG | BA | 3510 | 1/1 | 0.80 | 0.26 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3892 | 1/1 | 0.83 | 0.21 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3822 | 1/1 | 0.90 | 0.17 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3497 | 1/1 | 0.95 | 0.20 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3838 | 1/1 | 0.98 | 0.20 | - | 28,28,28,28 | 0 |
| 56 | MG | BA | 3386 | 1/1 | 0.97 | 0.17 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3617 | 1/1 | 0.99 | 0.07 | - | 58,58,58,58 | 0 |
| 56 | MG | DA | 3313 | 1/1 | 0.92 | 0.24 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1870 | 1/1 | 0.88 | 0.14 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3001 | 1/1 | 0.88 | 0.18 | - | 35,35,35,35 | 0 |
| 56 | MG | CA | 1812 | 1/1 | 0.65 | 0.28 | - | 114,114,114,114 | 0 |
| 56 | MG | BA | 3568 | 1/1 | 0.94 | 0.16 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3208 | 1/1 | 0.82 | 0.29 | - | 91,91,91,91 | 0 |
| 56 | MG | DA | 3236 | 1/1 | 0.81 | 0.47 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3136 | 1/1 | 0.97 | 0.26 | - | 32,32,32,32 | 0 |
| 56 | MG | DA | 3194 | 1/1 | 0.91 | 0.52 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3449 | 1/1 | 0.97 | 0.50 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 3619 | 1/1 | 0.95 | 0.12 | - | 39,39,39,39 | 0 |
| 56 | MG | BA | 3381 | 1/1 | 0.95 | 0.37 | - | 19,19,19,19 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3184 | 1/1 | 0.97 | 0.29 | - | 31,31,31,31 | 0 |
| 56 | MG | BA | 3174 | 1/1 | 0.91 | 0.25 | - | 62,62,62,62 | 0 |
| 56 | MG | DD | 304 | 1/1 | 0.92 | 0.38 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3158 | 1/1 | 0.92 | 0.65 | - | 82,82,82,82 | 0 |
| 56 | MG | AA | 1926 | 1/1 | 0.91 | 0.10 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3148 | 1/1 | 0.86 | 0.57 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3111 | 1/1 | 0.94 | 0.28 | - | 51,51,51,51 | 0 |
| 56 | MG | BD | 304 | 1/1 | 0.98 | 0.42 | - | 20,20,20,20 | 0 |
| 56 | MG | DA | 3365 | 1/1 | 0.94 | 0.12 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3869 | 1/1 | 0.94 | 0.10 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3577 | 1/1 | 0.91 | 0.12 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3275 | 1/1 | 0.91 | 0.24 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3835 | 1/1 | 0.91 | 0.29 | - | 86,86,86,86 | 0 |
| 56 | MG | BA | 3843 | 1/1 | 0.90 | 0.13 | - | 78,78,78,78 | 0 |
| 56 | MG | AA | 1719 | 1/1 | 0.81 | 0.26 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3588 | 1/1 | 0.97 | 0.18 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3409 | 1/1 | 0.94 | 0.16 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3613 | 1/1 | 0.94 | 0.25 | - | 40,40,40,40 | 0 |
| 56 | MG | CA | 1742 | 1/1 | 0.88 | 0.27 | - | 89,89,89,89 | 0 |
| 56 | MG | BA | 3785 | 1/1 | 0.91 | 0.17 | - | 69,69,69,69 | 0 |
| 56 | MG | AA | 1884 | 1/1 | 0.80 | 0.16 | - | 82,82,82,82 | 0 |
| 56 | MG | CA | 1780 | 1/1 | 0.58 | 0.15 | - | 90,90,90,90 | 0 |
| 56 | MG | AA | 1937 | 1/1 | 0.58 | 0.14 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3438 | 1/1 | 0.96 | 0.09 | - | 66,66,66,66 | 0 |
| 56 | MG | CA | 1614 | 1/1 | 0.94 | 0.11 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3456 | 1/1 | 0.97 | 0.18 | - | 56,56,56,56 | 0 |
| 56 | MG | DA | 3180 | 1/1 | 0.89 | 0.11 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3116 | 1/1 | 0.89 | 0.26 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3276 | 1/1 | 0.92 | 0.23 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3210 | 1/1 | 0.81 | 0.36 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3150 | 1/1 | 0.94 | 0.49 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3582 | 1/1 | 0.83 | 0.12 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3280 | 1/1 | 0.83 | 0.39 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1742 | 1/1 | 0.81 | 0.20 | - | 93,93,93,93 | 0 |
| 56 | MG | AA | 1655 | 1/1 | 0.92 | 0.27 | - | 77,77,77,77 | 0 |
| 56 | MG | AA | 1606 | 1/1 | 0.97 | 0.27 | - | 35,35,35,35 | 0 |
| 56 | MG | BA | 3420 | 1/1 | 0.85 | 0.23 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3765 | 1/1 | 0.98 | 0.06 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3263 | 1/1 | 0.97 | 0.16 | - | 41,41,41,41 | 0 |
| 56 | MG | DA | 3414 | 1/1 | 0.96 | 0.17 | - | 50,50,50,50 | 0 |
| 56 | MG | AA | 1752 | 1/1 | 0.87 | 0.38 | - | 88,88,88,88 | 0 |
| 56 | MG | BA | 3312 | 1/1 | 0.91 | 0.28 | - | 54,54,54,54 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3209 | 1/1 | 0.97 | 0.20 | - | 89,89,89,89 | 0 |
| 56 | MG | DA | 3305 | 1/1 | 0.94 | 0.19 | - | 76,76,76,76 | 0 |
| 56 | MG | CA | 1725 | 1/1 | 0.95 | 0.17 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3688 | 1/1 | 0.81 | 0.15 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3346 | 1/1 | 0.91 | 0.27 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3737 | 1/1 | 0.94 | 0.08 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3567 | 1/1 | 0.94 | 0.15 | - | 55,55,55,55 | 0 |
| 56 | MG | DA | 3093 | 1/1 | 0.96 | 0.29 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3057 | 1/1 | 0.90 | 0.31 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3116 | 1/1 | 0.98 | 0.29 | - | 37,37,37,37 | 0 |
| 56 | MG | BA | 3050 | 1/1 | 0.89 | 0.29 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3690 | 1/1 | 0.68 | 0.07 | - | 107,107,107,107 | 0 |
| 56 | MG | CA | 1752 | 1/1 | 0.90 | 0.20 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1702 | 1/1 | 0.92 | 0.24 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3653 | 1/1 | 0.97 | 0.19 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3268 | 1/1 | 0.97 | 0.14 | - | 52,52,52,52 | 0 |
| 56 | MG | AA | 1669 | 1/1 | 0.85 | 0.37 | - | 84,84,84,84 | 0 |
| 56 | MG | B7 | 101 | 1/1 | 0.89 | 0.22 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3684 | 1/1 | 0.95 | 0.20 | - | 42,42,42,42 | 0 |
| 56 | MG | AA | 1828 | 1/1 | 0.76 | 0.41 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3750 | 1/1 | 0.93 | 0.12 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3269 | 1/1 | 0.83 | 0.17 | - | 85,85,85,85 | 0 |
| 56 | MG | AA | 1709 | 1/1 | 0.86 | 0.12 | - | 86,86,86,86 | 0 |
| 56 | MG | AA | 1718 | 1/1 | 0.75 | 0.22 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3644 | 1/1 | 0.96 | 0.05 | - | 80,80,80,80 | 0 |
| 56 | MG | CA | 1787 | 1/1 | 0.86 | 0.17 | - | 98,98,98,98 | 0 |
| 56 | MG | DA | 3538 | 1/1 | 0.77 | 0.25 | - | 96,96,96,96 | 0 |
| 56 | MG | DA | 3096 | 1/1 | 0.96 | 0.20 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3349 | 1/1 | 0.91 | 0.20 | - | 52,52,52,52 | 0 |
| 56 | MG | DA | 3682 | 1/1 | 0.80 | 0.12 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3247 | 1/1 | 0.85 | 0.30 | - | 58,58,58,58 | 0 |
| 56 | MG | CA | 1715 | 1/1 | 0.97 | 0.13 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3447 | 1/1 | 0.97 | 0.11 | - | 45,45,45,45 | 0 |
| 56 | MG | AA | 1886 | 1/1 | 0.92 | 0.11 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3735 | 1/1 | 0.96 | 0.05 | - | 58,58,58,58 | 0 |
| 56 | MG | DA | 3234 | 1/1 | 0.84 | 0.35 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3279 | 1/1 | 0.85 | 0.24 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1760 | 1/1 | 0.81 | 0.83 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3194 | 1/1 | 0.82 | 0.30 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3162 | 1/1 | 0.91 | 0.18 | - | 36,36,36,36 | 0 |
| 56 | MG | CA | 1677 | 1/1 | 0.91 | 0.13 | - | 88,88,88,88 | 0 |
| 56 | MG | BA | 3345 | 1/1 | 0.93 | 0.19 | - | 74,74,74,74 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3842 | 1/1 | 0.88 | 0.16 | - | 85,85,85,85 | 0 |
| 56 | MG | CA | 1777 | 1/1 | 0.94 | 0.11 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3513 | 1/1 | 0.83 | 0.14 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3337 | 1/1 | 0.92 | 0.22 | - | 65,65,65,65 | 0 |
| 56 | MG | BP | 202 | 1/1 | 0.94 | 0.17 | - | 62,62,62,62 | 0 |
| 56 | MG | AA | 1784 | 1/1 | 0.80 | 0.32 | - | 69,69,69,69 | 0 |
| 56 | MG | CA | 1638 | 1/1 | 0.48 | 0.56 | - | 99,99,99,99 | 0 |
| 56 | MG | BA | 3060 | 1/1 | 0.94 | 0.14 | - | 52,52,52,52 | 0 |
| 56 | MG | AA | 1678 | 1/1 | 0.74 | 0.27 | - | 90,90,90,90 | 0 |
| 56 | MG | AV | 113 | 1/1 | 0.66 | 0.54 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3522 | 1/1 | 0.89 | 0.22 | - | 76,76,76,76 | 0 |
| 56 | MG | BF | 306 | 1/1 | 0.92 | 0.22 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3133 | 1/1 | 0.91 | 0.52 | - | 51,51,51,51 | 0 |
| 56 | MG | AA | 1817 | 1/1 | 0.84 | 0.83 | - | 93,93,93,93 | 0 |
| 56 | MG | CA | 1687 | 1/1 | 0.87 | 0.26 | - | 81,81,81,81 | 0 |
| 56 | MG | AA | 1848 | 1/1 | 0.92 | 0.43 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3492 | 1/1 | 0.88 | 0.25 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3616 | 1/1 | 0.73 | 0.48 | - | 115,115,115,115 | 0 |
| 56 | MG | DA | 3113 | 1/1 | 0.85 | 0.23 | - | 59,59,59,59 | 0 |
| 56 | MG | CA | 1779 | 1/1 | 0.98 | 0.18 | - | 95,95,95,95 | 0 |
| 56 | MG | AA | 1691 | 1/1 | 0.93 | 0.32 | - | 121,121,121,121 | 0 |
| 56 | MG | CA | 1699 | 1/1 | 0.71 | 0.23 | - | 97,97,97,97 | 0 |
| 56 | MG | DA | 3204 | 1/1 | 0.86 | 0.38 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3187 | 1/1 | 0.90 | 0.29 | - | 109,109,109,109 | 0 |
| 56 | MG | AA | 1896 | 1/1 | 0.99 | 0.10 | - | 88,88,88,88 | 0 |
| 56 | MG | AA | 1900 | 1/1 | 0.74 | 0.12 | - | 110,110,110,110 | 0 |
| 56 | MG | DA | 3212 | 1/1 | 0.96 | 0.28 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3327 | 1/1 | 0.96 | 0.41 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3259 | 1/1 | 0.54 | 0.53 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3239 | 1/1 | 0.89 | 0.47 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3603 | 1/1 | 0.81 | 0.51 | - | 100,100,100,100 | 0 |
| 56 | MG | BA | 3125 | 1/1 | 0.81 | 0.55 | - | 48,48,48,48 | 0 |
| 56 | MG | AA | 1840 | 1/1 | 0.96 | 0.16 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3701 | 1/1 | 0.98 | 0.13 | - | 26,26,26,26 | 0 |
| 56 | MG | CA | 1798 | 1/1 | 0.88 | 0.16 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3071 | 1/1 | 0.91 | 0.35 | - | 41,41,41,41 | 0 |
| 56 | MG | CA | 1762 | 1/1 | 0.89 | 0.22 | - | 76,76,76,76 | 0 |
| 56 | MG | AA | 1836 | 1/1 | 0.96 | 0.16 | - | 59,59,59,59 | 0 |
| 56 | MG | AA | 1916 | 1/1 | 0.97 | 0.07 | - | 82,82,82,82 | 0 |
| 56 | MG | BB | 209 | 1/1 | 0.83 | 0.36 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 1619 | 1/1 | 0.93 | 0.29 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3743 | 1/1 | 0.97 | 0.32 | - | 71,71,71,71 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3103 | 1/1 | 0.95 | 0.49 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3830 | 1/1 | 0.97 | 0.15 | - | 31,31,31,31 | 0 |
| 56 | MG | AA | 1612 | 1/1 | 0.83 | 0.26 | - | 60,60,60,60 | 0 |
| 56 | MG | AA | 1798 | 1/1 | 0.86 | 0.41 | - | 54,54,54,54 | 0 |
| 56 | MG | AA | 1914 | 1/1 | 0.85 | 0.19 | - | 104,104,104,104 | 0 |
| 56 | MG | CA | 1734 | 1/1 | 0.83 | 0.24 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3085 | 1/1 | 0.96 | 0.29 | - | 35,35,35,35 | 0 |
| 56 | MG | DA | 3676 | 1/1 | 0.80 | 0.28 | - | 94,94,94,94 | 0 |
| 56 | MG | DA | 3166 | 1/1 | 0.77 | 0.66 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3499 | 1/1 | 0.91 | 0.17 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3297 | 1/1 | 0.91 | 0.24 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3126 | 1/1 | 0.98 | 0.46 | - | 40,40,40,40 | 0 |
| 56 | MG | DA | 3242 | 1/1 | 0.92 | 0.28 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3569 | 1/1 | 0.90 | 0.09 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3237 | 1/1 | 0.90 | 0.25 | - | 61,61,61,61 | 0 |
| 56 | MG | BB | 214 | 1/1 | 0.92 | 0.21 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3002 | 1/1 | 0.82 | 0.34 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3234 | 1/1 | 0.91 | 0.29 | - | 43,43,43,43 | 0 |
| 56 | MG | DA | 3050 | 1/1 | 0.92 | 0.20 | - | 67,67,67,67 | 0 |
| 56 | MG | DA | 3442 | 1/1 | 0.96 | 0.19 | - | 56,56,56,56 | 0 |
| 56 | MG | DD | 301 | 1/1 | 0.93 | 0.17 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3115 | 1/1 | 0.94 | 0.59 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3534 | 1/1 | 0.98 | 0.12 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3333 | 1/1 | 0.86 | 0.42 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3308 | 1/1 | 0.94 | 0.20 | - | 51,51,51,51 | 0 |
| 56 | MG | AA | 1673 | 1/1 | 0.96 | 0.22 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3231 | 1/1 | 0.97 | 0.20 | - | 31,31,31,31 | 0 |
| 56 | MG | DA | 3611 | 1/1 | 0.85 | 0.27 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1624 | 1/1 | 0.93 | 0.50 | - | 57,57,57,57 | 0 |
| 56 | MG | CA | 1814 | 1/1 | 0.82 | 0.09 | - | 114,114,114,114 | 0 |
| 56 | MG | DA | 3126 | 1/1 | 0.85 | 0.24 | - | 69,69,69,69 | 0 |
| 56 | MG | AA | 1922 | 1/1 | 0.71 | 0.18 | - | 106,106,106,106 | 0 |
| 56 | MG | AA | 1757 | 1/1 | 0.94 | 0.20 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1769 | 1/1 | 0.96 | 0.14 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3009 | 1/1 | 0.63 | 0.10 | - | 90,90,90,90 | 0 |
| 56 | MG | AA | 1946 | 1/1 | 0.98 | 0.11 | - | 81,81,81,81 | 0 |
| 56 | MG | CA | 1671 | 1/1 | 0.81 | 0.20 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3746 | 1/1 | 0.93 | 0.27 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3712 | 1/1 | 0.99 | 0.21 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3073 | 1/1 | 0.84 | 0.57 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1802 | 1/1 | 0.78 | 0.40 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3733 | 1/1 | 0.95 | 0.17 | - | 49,49,49,49 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3546 | 1/1 | 0.91 | 0.10 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3138 | 1/1 | 0.88 | 0.41 | - | 58,58,58,58 | 0 |
| 56 | MG | CV | 104 | 1/1 | 0.94 | 0.22 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3068 | 1/1 | 0.93 | 0.10 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3217 | 1/1 | 0.91 | 0.15 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3016 | 1/1 | 0.92 | 0.29 | - | 42,42,42,42 | 0 |
| 56 | MG | BO | 202 | 1/1 | 0.90 | 0.34 | - | 42,42,42,42 | 0 |
| 56 | MG | CA | 1655 | 1/1 | 0.90 | 0.51 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3507 | 1/1 | 0.86 | 0.20 | - | 109,109,109,109 | 0 |
| 56 | MG | BA | 3223 | 1/1 | 0.82 | 0.24 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3597 | 1/1 | 0.93 | 0.08 | - | 66,66,66,66 | 0 |
| 56 | MG | AA | 1847 | 1/1 | 0.97 | 0.28 | - | 98,98,98,98 | 0 |
| 56 | MG | BA | 3164 | 1/1 | 0.97 | 0.14 | - | 26,26,26,26 | 0 |
| 56 | MG | BA | 3380 | 1/1 | 0.95 | 0.19 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3551 | 1/1 | 0.95 | 0.25 | - | 42,42,42,42 | 0 |
| 56 | MG | DA | 3415 | 1/1 | 0.98 | 0.43 | - | 33,33,33,33 | 0 |
| 56 | MG | BA | 3213 | 1/1 | 0.91 | 0.22 | - | 37,37,37,37 | 0 |
| 56 | MG | BA | 3761 | 1/1 | 0.96 | 0.21 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3053 | 1/1 | 0.93 | 0.21 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3607 | 1/1 | 0.87 | 0.14 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3366 | 1/1 | 0.85 | 0.16 | - | 81,81,81,81 | 0 |
| 56 | MG | BA | 3578 | 1/1 | 0.97 | 0.16 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3108 | 1/1 | 0.95 | 0.12 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3332 | 1/1 | 0.69 | 0.36 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1672 | 1/1 | 0.78 | 0.29 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3719 | 1/1 | 0.94 | 0.12 | - | 71,71,71,71 | 0 |
| 56 | MG | CA | 1630 | 1/1 | 0.94 | 0.53 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3379 | 1/1 | 0.88 | 0.29 | - | 39,39,39,39 | 0 |
| 56 | MG | BA | 3793 | 1/1 | 0.96 | 0.46 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3217 | 1/1 | 0.75 | 0.18 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3189 | 1/1 | 0.82 | 0.20 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3361 | 1/1 | 0.95 | 0.23 | - | 60,60,60,60 | 0 |
| 56 | MG | AA | 1907 | 1/1 | 0.91 | 0.16 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3181 | 1/1 | 0.92 | 0.22 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3028 | 1/1 | 0.95 | 0.52 | - | 56,56,56,56 | 0 |
| 56 | MG | CA | 1653 | 1/1 | 0.80 | 0.39 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3440 | 1/1 | 0.99 | 0.06 | - | 47,47,47,47 | 0 |
| 56 | MG | AA | 1905 | 1/1 | 0.78 | 0.15 | - | 130,130,130,130 | 0 |
| 56 | MG | BA | 3655 | 1/1 | 0.94 | 0.12 | - | 46,46,46,46 | 0 |
| 56 | MG | DE | 301 | 1/1 | 0.82 | 0.21 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3253 | 1/1 | 0.96 | 0.38 | - | 20,20,20,20 | 0 |
| 56 | MG | DA | 3240 | 1/1 | 0.91 | 0.13 | - | 74,74,74,74 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1927 | 1/1 | 0.97 | 0.11 | - | 85,85,85,85 | 0 |
| 56 | MG | AA | 1887 | 1/1 | 0.86 | 0.24 | - | 90,90,90,90 | 0 |
| 56 | MG | CA | 1774 | 1/1 | 0.88 | 0.17 | - | 111,111,111,111 | 0 |
| 56 | MG | CA | 1609 | 1/1 | 0.95 | 0.12 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3617 | 1/1 | 0.95 | 0.10 | - | 86,86,86,86 | 0 |
| 56 | MG | BA | 3786 | 1/1 | 0.95 | 0.16 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3277 | 1/1 | 0.90 | 0.17 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3399 | 1/1 | 0.85 | 0.09 | - | 95,95,95,95 | 0 |
| 56 | MG | BA | 3097 | 1/1 | 0.98 | 0.14 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 3193 | 1/1 | 0.91 | 0.15 | - | 67,67,67,67 | 0 |
| 56 | MG | AA | 1866 | 1/1 | 0.94 | 0.34 | - | 86,86,86,86 | 0 |
| 56 | MG | BA | 3499 | 1/1 | 0.71 | 0.30 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3491 | 1/1 | 0.76 | 0.15 | - | 101,101,101,101 | 0 |
| 56 | MG | CA | 1651 | 1/1 | 0.93 | 0.37 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3471 | 1/1 | 0.90 | 0.26 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1603 | 1/1 | 0.87 | 0.12 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3381 | 1/1 | 0.80 | 0.19 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3497 | 1/1 | 0.72 | 0.20 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3144 | 1/1 | 0.88 | 0.38 | - | 71,71,71,71 | 0 |
| 56 | MG | AA | 1671 | 1/1 | 0.93 | 0.64 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3138 | 1/1 | 0.98 | 0.20 | - | 33,33,33,33 | 0 |
| 56 | MG | DA | 3253 | 1/1 | 0.96 | 0.36 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3718 | 1/1 | 0.94 | 0.12 | - | 87,87,87,87 | 0 |
| 56 | MG | BA | 3493 | 1/1 | 0.70 | 0.40 | - | 62,62,62,62 | 0 |
| 56 | MG | DB | 206 | 1/1 | 0.86 | 0.29 | - | 77,77,77,77 | 0 |
| 56 | MG | BX | 101 | 1/1 | 0.64 | 0.44 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3301 | 1/1 | 0.89 | 0.12 | - | 70,70,70,70 | 0 |
| 56 | MG | AA | 1826 | 1/1 | 0.75 | 0.14 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3429 | 1/1 | 0.97 | 0.06 | - | 73,73,73,73 | 0 |
| 56 | MG | AA | 1932 | 1/1 | 0.55 | 0.26 | - | 116,116,116,116 | 0 |
| 56 | MG | BA | 3825 | 1/1 | 0.98 | 0.05 | - | 37,37,37,37 | 0 |
| 56 | MG | BA | 3526 | 1/1 | 0.97 | 0.08 | - | 40,40,40,40 | 0 |
| 56 | MG | DA | 3604 | 1/1 | 0.94 | 0.17 | - | 97,97,97,97 | 0 |
| 56 | MG | DA | 3125 | 1/1 | 0.95 | 0.19 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3170 | 1/1 | 0.92 | 0.32 | - | 96,96,96,96 | 0 |
| 56 | MG | BA | 3242 | 1/1 | 0.96 | 0.24 | - | 47,47,47,47 | 0 |
| 56 | MG | BA | 3267 | 1/1 | 0.89 | 0.31 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3626 | 1/1 | 0.95 | 0.08 | - | 70,70,70,70 | 0 |
| 56 | MG | AA | 1849 | 1/1 | 0.95 | 0.21 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3170 | 1/1 | 0.97 | 0.19 | - | 43,43,43,43 | 0 |
| 56 | MG | CA | 1633 | 1/1 | 0.91 | 0.43 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3591 | 1/1 | 0.91 | 0.18 | - | 86,86,86,86 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3716 | 1/1 | 0.97 | 0.16 | - | 40,40,40,40 | 0 |
| 56 | MG | DA | 3648 | 1/1 | 0.91 | 0.23 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3191 | 1/1 | 0.89 | 0.18 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3430 | 1/1 | 0.85 | 0.21 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3775 | 1/1 | 0.96 | 0.27 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1765 | 1/1 | 0.95 | 0.16 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3174 | 1/1 | 0.85 | 0.53 | - | 68,68,68,68 | 0 |
| 56 | MG | AA | 1767 | 1/1 | 0.90 | 0.20 | - | 59,59,59,59 | 0 |
| 56 | MG | CA | 1623 | 1/1 | 0.92 | 0.26 | - | 68,68,68,68 | 0 |
| 56 | MG | AA | 1675 | 1/1 | 0.90 | 1.11 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3614 | 1/1 | 0.81 | 0.38 | - | 98,98,98,98 | 0 |
| 56 | MG | BA | 3554 | 1/1 | 0.98 | 0.14 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3115 | 1/1 | 0.95 | 0.24 | - | 52,52,52,52 | 0 |
| 56 | MG | DA | 3533 | 1/1 | 0.90 | 0.17 | - | 95,95,95,95 | 0 |
| 56 | MG | D5 | 101 | 1/1 | 0.95 | 0.61 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3283 | 1/1 | 0.87 | 0.56 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3105 | 1/1 | 0.96 | 0.16 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3338 | 1/1 | 0.91 | 0.35 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1909 | 1/1 | 0.92 | 0.05 | - | 91,91,91,91 | 0 |
| 56 | MG | BA | 3046 | 1/1 | 0.92 | 0.14 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1750 | 1/1 | 0.96 | 0.15 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3314 | 1/1 | 0.87 | 0.31 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3503 | 1/1 | 0.95 | 0.25 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3206 | 1/1 | 0.92 | 0.32 | - | 31,31,31,31 | 0 |
| 56 | MG | BB | 203 | 1/1 | 0.79 | 0.35 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3382 | 1/1 | 0.95 | 0.16 | - | 68,68,68,68 | 0 |
| 56 | MG | AA | 1729 | 1/1 | 0.94 | 0.18 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3350 | 1/1 | 0.90 | 0.29 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3205 | 1/1 | 0.79 | 0.23 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3335 | 1/1 | 0.60 | 0.48 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3662 | 1/1 | 0.98 | 0.15 | - | 30,30,30,30 | 0 |
| 56 | MG | BA | 3103 | 1/1 | 0.88 | 0.41 | - | 54,54,54,54 | 0 |
| 56 | MG | AA | 1677 | 1/1 | 0.89 | 0.55 | - | 84,84,84,84 | 0 |
| 56 | MG | BB | 216 | 1/1 | 0.89 | 0.19 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3652 | 1/1 | 0.98 | 0.08 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3142 | 1/1 | 0.92 | 0.36 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3306 | 1/1 | 0.95 | 0.18 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3415 | 1/1 | 0.82 | 0.31 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3517 | 1/1 | 0.79 | 0.40 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1947 | 1/1 | 0.96 | 0.07 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3616 | 1/1 | 0.98 | 0.23 | - | 40,40,40,40 | 0 |
| 56 | MG | AA | 1772 | 1/1 | 0.92 | 0.33 | - | 77,77,77,77 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1639 | 1/1 | 0.91 | 0.12 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3623 | 1/1 | 0.97 | 0.05 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3776 | 1/1 | 0.95 | 0.53 | - | 68,68,68,68 | 0 |
| 56 | MG | AA | 1791 | 1/1 | 0.89 | 0.26 | - | 99,99,99,99 | 0 |
| 56 | MG | AA | 1920 | 1/1 | 0.92 | 0.11 | - | 86,86,86,86 | 0 |
| 56 | MG | D8 | 201 | 1/1 | 0.92 | 0.22 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3530 | 1/1 | 0.97 | 0.12 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3485 | 1/1 | 0.84 | 0.24 | - | 52,52,52,52 | 0 |
| 56 | MG | AE | 201 | 1/1 | 0.79 | 0.47 | - | 83,83,83,83 | 0 |
| 56 | MG | BA | 3762 | 1/1 | 0.95 | 0.14 | - | 48,48,48,48 | 0 |
| 56 | MG | CA | 1807 | 1/1 | 0.74 | 0.13 | - | 100,100,100,100 | 0 |
| 56 | MG | AA | 1902 | 1/1 | 0.87 | 0.27 | - | 121,121,121,121 | 0 |
| 56 | MG | BA | 3036 | 1/1 | 0.96 | 0.33 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3089 | 1/1 | 0.80 | 0.51 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3684 | 1/1 | 0.91 | 0.19 | - | 98,98,98,98 | 0 |
| 56 | MG | DA | 3683 | 1/1 | 0.91 | 0.28 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3857 | 1/1 | 0.63 | 0.22 | - | 78,78,78,78 | 0 |
| 56 | MG | CA | 1662 | 1/1 | 0.89 | 0.47 | - | 92,92,92,92 | 0 |
| 56 | MG | CA | 1627 | 1/1 | 0.96 | 0.56 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3545 | 1/1 | 0.97 | 0.12 | - | 53,53,53,53 | 0 |
| 56 | MG | BV | 202 | 1/1 | 0.96 | 0.19 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3272 | 1/1 | 0.68 | 0.41 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3223 | 1/1 | 0.83 | 0.58 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3890 | 1/1 | 0.95 | 0.08 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3730 | 1/1 | 0.94 | 0.06 | - | 63,63,63,63 | 0 |
| 56 | MG | AV | 110 | 1/1 | 0.85 | 0.28 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1708 | 1/1 | 0.81 | 0.28 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3512 | 1/1 | 0.99 | 0.32 | - | 49,49,49,49 | 0 |
| 56 | MG | CA | 1601 | 1/1 | 0.91 | 0.83 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3401 | 1/1 | 0.90 | 0.23 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3363 | 1/1 | 0.82 | 0.24 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3353 | 1/1 | 0.93 | 0.21 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3661 | 1/1 | 0.97 | 0.24 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3159 | 1/1 | 0.97 | 0.27 | - | 43,43,43,43 | 0 |
| 56 | MG | AA | 1780 | 1/1 | 0.97 | 0.23 | - | 55,55,55,55 | 0 |
| 56 | MG | DA | 3131 | 1/1 | 0.96 | 0.34 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3538 | 1/1 | 0.90 | 0.14 | - | 33,33,33,33 | 0 |
| 56 | MG | CA | 1746 | 1/1 | 0.94 | 0.09 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3011 | 1/1 | 0.90 | 0.15 | - | 66,66,66,66 | 0 |
| 56 | MG | B5 | 101 | 1/1 | 0.90 | 0.27 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3505 | 1/1 | 0.90 | 0.34 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 1747 | 1/1 | 0.88 | 0.17 | - | 96,96,96,96 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3271 | 1/1 | 0.96 | 0.16 | - | 44,44,44,44 | 0 |
| 56 | MG | AY | 201 | 1/1 | 0.80 | 0.21 | - | 111,111,111,111 | 0 |
| 56 | MG | BA | 3451 | 1/1 | 0.95 | 0.21 | - | 47,47,47,47 | 0 |
| 56 | MG | BZ | 302 | 1/1 | 0.88 | 0.53 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3056 | 1/1 | 0.86 | 0.30 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3196 | 1/1 | 0.93 | 0.13 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3025 | 1/1 | 0.49 | 0.35 | - | 76,76,76,76 | 0 |
| 56 | MG | CA | 1672 | 1/1 | 0.91 | 0.34 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3319 | 1/1 | 0.70 | 0.54 | - | 69,69,69,69 | 0 |
| 56 | MG | AA | 1699 | 1/1 | 0.67 | 0.21 | - | 109,109,109,109 | 0 |
| 56 | MG | BA | 3151 | 1/1 | 0.92 | 0.23 | - | 38,38,38,38 | 0 |
| 56 | MG | BA | 3266 | 1/1 | 0.88 | 0.45 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3860 | 1/1 | 0.94 | 0.04 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3685 | 1/1 | 0.82 | 0.20 | - | 96,96,96,96 | 0 |
| 56 | MG | DA | 3560 | 1/1 | 0.97 | 0.21 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3354 | 1/1 | 0.93 | 0.11 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 3663 | 1/1 | 0.89 | 0.11 | - | 81,81,81,81 | 0 |
| 56 | MG | AA | 1741 | 1/1 | 0.78 | 0.49 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3319 | 1/1 | 0.92 | 0.15 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3861 | 1/1 | 0.90 | 0.08 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3581 | 1/1 | 0.93 | 0.10 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3091 | 1/1 | 0.91 | 0.33 | - | 60,60,60,60 | 0 |
| 56 | MG | BZ | 301 | 1/1 | 0.93 | 0.21 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3039 | 1/1 | 0.91 | 0.18 | - | 34,34,34,34 | 0 |
| 56 | MG | AA | 1712 | 1/1 | 0.80 | 0.19 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3133 | 1/1 | 0.94 | 0.54 | - | 27,27,27,27 | 0 |
| 56 | MG | AA | 1773 | 1/1 | 0.82 | 0.31 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1854 | 1/1 | 0.96 | 0.17 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3285 | 1/1 | 0.95 | 0.14 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3870 | 1/1 | 0.90 | 0.28 | - | 100,100,100,100 | 0 |
| 56 | MG | CA | 1688 | 1/1 | 0.82 | 0.34 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3329 | 1/1 | 0.83 | 0.14 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3294 | 1/1 | 0.85 | 0.22 | - | 82,82,82,82 | 0 |
| 56 | MG | BY | 202 | 1/1 | 0.92 | 0.28 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3208 | 1/1 | 0.96 | 0.12 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3444 | 1/1 | 0.91 | 0.19 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3322 | 1/1 | 0.93 | 0.23 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3291 | 1/1 | 0.88 | 0.17 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3362 | 1/1 | 0.93 | 0.42 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3529 | 1/1 | 0.95 | 0.14 | - | 49,49,49,49 | 0 |
| 56 | MG | CA | 1811 | 1/1 | 0.78 | 0.07 | - | 102,102,102,102 | 0 |
| 56 | MG | BA | 3482 | 1/1 | 0.92 | 0.15 | - | 73,73,73,73 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3055 | 1/1 | 0.91 | 0.15 | - | 37,37,37,37 | 0 |
| 56 | MG | BA | 3512 | 1/1 | 0.88 | 0.32 | - | 56,56,56,56 | 0 |
| 56 | MG | AA | 1654 | 1/1 | 0.95 | 0.34 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3636 | 1/1 | 0.98 | 0.13 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3641 | 1/1 | 0.97 | 0.11 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3725 | 1/1 | 0.94 | 0.13 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3430 | 1/1 | 0.92 | 0.18 | - | 69,69,69,69 | 0 |
| 56 | MG | AA | 1768 | 1/1 | 0.88 | 0.26 | - | 88,88,88,88 | 0 |
| 56 | MG | AA | 1710 | 1/1 | 0.93 | 0.11 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3795 | 1/1 | 0.97 | 0.17 | - | 84,84,84,84 | 0 |
| 56 | MG | AA | 1918 | 1/1 | 0.95 | 0.13 | - | 68,68,68,68 | 0 |
| 56 | MG | CA | 1713 | 1/1 | 0.86 | 0.11 | - | 71,71,71,71 | 0 |
| 56 | MG | AA | 1666 | 1/1 | 0.95 | 0.25 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3364 | 1/1 | 0.89 | 0.20 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3069 | 1/1 | 0.90 | 0.37 | - | 83,83,83,83 | 0 |
| 56 | MG | CA | 1659 | 1/1 | 0.82 | 0.11 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3314 | 1/1 | 0.88 | 0.17 | - | 52,52,52,52 | 0 |
| 56 | MG | BA | 3388 | 1/1 | 0.86 | 0.32 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3245 | 1/1 | 0.97 | 0.14 | - | 39,39,39,39 | 0 |
| 56 | MG | AA | 1899 | 1/1 | 0.58 | 0.22 | - | 115,115,115,115 | 0 |
| 56 | MG | DU | 201 | 1/1 | 0.87 | 0.31 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3136 | 1/1 | 0.68 | 1.07 | - | 67,67,67,67 | 0 |
| 56 | MG | DA | 3478 | 1/1 | 0.95 | 0.35 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3268 | 1/1 | 0.90 | 0.32 | - | 64,64,64,64 | 0 |
| 56 | MG | AA | 1851 | 1/1 | 0.85 | 0.14 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3457 | 1/1 | 0.92 | 0.30 | - | 102,102,102,102 | 0 |
| 56 | MG | CA | 1664 | 1/1 | 0.59 | 0.36 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3536 | 1/1 | 0.96 | 0.15 | - | 42,42,42,42 | 0 |
| 56 | MG | CA | 1654 | 1/1 | 0.76 | 0.48 | - | 74,74,74,74 | 0 |
| 56 | MG | CV | 108 | 1/1 | 0.91 | 0.29 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3705 | 1/1 | 0.98 | 0.25 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3221 | 1/1 | 0.90 | 0.38 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3287 | 1/1 | 0.91 | 0.24 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3457 | 1/1 | 0.87 | 0.20 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3846 | 1/1 | 0.98 | 0.18 | - | 27,27,27,27 | 0 |
| 56 | MG | BA | 3343 | 1/1 | 0.95 | 0.26 | - | 37,37,37,37 | 0 |
| 56 | MG | AA | 1827 | 1/1 | 0.72 | 0.20 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3751 | 1/1 | 0.95 | 0.08 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3427 | 1/1 | 0.95 | 0.22 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3364 | 1/1 | 0.85 | 0.17 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3119 | 1/1 | 0.94 | 0.16 | - | 50,50,50,50 | 0 |
| 56 | MG | DB | 216 | 1/1 | 0.85 | 0.10 | - | 109,109,109,109 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3606 | 1/1 | 0.98 | 0.09 | - | 63,63,63,63 | 0 |
| 56 | MG | CA | 1709 | 1/1 | 0.88 | 0.66 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3120 | 1/1 | 0.96 | 0.15 | - | 42,42,42,42 | 0 |
| 56 | MG | DA | 3542 | 1/1 | 0.96 | 0.09 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 3295 | 1/1 | 0.96 | 0.23 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3500 | 1/1 | 0.96 | 0.10 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3886 | 1/1 | 0.90 | 0.27 | - | 94,94,94,94 | 0 |
| 56 | MG | CA | 1771 | 1/1 | 0.97 | 0.21 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3564 | 1/1 | 0.97 | 0.10 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3291 | 1/1 | 0.83 | 0.35 | - | 61,61,61,61 | 0 |
| 56 | MG | AA | 1730 | 1/1 | 0.95 | 0.17 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3195 | 1/1 | 0.97 | 0.35 | - | 19,19,19,19 | 0 |
| 56 | MG | BA | 3255 | 1/1 | 0.96 | 0.34 | - | 16,16,16,16 | 0 |
| 56 | MG | DA | 3374 | 1/1 | 0.92 | 0.41 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3140 | 1/1 | 0.98 | 0.52 | - | 44,44,44,44 | 0 |
| 56 | MG | BB | 207 | 1/1 | 0.96 | 0.27 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3244 | 1/1 | 0.89 | 0.40 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3557 | 1/1 | 0.97 | 0.05 | - | 62,62,62,62 | 0 |
| 56 | MG | AA | 1615 | 1/1 | 0.92 | 0.09 | - | 75,75,75,75 | 0 |
| 56 | MG | DF | 301 | 1/1 | 0.88 | 0.30 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3145 | 1/1 | 0.94 | 0.17 | - | 41,41,41,41 | 0 |
| 56 | MG | AV | 108 | 1/1 | 0.89 | 0.19 | - | 98,98,98,98 | 0 |
| 56 | MG | CA | 1818 | 1/1 | 0.67 | 0.25 | - | 87,87,87,87 | 0 |
| 56 | MG | DA | 3474 | 1/1 | 0.91 | 0.11 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3673 | 1/1 | 0.85 | 0.39 | - | 111,111,111,111 | 0 |
| 56 | MG | BA | 3794 | 1/1 | 0.96 | 0.17 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3339 | 1/1 | 0.75 | 0.34 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3440 | 1/1 | 0.77 | 0.72 | - | 56,56,56,56 | 0 |
| 56 | MG | CA | 1770 | 1/1 | 0.74 | 0.15 | - | 93,93,93,93 | 0 |
| 56 | MG | CA | 1768 | 1/1 | 0.93 | 0.24 | - | 94,94,94,94 | 0 |
| 56 | MG | BA | 3528 | 1/1 | 0.96 | 0.09 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3462 | 1/1 | 0.93 | 0.12 | - | 50,50,50,50 | 0 |
| 56 | MG | AA | 1633 | 1/1 | 0.95 | 0.49 | - | 32,32,32,32 | 0 |
| 56 | MG | DA | 3233 | 1/1 | 0.81 | 0.32 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3039 | 1/1 | 0.91 | 0.21 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3327 | 1/1 | 0.95 | 0.25 | - | 80,80,80,80 | 0 |
| 56 | MG | CA | 1754 | 1/1 | 0.94 | 0.21 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3106 | 1/1 | 0.94 | 0.28 | - | 48,48,48,48 | 0 |
| 56 | MG | BB | 210 | 1/1 | 0.94 | 0.41 | - | 53,53,53,53 | 0 |
| 56 | MG | BE | 304 | 1/1 | 0.96 | 0.44 | - | 14,14,14,14 | 0 |
| 56 | MG | BA | 3047 | 1/1 | 0.97 | 0.32 | - | 32,32,32,32 | 0 |
| 56 | MG | BA | 3428 | 1/1 | 0.91 | 0.24 | - | 63,63,63,63 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3010 | 1/1 | 0.84 | 0.23 | - | 78,78,78,78 | 0 |
| 56 | MG | BB | 224 | 1/1 | 0.92 | 0.12 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3254 | 1/1 | 0.81 | 0.36 | - | 71,71,71,71 | 0 |
| 56 | MG | AA | 1889 | 1/1 | 0.97 | 0.17 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3479 | 1/1 | 0.81 | 0.42 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3290 | 1/1 | 0.86 | 0.36 | - | 79,79,79,79 | 0 |
| 56 | MG | AA | 1618 | 1/1 | 0.90 | 0.30 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3313 | 1/1 | 0.88 | 0.28 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3668 | 1/1 | 0.93 | 0.13 | - | 29,29,29,29 | 0 |
| 56 | MG | DA | 3379 | 1/1 | 0.76 | 0.41 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3736 | 1/1 | 0.80 | 0.21 | - | 59,59,59,59 | 0 |
| 56 | MG | AA | 1653 | 1/1 | 0.89 | 0.71 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3596 | 1/1 | 0.97 | 0.06 | - | 39,39,39,39 | 0 |
| 56 | MG | AA | 1693 | 1/1 | 0.81 | 0.39 | - | 103,103,103,103 | 0 |
| 56 | MG | AA | 1704 | 1/1 | 0.85 | 0.29 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 1772 | 1/1 | 0.93 | 0.11 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3385 | 1/1 | 0.95 | 0.16 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3049 | 1/1 | 0.89 | 0.44 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3772 | 1/1 | 0.92 | 0.10 | - | 26,26,26,26 | 0 |
| 56 | MG | AA | 1751 | 1/1 | 0.86 | 0.20 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1667 | 1/1 | 0.75 | 0.34 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3195 | 1/1 | 0.95 | 0.17 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3549 | 1/1 | 0.99 | 0.24 | - | 19,19,19,19 | 0 |
| 56 | MG | BA | 3326 | 1/1 | 0.92 | 0.13 | - | 100,100,100,100 | 0 |
| 56 | MG | CA | 1721 | 1/1 | 0.95 | 0.10 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3098 | 1/1 | 0.92 | 0.22 | - | 39,39,39,39 | 0 |
| 56 | MG | DA | 3453 | 1/1 | 0.95 | 0.15 | - | 77,77,77,77 | 0 |
| 56 | MG | DB | 204 | 1/1 | 0.92 | 0.26 | - | 107,107,107,107 | 0 |
| 56 | MG | CA | 1711 | 1/1 | 0.91 | 0.31 | - | 70,70,70,70 | 0 |
| 56 | MG | AA | 1898 | 1/1 | 0.86 | 0.13 | - | 98,98,98,98 | 0 |
| 56 | MG | DA | 3651 | 1/1 | 0.96 | 0.04 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3577 | 1/1 | 0.98 | 0.21 | - | 95,95,95,95 | 0 |
| 56 | MG | BA | 3158 | 1/1 | 0.82 | 0.40 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3671 | 1/1 | 0.81 | 0.11 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3261 | 1/1 | 0.93 | 0.19 | - | 69,69,69,69 | 0 |
| 56 | MG | DB | 210 | 1/1 | 0.96 | 0.18 | - | 91,91,91,91 | 0 |
| 56 | MG | CA | 1685 | 1/1 | 0.84 | 0.31 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3422 | 1/1 | 0.97 | 0.07 | - | 82,82,82,82 | 0 |
| 56 | MG | B8 | 101 | 1/1 | 0.97 | 0.55 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1746 | 1/1 | 0.72 | 0.36 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3117 | 1/1 | 0.61 | 0.30 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3498 | 1/1 | 0.89 | 0.20 | - | 54,54,54,54 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3063 | 1/1 | 0.95 | 0.45 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3135 | 1/1 | 0.89 | 0.31 | - | 58,58,58,58 | 0 |
| 56 | MG | DA | 3519 | 1/1 | 0.59 | 0.09 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3452 | 1/1 | 0.97 | 0.33 | - | 55,55,55,55 | 0 |
| 56 | MG | DA | 3152 | 1/1 | 0.90 | 0.36 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3141 | 1/1 | 0.95 | 0.15 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3005 | 1/1 | 0.80 | 0.37 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 1624 | 1/1 | 0.83 | 0.25 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3649 | 1/1 | 0.91 | 0.12 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3494 | 1/1 | 0.87 | 0.30 | - | 62,62,62,62 | 0 |
| 56 | MG | AA | 1701 | 1/1 | 0.88 | 0.28 | - | 57,57,57,57 | 0 |
| 56 | MG | AA | 1770 | 1/1 | 0.95 | 0.39 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3803 | 1/1 | 0.92 | 0.21 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3139 | 1/1 | 0.94 | 0.45 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3272 | 1/1 | 0.92 | 0.19 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3583 | 1/1 | 0.98 | 0.10 | - | 22,22,22,22 | 0 |
| 56 | MG | CA | 1698 | 1/1 | 0.92 | 0.72 | - | 114,114,114,114 | 0 |
| 56 | MG | AK | 201 | 1/1 | 0.66 | 0.47 | - | 107,107,107,107 | 0 |
| 56 | MG | BA | 3720 | 1/1 | 0.98 | 0.17 | - | 22,22,22,22 | 0 |
| 56 | MG | DA | 3448 | 1/1 | 0.86 | 0.16 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3490 | 1/1 | 0.89 | 0.30 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1789 | 1/1 | 0.69 | 0.37 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3621 | 1/1 | 0.96 | 0.19 | - | 30,30,30,30 | 0 |
| 56 | MG | DA | 3092 | 1/1 | 0.89 | 0.19 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3070 | 1/1 | 0.90 | 0.42 | - | 51,51,51,51 | 0 |
| 56 | MG | DA | 3360 | 1/1 | 0.84 | 0.25 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3778 | 1/1 | 0.78 | 0.17 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3456 | 1/1 | 0.64 | 0.42 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3165 | 1/1 | 0.90 | 0.57 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3182 | 1/1 | 0.88 | 0.28 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3149 | 1/1 | 0.91 | 0.17 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3190 | 1/1 | 0.92 | 0.22 | - | 42,42,42,42 | 0 |
| 56 | MG | AA | 1882 | 1/1 | 0.96 | 0.13 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3435 | 1/1 | 0.88 | 0.14 | - | 84,84,84,84 | 0 |
| 56 | MG | CA | 1694 | 1/1 | 0.73 | 0.48 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3330 | 1/1 | 0.91 | 0.65 | - | 78,78,78,78 | 0 |
| 56 | MG | AV | 114 | 1/1 | 0.88 | 0.22 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3677 | 1/1 | 0.98 | 0.20 | - | 29,29,29,29 | 0 |
| 56 | MG | BA | 3024 | 1/1 | 0.96 | 0.27 | - | 36,36,36,36 | 0 |
| 56 | MG | AA | 1740 | 1/1 | 0.94 | 0.49 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3867 | 1/1 | 0.93 | 0.19 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3738 | 1/1 | 0.98 | 0.36 | - | 42,42,42,42 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3134 | 1/1 | 0.91 | 0.16 | - | 61,61,61,61 | 0 |
| 56 | MG | AA | 1835 | 1/1 | 0.98 | 0.08 | - | 88,88,88,88 | 0 |
| 56 | MG | AA | 1627 | 1/1 | 0.73 | 0.67 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3173 | 1/1 | 0.95 | 0.27 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3187 | 1/1 | 0.89 | 0.21 | - | 47,47,47,47 | 0 |
| 56 | MG | BA | 3522 | 1/1 | 0.92 | 0.32 | - | 62,62,62,62 | 0 |
| 56 | MG | BF | 302 | 1/1 | 0.90 | 0.41 | - | 41,41,41,41 | 0 |
| 56 | MG | BA | 3469 | 1/1 | 0.89 | 0.31 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3025 | 1/1 | 0.71 | 0.50 | - | 68,68,68,68 | 0 |
| 56 | MG | BB | 215 | 1/1 | 0.94 | 0.16 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3102 | 1/1 | 0.79 | 0.16 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 3634 | 1/1 | 0.94 | 0.08 | - | 46,46,46,46 | 0 |
| 56 | MG | BE | 303 | 1/1 | 0.95 | 0.18 | - | 32,32,32,32 | 0 |
| 56 | MG | DA | 3282 | 1/1 | 0.80 | 0.60 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3355 | 1/1 | 0.95 | 0.34 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3797 | 1/1 | 0.82 | 0.21 | - | 91,91,91,91 | 0 |
| 56 | MG | BA | 3323 | 1/1 | 0.93 | 0.28 | - | 45,45,45,45 | 0 |
| 56 | MG | CA | 1729 | 1/1 | 0.96 | 0.18 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3575 | 1/1 | 0.84 | 0.11 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3895 | 1/1 | 0.87 | 0.12 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3167 | 1/1 | 0.94 | 0.25 | - | 31,31,31,31 | 0 |
| 56 | MG | BA | 3143 | 1/1 | 0.96 | 0.32 | - | 20,20,20,20 | 0 |
| 56 | MG | BA | 3008 | 1/1 | 0.83 | 0.20 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 3344 | 1/1 | 0.90 | 0.16 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3383 | 1/1 | 0.84 | 0.44 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3827 | 1/1 | 0.84 | 0.16 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3058 | 1/1 | 0.93 | 0.29 | - | 46,46,46,46 | 0 |
| 56 | MG | AA | 1812 | 1/1 | 0.82 | 0.33 | - | 122,122,122,122 | 0 |
| 56 | MG | DA | 3216 | 1/1 | 0.84 | 0.23 | - | 46,46,46,46 | 0 |
| 56 | MG | AA | 1620 | 1/1 | 0.63 | 0.54 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1929 | 1/1 | 0.95 | 0.15 | - | 48,48,48,48 | 0 |
| 56 | MG | AA | 1779 | 1/1 | 0.92 | 0.30 | - | 60,60,60,60 | 0 |
| 56 | MG | AA | 1745 | 1/1 | 0.97 | 0.28 | - | 64,64,64,64 | 0 |
| 56 | MG | AA | 1689 | 1/1 | 0.77 | 0.18 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3371 | 1/1 | 0.85 | 0.18 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3307 | 1/1 | 0.84 | 0.26 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3336 | 1/1 | 0.89 | 0.26 | - | 46,46,46,46 | 0 |
| 56 | MG | CA | 1803 | 1/1 | 0.90 | 0.19 | - | 102,102,102,102 | 0 |
| 56 | MG | DA | 3099 | 1/1 | 0.98 | 0.42 | - | 42,42,42,42 | 0 |
| 56 | MG | AA | 1948 | 1/1 | 0.78 | 0.10 | - | 88,88,88,88 | 0 |
| 56 | MG | BA | 3722 | 1/1 | 0.96 | 0.05 | - | 61,61,61,61 | 0 |
| 56 | MG | CA | 1634 | 1/1 | 0.98 | 0.39 | - | 63,63,63,63 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3305 | 1/1 | 0.92 | 0.16 | - | 35,35,35,35 | 0 |
| 56 | MG | DA | 3275 | 1/1 | 0.95 | 0.33 | - | 42,42,42,42 | 0 |
| 56 | MG | BA | 3742 | 1/1 | 0.69 | 0.22 | - | 72,72,72,72 | 0 |
| 56 | MG | CA | 1755 | 1/1 | 0.95 | 0.17 | - | 93,93,93,93 | 0 |
| 56 | MG | BA | 3808 | 1/1 | 0.90 | 0.13 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3572 | 1/1 | 0.97 | 0.07 | - | 66,66,66,66 | 0 |
| 56 | MG | AA | 1837 | 1/1 | 0.85 | 0.17 | - | 66,66,66,66 | 0 |
| 56 | MG | AA | 1737 | 1/1 | 0.68 | 0.42 | - | 88,88,88,88 | 0 |
| 56 | MG | BA | 3013 | 1/1 | 0.94 | 0.30 | - | 57,57,57,57 | 0 |
| 56 | MG | BB | 226 | 1/1 | 0.98 | 0.07 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3297 | 1/1 | 0.92 | 0.21 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3303 | 1/1 | 0.86 | 0.28 | - | 54,54,54,54 | 0 |
| 56 | MG | AA | 1825 | 1/1 | 0.86 | 0.28 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3333 | 1/1 | 0.89 | 0.24 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1814 | 1/1 | 0.93 | 0.30 | - | 81,81,81,81 | 0 |
| 56 | MG | BA | 3074 | 1/1 | 0.96 | 0.15 | - | 52,52,52,52 | 0 |
| 56 | MG | DA | 3036 | 1/1 | 0.83 | 0.18 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3541 | 1/1 | 0.98 | 0.08 | - | 35,35,35,35 | 0 |
| 56 | MG | BA | 3773 | 1/1 | 0.96 | 0.07 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3565 | 1/1 | 0.98 | 0.12 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3570 | 1/1 | 0.80 | 0.22 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 1666 | 1/1 | 0.72 | 0.28 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3201 | 1/1 | 0.90 | 0.58 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3034 | 1/1 | 0.89 | 0.44 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3206 | 1/1 | 0.82 | 0.17 | - | 92,92,92,92 | 0 |
| 56 | MG | DA | 3071 | 1/1 | 0.96 | 0.38 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3487 | 1/1 | 0.91 | 0.20 | - | 53,53,53,53 | 0 |
| 56 | MG | CA | 1749 | 1/1 | 0.90 | 0.21 | - | 92,92,92,92 | 0 |
| 56 | MG | BA | 3147 | 1/1 | 0.87 | 0.14 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3241 | 1/1 | 0.94 | 0.13 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3595 | 1/1 | 0.97 | 0.14 | - | 43,43,43,43 | 0 |
| 56 | MG | DA | 3476 | 1/1 | 0.93 | 0.17 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3659 | 1/1 | 0.89 | 0.22 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3622 | 1/1 | 0.97 | 0.16 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3502 | 1/1 | 0.97 | 0.27 | - | 33,33,33,33 | 0 |
| 56 | MG | AA | 1833 | 1/1 | 0.84 | 0.19 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3518 | 1/1 | 0.96 | 0.24 | - | 33,33,33,33 | 0 |
| 56 | MG | AA | 1696 | 1/1 | 0.90 | 0.53 | - | 95,95,95,95 | 0 |
| 56 | MG | BA | 3496 | 1/1 | 0.94 | 0.25 | - | 61,61,61,61 | 0 |
| 56 | MG | DR | 201 | 1/1 | 0.95 | 0.23 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3763 | 1/1 | 0.74 | 0.10 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 3016 | 1/1 | 0.95 | 0.43 | - | 52,52,52,52 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3310 | 1/1 | 0.89 | 0.27 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3140 | 1/1 | 0.87 | 0.24 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3663 | 1/1 | 0.86 | 0.16 | - | 21,21,21,21 | 0 |
| 56 | MG | AA | 1759 | 1/1 | 0.92 | 0.30 | - | 60,60,60,60 | 0 |
| 56 | MG | AA | 1610 | 1/1 | 0.91 | 0.40 | - | 48,48,48,48 | 0 |
| 56 | MG | BA | 3551 | 1/1 | 0.99 | 0.03 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3866 | 1/1 | 0.86 | 0.07 | - | 82,82,82,82 | 0 |
| 56 | MG | AA | 1688 | 1/1 | 0.89 | 0.11 | - | 96,96,96,96 | 0 |
| 56 | MG | BA | 3535 | 1/1 | 0.87 | 0.15 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3656 | 1/1 | 0.90 | 0.08 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3714 | 1/1 | 0.94 | 0.30 | - | 62,62,62,62 | 0 |
| 56 | MG | B5 | 102 | 1/1 | 0.95 | 0.18 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3425 | 1/1 | 0.92 | 0.30 | - | 46,46,46,46 | 0 |
| 56 | MG | BA | 3741 | 1/1 | 0.90 | 0.12 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3035 | 1/1 | 0.82 | 0.20 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3292 | 1/1 | 0.93 | 0.15 | - | 47,47,47,47 | 0 |
| 56 | MG | BA | 3186 | 1/1 | 0.95 | 0.46 | - | 27,27,27,27 | 0 |
| 56 | MG | DA | 3669 | 1/1 | 0.93 | 0.10 | - | 93,93,93,93 | 0 |
| 56 | MG | CV | 106 | 1/1 | 0.71 | 0.36 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3475 | 1/1 | 0.94 | 0.21 | - | 42,42,42,42 | 0 |
| 56 | MG | BA | 3740 | 1/1 | 0.94 | 0.17 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3494 | 1/1 | 0.98 | 0.19 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3355 | 1/1 | 0.85 | 0.26 | - | 55,55,55,55 | 0 |
| 56 | MG | AA | 1813 | 1/1 | 0.90 | 0.13 | - | 121,121,121,121 | 0 |
| 56 | MG | BA | 3176 | 1/1 | 0.92 | 0.15 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1901 | 1/1 | 0.53 | 0.17 | - | 119,119,119,119 | 0 |
| 56 | MG | AA | 1792 | 1/1 | 0.95 | 0.17 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3633 | 1/1 | 0.97 | 0.26 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3579 | 1/1 | 0.85 | 0.20 | - | 104,104,104,104 | 0 |
| 56 | MG | AA | 1903 | 1/1 | 0.87 | 0.19 | - | 117,117,117,117 | 0 |
| 56 | MG | BA | 3246 | 1/1 | 0.88 | 0.45 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3549 | 1/1 | 0.87 | 0.18 | - | 87,87,87,87 | 0 |
| 56 | MG | CA | 1776 | 1/1 | 0.92 | 0.54 | - | 90,90,90,90 | 0 |
| 56 | MG | AA | 1936 | 1/1 | 0.97 | 0.18 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 3659 | 1/1 | 0.97 | 0.18 | - | 60,60,60,60 | 0 |
| 56 | MG | BA | 3373 | 1/1 | 0.73 | 0.39 | - | 69,69,69,69 | 0 |
| 56 | MG | BB | 212 | 1/1 | 0.89 | 0.27 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3104 | 1/1 | 0.94 | 0.43 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3147 | 1/1 | 0.92 | 0.30 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3569 | 1/1 | 0.97 | 0.24 | - | 49,49,49,49 | 0 |
| 56 | MG | BA | 3504 | 1/1 | 0.93 | 0.23 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 3524 | 1/1 | 0.79 | 0.17 | - | 81,81,81,81 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3152 | 1/1 | 0.91 | 0.11 | - | 42,42,42,42 | 0 |
| 56 | MG | DA | 3404 | 1/1 | 0.99 | 0.11 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3088 | 1/1 | 0.96 | 0.27 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3464 | 1/1 | 0.91 | 0.34 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3122 | 1/1 | 0.82 | 0.71 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3481 | 1/1 | 0.94 | 0.38 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3488 | 1/1 | 0.95 | 0.70 | - | 73,73,73,73 | 0 |
| 56 | MG | AA | 1781 | 1/1 | 0.90 | 0.49 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3263 | 1/1 | 0.90 | 0.30 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3462 | 1/1 | 0.96 | 0.34 | - | 47,47,47,47 | 0 |
| 56 | MG | BA | 3814 | 1/1 | 0.96 | 0.27 | - | 86,86,86,86 | 0 |
| 56 | MG | BA | 3101 | 1/1 | 0.98 | 0.34 | - | 26,26,26,26 | 0 |
| 56 | MG | AA | 1715 | 1/1 | 0.63 | 0.46 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3852 | 1/1 | 0.97 | 0.22 | - | 59,59,59,59 | 0 |
| 56 | MG | CA | 1661 | 1/1 | 0.63 | 0.15 | - | 101,101,101,101 | 0 |
| 56 | MG | DA | 3088 | 1/1 | 0.87 | 0.30 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3132 | 1/1 | 0.94 | 0.17 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3699 | 1/1 | 0.98 | 0.14 | - | 38,38,38,38 | 0 |
| 56 | MG | AA | 1871 | 1/1 | 0.97 | 0.07 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3302 | 1/1 | 0.92 | 0.22 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3689 | 1/1 | 0.90 | 0.20 | - | 104,104,104,104 | 0 |
| 56 | MG | DA | 3332 | 1/1 | 0.85 | 0.39 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1661 | 1/1 | 0.92 | 0.40 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3421 | 1/1 | 0.90 | 0.29 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3802 | 1/1 | 0.93 | 0.20 | - | 71,71,71,71 | 0 |
| 56 | MG | BA | 3171 | 1/1 | 0.97 | 0.36 | - | 38,38,38,38 | 0 |
| 56 | MG | BA | 3369 | 1/1 | 0.97 | 0.43 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3295 | 1/1 | 0.84 | 0.11 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3590 | 1/1 | 0.84 | 0.29 | - | 89,89,89,89 | 0 |
| 56 | MG | AA | 1891 | 1/1 | 0.96 | 0.05 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3003 | 1/1 | 0.97 | 0.11 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3198 | 1/1 | 0.97 | 0.21 | - | 17,17,17,17 | 0 |
| 56 | MG | DA | 3324 | 1/1 | 0.95 | 0.14 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3600 | 1/1 | 0.98 | 0.26 | - | 36,36,36,36 | 0 |
| 56 | MG | BA | 3546 | 1/1 | 0.98 | 0.07 | - | 48,48,48,48 | 0 |
| 56 | MG | BA | 3653 | 1/1 | 0.97 | 0.17 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3289 | 1/1 | 0.80 | 0.18 | - | 86,86,86,86 | 0 |
| 56 | MG | CA | 1816 | 1/1 | 0.77 | 0.25 | - | 110,110,110,110 | 0 |
| 56 | MG | BA | 3357 | 1/1 | 0.91 | 0.24 | - | 82,82,82,82 | 0 |
| 56 | MG | CA | 1794 | 1/1 | 0.99 | 0.13 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3598 | 1/1 | 0.96 | 0.04 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3201 | 1/1 | 0.88 | 0.28 | - | 54,54,54,54 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1860 | 1/1 | 0.97 | 0.11 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3612 | 1/1 | 0.94 | 0.08 | - | 61,61,61,61 | 0 |
| 56 | MG | BD | 305 | 1/1 | 0.94 | 0.39 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3467 | 1/1 | 0.93 | 0.17 | - | 91,91,91,91 | 0 |
| 56 | MG | DA | 3418 | 1/1 | 0.95 | 0.34 | - | 52,52,52,52 | 0 |
| 56 | MG | AV | 102 | 1/1 | 0.91 | 0.19 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3289 | 1/1 | 0.96 | 0.23 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3161 | 1/1 | 0.98 | 0.20 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3219 | 1/1 | 0.95 | 0.43 | - | 43,43,43,43 | 0 |
| 56 | MG | DA | 3356 | 1/1 | 0.88 | 0.15 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3505 | 1/1 | 0.94 | 0.16 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3352 | 1/1 | 0.91 | 0.41 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3680 | 1/1 | 0.97 | 0.09 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3610 | 1/1 | 0.75 | 0.26 | - | 97,97,97,97 | 0 |
| 56 | MG | CA | 1702 | 1/1 | 0.79 | 0.34 | - | 114,114,114,114 | 0 |
| 56 | MG | CA | 1763 | 1/1 | 0.98 | 0.09 | - | 62,62,62,62 | 0 |
| 56 | MG | CA | 1676 | 1/1 | 0.80 | 0.17 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3373 | 1/1 | 0.94 | 0.35 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3423 | 1/1 | 0.97 | 0.26 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3635 | 1/1 | 0.97 | 0.17 | - | 88,88,88,88 | 0 |
| 56 | MG | BA | 3089 | 1/1 | 0.82 | 0.43 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3109 | 1/1 | 0.89 | 0.24 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1724 | 1/1 | 0.72 | 0.36 | - | 92,92,92,92 | 0 |
| 56 | MG | AV | 105 | 1/1 | 0.93 | 0.20 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3792 | 1/1 | 0.85 | 0.20 | - | 48,48,48,48 | 0 |
| 56 | MG | BA | 3177 | 1/1 | 0.96 | 0.22 | - | 46,46,46,46 | 0 |
| 56 | MG | DA | 3066 | 1/1 | 0.91 | 0.55 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3446 | 1/1 | 0.74 | 0.23 | - | 87,87,87,87 | 0 |
| 56 | MG | CA | 1648 | 1/1 | 0.83 | 0.20 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 1793 | 1/1 | 0.86 | 0.26 | - | 73,73,73,73 | 0 |
| 56 | MG | AV | 115 | 1/1 | 0.92 | 0.20 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3238 | 1/1 | 0.72 | 0.30 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3650 | 1/1 | 0.96 | 0.09 | - | 46,46,46,46 | 0 |
| 56 | MG | CA | 1809 | 1/1 | 0.89 | 0.09 | - | 101,101,101,101 | 0 |
| 56 | MG | DA | 3605 | 1/1 | 0.95 | 0.21 | - | 101,101,101,101 | 0 |
| 56 | MG | AA | 1880 | 1/1 | 0.85 | 0.41 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3602 | 1/1 | 0.98 | 0.19 | - | 47,47,47,47 | 0 |
| 56 | MG | DA | 3562 | 1/1 | 0.97 | 0.26 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3520 | 1/1 | 0.94 | 0.06 | - | 67,67,67,67 | 0 |
| 56 | MG | BA | 3787 | 1/1 | 0.95 | 0.06 | - | 35,35,35,35 | 0 |
| 56 | MG | DA | 3203 | 1/1 | 0.71 | 0.32 | - | 91,91,91,91 | 0 |
| 56 | MG | AA | 1774 | 1/1 | 0.86 | 0.29 | - | 69,69,69,69 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1794 | 1/1 | 0.86 | 0.52 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3483 | 1/1 | 0.88 | 0.16 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 3022 | 1/1 | 0.92 | 0.12 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3468 | 1/1 | 0.87 | 0.08 | - | 80,80,80,80 | 0 |
| 56 | MG | BB | 221 | 1/1 | 0.97 | 0.10 | - | 44,44,44,44 | 0 |
| 56 | MG | BO | 201 | 1/1 | 0.80 | 0.33 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3620 | 1/1 | 0.86 | 0.28 | - | 95,95,95,95 | 0 |
| 56 | MG | DA | 3361 | 1/1 | 0.96 | 0.20 | - | 60,60,60,60 | 0 |
| 56 | MG | AA | 1855 | 1/1 | 0.96 | 0.18 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3521 | 1/1 | 0.98 | 0.51 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3626 | 1/1 | 0.93 | 0.25 | - | 103,103,103,103 | 0 |
| 56 | MG | DA | 3171 | 1/1 | 0.90 | 0.25 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3309 | 1/1 | 0.76 | 0.47 | - | 56,56,56,56 | 0 |
| 56 | MG | CA | 1740 | 1/1 | 0.88 | 0.16 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3881 | 1/1 | 0.93 | 0.10 | - | 75,75,75,75 | 0 |
| 56 | MG | AV | 109 | 1/1 | 0.95 | 0.19 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3413 | 1/1 | 0.97 | 0.29 | - | 40,40,40,40 | 0 |
| 56 | MG | BA | 3214 | 1/1 | 0.89 | 0.14 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1829 | 1/1 | 0.91 | 0.17 | - | 63,63,63,63 | 0 |
| 56 | MG | CA | 1668 | 1/1 | 0.93 | 0.13 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3177 | 1/1 | 0.91 | 0.46 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1890 | 1/1 | 0.90 | 0.19 | - | 89,89,89,89 | 0 |
| 56 | MG | DA | 3329 | 1/1 | 0.83 | 0.46 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1853 | 1/1 | 0.94 | 0.20 | - | 93,93,93,93 | 0 |
| 56 | MG | CA | 1767 | 1/1 | 0.86 | 0.25 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3514 | 1/1 | 0.86 | 0.27 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1716 | 1/1 | 0.95 | 0.14 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3654 | 1/1 | 0.50 | 0.41 | - | 118,118,118,118 | 0 |
| 56 | MG | CA | 1629 | 1/1 | 0.84 | 0.74 | - | 74,74,74,74 | 0 |
| 56 | MG | B3 | 102 | 1/1 | 0.89 | 0.28 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3280 | 1/1 | 0.80 | 0.31 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3153 | 1/1 | 0.94 | 0.20 | - | 56,56,56,56 | 0 |
| 56 | MG | BA | 3708 | 1/1 | 0.87 | 0.07 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3511 | 1/1 | 0.92 | 0.35 | - | 48,48,48,48 | 0 |
| 56 | MG | AA | 1764 | 1/1 | 0.90 | 0.28 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3020 | 1/1 | 0.93 | 0.44 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3668 | 1/1 | 0.91 | 0.17 | - | 100,100,100,100 | 0 |
| 56 | MG | DA | 3118 | 1/1 | 0.92 | 0.24 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 3407 | 1/1 | 0.87 | 0.22 | - | 44,44,44,44 | 0 |
| 56 | MG | BA | 3607 | 1/1 | 0.96 | 0.29 | - | 59,59,59,59 | 0 |
| 56 | MG | AA | 1807 | 1/1 | 0.77 | 0.36 | - | 84,84,84,84 | 0 |
| 56 | MG | AA | 1743 | 1/1 | 0.78 | 0.53 | - | 80,80,80,80 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3358 | 1/1 | 0.90 | 0.80 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3090 | 1/1 | 0.92 | 0.52 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3267 | 1/1 | 0.83 | 0.46 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3412 | 1/1 | 0.93 | 0.21 | - | 56,56,56,56 | 0 |
| 56 | MG | AA | 1703 | 1/1 | 0.85 | 0.34 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3382 | 1/1 | 0.86 | 0.70 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3163 | 1/1 | 0.88 | 0.64 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3681 | 1/1 | 0.97 | 0.14 | - | 52,52,52,52 | 0 |
| 56 | MG | BA | 3245 | 1/1 | 0.96 | 0.33 | - | 42,42,42,42 | 0 |
| 56 | MG | CA | 1741 | 1/1 | 0.88 | 0.06 | - | 92,92,92,92 | 0 |
| 56 | MG | AA | 1793 | 1/1 | 0.83 | 0.25 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3286 | 1/1 | 0.96 | 0.17 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3084 | 1/1 | 0.85 | 0.33 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3642 | 1/1 | 0.93 | 0.07 | - | 78,78,78,78 | 0 |
| 56 | MG | AA | 1727 | 1/1 | 0.95 | 0.48 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3391 | 1/1 | 0.94 | 0.25 | - | 27,27,27,27 | 0 |
| 56 | MG | BA | 3480 | 1/1 | 0.92 | 0.31 | - | 59,59,59,59 | 0 |
| 56 | MG | BA | 3288 | 1/1 | 0.89 | 0.12 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3727 | 1/1 | 0.96 | 0.12 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3318 | 1/1 | 0.94 | 0.16 | - | 63,63,63,63 | 0 |
| 56 | MG | BA | 3542 | 1/1 | 0.83 | 0.14 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3566 | 1/1 | 0.85 | 0.18 | - | 84,84,84,84 | 0 |
| 56 | MG | AA | 1736 | 1/1 | 0.72 | 0.52 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3609 | 1/1 | 0.89 | 0.25 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 3347 | 1/1 | 0.99 | 0.48 | - | 20,20,20,20 | 0 |
| 56 | MG | AA | 1748 | 1/1 | 0.96 | 0.16 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3149 | 1/1 | 0.92 | 0.21 | - | 35,35,35,35 | 0 |
| 56 | MG | DA | 3334 | 1/1 | 0.85 | 0.34 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3114 | 1/1 | 0.87 | 0.19 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 1719 | 1/1 | 0.94 | 0.23 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3055 | 1/1 | 0.83 | 0.25 | - | 57,57,57,57 | 0 |
| 56 | MG | AA | 1638 | 1/1 | 0.86 | 0.31 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 3625 | 1/1 | 0.95 | 0.10 | - | 41,41,41,41 | 0 |
| 56 | MG | DA | 3409 | 1/1 | 0.98 | 0.07 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3574 | 1/1 | 0.96 | 0.14 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3224 | 1/1 | 0.68 | 0.46 | - | 75,75,75,75 | 0 |
| 56 | MG | DT | 202 | 1/1 | 0.93 | 0.18 | - | 38,38,38,38 | 0 |
| 56 | MG | AA | 1863 | 1/1 | 0.96 | 0.26 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3441 | 1/1 | 0.94 | 0.32 | - | 47,47,47,47 | 0 |
| 56 | MG | DA | 3359 | 1/1 | 0.86 | 0.16 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3261 | 1/1 | 0.92 | 0.31 | - | 69,69,69,69 | 0 |
| 56 | MG | CA | 1739 | 1/1 | 0.95 | 0.19 | - | 79,79,79,79 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3780 | 1/1 | 0.83 | 0.25 | - | 86,86,86,86 | 0 |
| 56 | MG | BA | 3470 | 1/1 | 0.96 | 0.28 | - | 52,52,52,52 | 0 |
| 56 | MG | DA | 3394 | 1/1 | 0.95 | 0.10 | - | 36,36,36,36 | 0 |
| 56 | MG | DA | 3631 | 1/1 | 0.90 | 0.30 | - | 94,94,94,94 | 0 |
| 56 | MG | AA | 1856 | 1/1 | 0.93 | 0.11 | - | 66,66,66,66 | 0 |
| 56 | MG | BR | 202 | 1/1 | 0.95 | 0.28 | - | 30,30,30,30 | 0 |
| 56 | MG | CA | 1727 | 1/1 | 0.89 | 0.22 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1684 | 1/1 | 0.95 | 0.18 | - | 102,102,102,102 | 0 |
| 56 | MG | AA | 1805 | 1/1 | 0.91 | 0.84 | - | 89,89,89,89 | 0 |
| 56 | MG | BA | 3755 | 1/1 | 1.00 | 0.10 | - | 40,40,40,40 | 0 |
| 56 | MG | BA | 3592 | 1/1 | 0.92 | 0.08 | - | 52,52,52,52 | 0 |
| 56 | MG | AA | 1668 | 1/1 | 0.72 | 0.35 | - | 65,65,65,65 | 0 |
| 56 | MG | CA | 1786 | 1/1 | 0.91 | 0.13 | - | 80,80,80,80 | 0 |
| 56 | MG | AV | 112 | 1/1 | 0.73 | 0.38 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 3196 | 1/1 | 0.91 | 0.14 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3350 | 1/1 | 0.83 | 0.20 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3260 | 1/1 | 0.89 | 0.27 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3480 | 1/1 | 0.86 | 0.20 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3378 | 1/1 | 0.91 | 0.20 | - | 40,40,40,40 | 0 |
| 56 | MG | BA | 3279 | 1/1 | 0.95 | 0.11 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3471 | 1/1 | 0.94 | 0.08 | - | 87,87,87,87 | 0 |
| 56 | MG | CA | 1730 | 1/1 | 0.95 | 0.35 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3516 | 1/1 | 0.95 | 0.17 | - | 50,50,50,50 | 0 |
| 56 | MG | AA | 1662 | 1/1 | 0.84 | 0.47 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3559 | 1/1 | 0.97 | 0.13 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3083 | 1/1 | 0.93 | 0.18 | - | 48,48,48,48 | 0 |
| 56 | MG | AA | 1761 | 1/1 | 0.89 | 0.31 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3848 | 1/1 | 0.91 | 0.20 | - | 43,43,43,43 | 0 |
| 56 | MG | BA | 3405 | 1/1 | 0.87 | 0.41 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3081 | 1/1 | 0.84 | 0.22 | - | 53,53,53,53 | 0 |
| 56 | MG | BA | 3489 | 1/1 | 0.96 | 0.13 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3739 | 1/1 | 0.97 | 0.07 | - | 42,42,42,42 | 0 |
| 56 | MG | CA | 1703 | 1/1 | 0.61 | 0.34 | - | 100,100,100,100 | 0 |
| 56 | MG | AA | 1939 | 1/1 | 0.70 | 0.34 | - | 105,105,105,105 | 0 |
| 56 | MG | BA | 3249 | 1/1 | 0.98 | 0.29 | - | 24,24,24,24 | 0 |
| 56 | MG | DA | 3580 | 1/1 | 0.90 | 0.11 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3020 | 1/1 | 0.91 | 0.14 | - | 44,44,44,44 | 0 |
| 56 | MG | CA | 1632 | 1/1 | 0.83 | 0.39 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 3815 | 1/1 | 0.89 | 0.10 | - | 51,51,51,51 | 0 |
| 56 | MG | DA | 3432 | 1/1 | 0.69 | 0.14 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3151 | 1/1 | 0.97 | 0.22 | - | 45,45,45,45 | 0 |
| 56 | MG | BA | 3644 | 1/1 | 0.94 | 0.11 | - | 72,72,72,72 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3320 | 1/1 | 0.97 | 0.32 | - | 58,58,58,58 | 0 |
| 56 | MG | DA | 3670 | 1/1 | 0.91 | 0.11 | - | 83,83,83,83 | 0 |
| 56 | MG | CX | 101 | 1/1 | 0.85 | 0.25 | - | 99,99,99,99 | 0 |
| 56 | MG | BA | 3397 | 1/1 | 0.70 | 0.36 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3449 | 1/1 | 0.98 | 0.27 | - | 45,45,45,45 | 0 |
| 56 | MG | AA | 1867 | 1/1 | 0.64 | 1.13 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3049 | 1/1 | 0.94 | 0.17 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3300 | 1/1 | 0.81 | 0.12 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 3346 | 1/1 | 0.78 | 0.26 | - | 43,43,43,43 | 0 |
| 56 | MG | AA | 1658 | 1/1 | 0.79 | 0.78 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 1805 | 1/1 | 0.97 | 0.13 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3344 | 1/1 | 0.85 | 0.34 | - | 88,88,88,88 | 0 |
| 56 | MG | DA | 3622 | 1/1 | 0.93 | 0.19 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 3744 | 1/1 | 0.90 | 0.43 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3592 | 1/1 | 0.96 | 0.13 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3628 | 1/1 | 0.93 | 0.14 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 3647 | 1/1 | 0.94 | 0.13 | - | 61,61,61,61 | 0 |
| 56 | MG | AA | 1695 | 1/1 | 0.67 | 0.22 | - | 102,102,102,102 | 0 |
| 56 | MG | BA | 3580 | 1/1 | 0.93 | 0.10 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3213 | 1/1 | 0.82 | 0.40 | - | 89,89,89,89 | 0 |
| 56 | MG | DA | 3650 | 1/1 | 0.98 | 0.16 | - | 43,43,43,43 | 0 |
| 56 | MG | DA | 3176 | 1/1 | 0.91 | 0.28 | - | 67,67,67,67 | 0 |
| 56 | MG | DA | 3298 | 1/1 | 0.92 | 0.23 | - | 55,55,55,55 | 0 |
| 56 | MG | AV | 117 | 1/1 | 0.92 | 0.10 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3099 | 1/1 | 0.92 | 0.21 | - | 32,32,32,32 | 0 |
| 56 | MG | AA | 1820 | 1/1 | 0.83 | 0.28 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3215 | 1/1 | 0.98 | 0.60 | - | 46,46,46,46 | 0 |
| 56 | MG | AA | 1819 | 1/1 | 0.77 | 0.61 | - | 91,91,91,91 | 0 |
| 56 | MG | DA | 3003 | 1/1 | 0.90 | 0.20 | - | 43,43,43,43 | 0 |
| 56 | MG | CA | 1797 | 1/1 | 0.52 | 0.40 | - | 121,121,121,121 | 0 |
| 56 | MG | DX | 101 | 1/1 | 0.89 | 0.24 | - | 55,55,55,55 | 0 |
| 56 | MG | CA | 1670 | 1/1 | 0.97 | 0.18 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3561 | 1/1 | 0.94 | 0.14 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3495 | 1/1 | 0.93 | 0.54 | - | 56,56,56,56 | 0 |
| 56 | MG | DA | 3292 | 1/1 | 0.85 | 0.24 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 3222 | 1/1 | 0.97 | 0.37 | - | 28,28,28,28 | 0 |
| 56 | MG | BA | 3876 | 1/1 | 0.99 | 0.09 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3278 | 1/1 | 0.49 | 0.60 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3623 | 1/1 | 0.85 | 0.30 | - | 85,85,85,85 | 0 |
| 56 | MG | BA | 3649 | 1/1 | 0.91 | 0.12 | - | 60,60,60,60 | 0 |
| 56 | MG | DA | 3514 | 1/1 | 0.94 | 0.20 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3093 | 1/1 | 0.97 | 0.12 | - | 42,42,42,42 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3696 | 1/1 | 0.81 | 0.23 | - | 96,96,96,96 | 0 |
| 56 | MG | BA | 3160 | 1/1 | 0.96 | 0.43 | - | 41,41,41,41 | 0 |
| 56 | MG | AA | 1881 | 1/1 | 0.96 | 0.15 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3338 | 1/1 | 0.84 | 0.46 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3150 | 1/1 | 0.90 | 0.10 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3479 | 1/1 | 0.94 | 0.12 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3458 | 1/1 | 0.99 | 0.12 | - | 49,49,49,49 | 0 |
| 56 | MG | DA | 3509 | 1/1 | 0.53 | 0.29 | - | 122,122,122,122 | 0 |
| 56 | MG | BY | 203 | 1/1 | 0.89 | 0.57 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 3387 | 1/1 | 0.96 | 0.16 | - | 48,48,48,48 | 0 |
| 56 | MG | AA | 1705 | 1/1 | 0.93 | 0.19 | - | 55,55,55,55 | 0 |
| 56 | MG | DA | 3053 | 1/1 | 0.94 | 0.16 | - | 55,55,55,55 | 0 |
| 56 | MG | BA | 3858 | 1/1 | 0.83 | 0.26 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3265 | 1/1 | 0.69 | 0.39 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3311 | 1/1 | 0.92 | 0.19 | - | 59,59,59,59 | 0 |
| 56 | MG | B1 | 103 | 1/1 | 0.98 | 0.22 | - | 36,36,36,36 | 0 |
| 56 | MG | DA | 3070 | 1/1 | 0.94 | 0.14 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3316 | 1/1 | 0.84 | 0.13 | - | 80,80,80,80 | 0 |
| 56 | MG | BA | 3889 | 1/1 | 0.95 | 0.17 | - | 80,80,80,80 | 0 |
| 56 | MG | B8 | 102 | 1/1 | 0.99 | 0.14 | - | 49,49,49,49 | 0 |
| 56 | MG | DA | 3686 | 1/1 | 0.99 | 0.23 | - | 74,74,74,74 | 0 |
| 56 | MG | CA | 1660 | 1/1 | 0.96 | 0.23 | - | 92,92,92,92 | 0 |
| 56 | MG | AA | 1788 | 1/1 | 0.79 | 0.47 | - | 62,62,62,62 | 0 |
| 56 | MG | BA | 3466 | 1/1 | 0.91 | 0.32 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3202 | 1/1 | 0.76 | 0.20 | - | 73,73,73,73 | 0 |
| 56 | MG | BA | 3566 | 1/1 | 0.97 | 0.05 | - | 54,54,54,54 | 0 |
| 56 | MG | AA | 1944 | 1/1 | 0.70 | 0.27 | - | 97,97,97,97 | 0 |
| 56 | MG | BA | 3562 | 1/1 | 0.96 | 0.21 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3662 | 1/1 | 0.84 | 0.09 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3014 | 1/1 | 0.98 | 0.21 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3083 | 1/1 | 0.73 | 0.41 | - | 82,82,82,82 | 0 |
| 56 | MG | BA | 3392 | 1/1 | 0.89 | 0.24 | - | 54,54,54,54 | 0 |
| 56 | MG | BA | 3833 | 1/1 | 0.98 | 0.12 | - | 41,41,41,41 | 0 |
| 56 | MG | AA | 1858 | 1/1 | 0.98 | 0.04 | - | 90,90,90,90 | 0 |
| 56 | MG | BA | 3683 | 1/1 | 0.92 | 0.17 | - | 31,31,31,31 | 0 |
| 56 | MG | BA | 3328 | 1/1 | 0.92 | 0.10 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 3394 | 1/1 | 0.89 | 0.30 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3556 | 1/1 | 0.95 | 0.22 | - | 52,52,52,52 | 0 |
| 56 | MG | DA | 3378 | 1/1 | 0.79 | 0.32 | - | 64,64,64,64 | 0 |
| 56 | MG | DA | 3612 | 1/1 | 0.87 | 0.20 | - | 87,87,87,87 | 0 |
| 56 | MG | BA | 3729 | 1/1 | 0.98 | 0.09 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3618 | 1/1 | 0.84 | 0.20 | - | 80,80,80,80 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 1790 | 1/1 | 0.96 | 0.30 | - | 64,64,64,64 | 0 |
| 56 | MG | BA | 3307 | 1/1 | 0.87 | 0.30 | - | 48,48,48,48 | 0 |
| 56 | MG | DA | 3255 | 1/1 | 0.75 | 0.24 | - | 72,72,72,72 | 0 |
| 56 | MG | BA | 3821 | 1/1 | 0.93 | 0.09 | - | 76,76,76,76 | 0 |
| 56 | MG | BA | 3096 | 1/1 | 0.96 | 0.13 | - | 37,37,37,37 | 0 |
| 56 | MG | BA | 3215 | 1/1 | 0.96 | 0.40 | - | 16,16,16,16 | 0 |
| 56 | MG | DA | 3647 | 1/1 | 0.94 | 0.20 | - | 70,70,70,70 | 0 |
| 56 | MG | AA | 1925 | 1/1 | 0.82 | 0.10 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3095 | 1/1 | 0.94 | 0.37 | - | 41,41,41,41 | 0 |
| 56 | MG | DA | 3188 | 1/1 | 0.85 | 0.49 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3400 | 1/1 | 0.85 | 0.28 | - | 53,53,53,53 | 0 |
| 56 | MG | AA | 1893 | 1/1 | 0.68 | 0.32 | - | 95,95,95,95 | 0 |
| 56 | MG | BA | 3454 | 1/1 | 0.91 | 0.24 | - | 58,58,58,58 | 0 |
| 56 | MG | AA | 1815 | 1/1 | 0.75 | 0.52 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3214 | 1/1 | 0.80 | 0.30 | - | 64,64,64,64 | 0 |
| 56 | MG | AA | 1844 | 1/1 | 0.81 | 0.35 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3006 | 1/1 | 0.97 | 0.19 | - | 56,56,56,56 | 0 |
| 56 | MG | DA | 3107 | 1/1 | 0.90 | 0.21 | - | 58,58,58,58 | 0 |
| 56 | MG | BA | 3558 | 1/1 | 0.91 | 0.14 | - | 61,61,61,61 | 0 |
| 56 | MG | BA | 3104 | 1/1 | 0.77 | 0.26 | - | 50,50,50,50 | 0 |
| 56 | MG | BB | 211 | 1/1 | 0.71 | 0.20 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3639 | 1/1 | 0.94 | 0.10 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3222 | 1/1 | 0.92 | 0.52 | - | 73,73,73,73 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.