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

Feb 1, 2016 – 07:03 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 4L47 |
| Title | : | Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U on the Ribosome |
| Authors | : | Maehigashi, T.; Dunkle, J.A.; Dunham, C.M. |
| Deposited on | : | 2013-06-07 |
| Resolution | : | 3.22 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

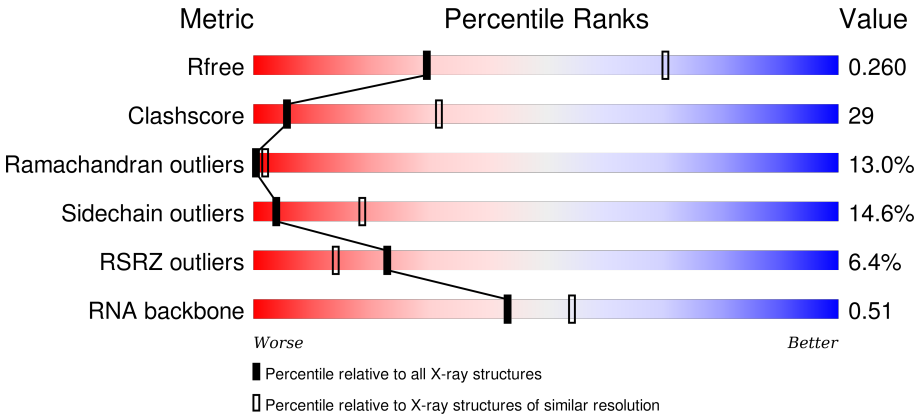
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| 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 3.22 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 | 1095 (3.26-3.18) |
| Clashscore | 102246 | 1046 (3.24-3.20) |
| Ramachandran outliers | 100387 | 1026 (3.24-3.20) |
| Sidechain outliers | 100360 | 1025 (3.24-3.20) |
| RSRZ outliers | 91569 | 1100 (3.26-3.18) |
| RNA backbone | 2183 | 1004 (3.72-2.72) |

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 <=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 | QA | 1522 | 3% 54% 34% 9% •• |
| 1 | XA | 1522 | 3% 54% 33% 10% •• |
| 2 | QB | 256 | 8% 16% 59% 16% • 7% |
| 2 | XB | 256 | 6% 17% 59% 16% • 7% |

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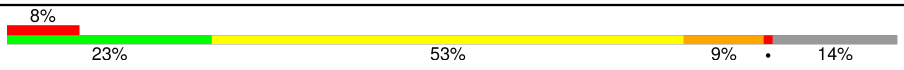
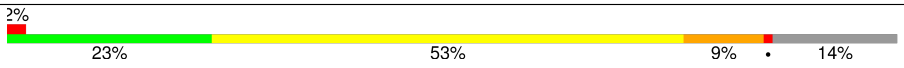
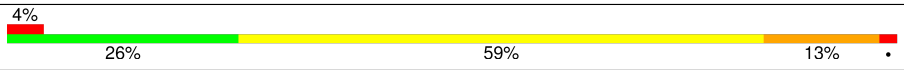
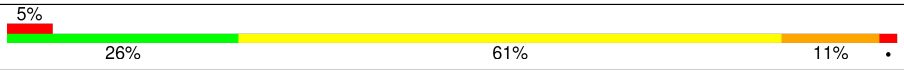
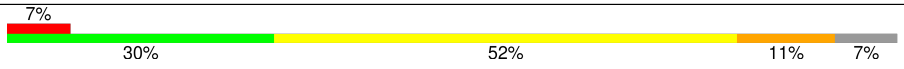
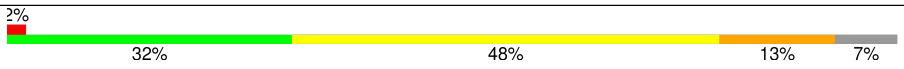
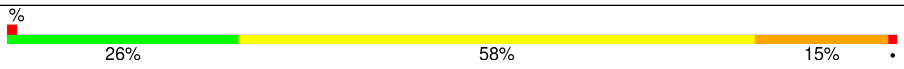
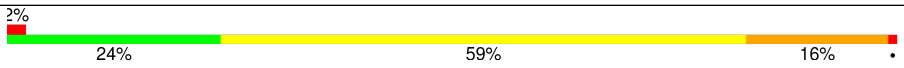
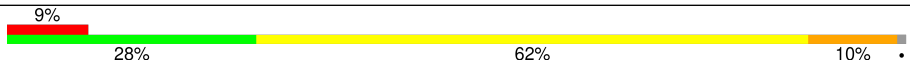
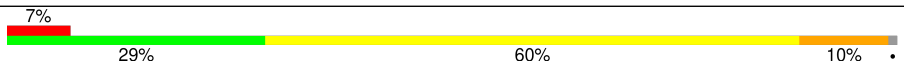
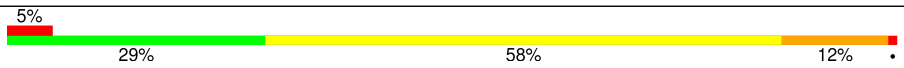
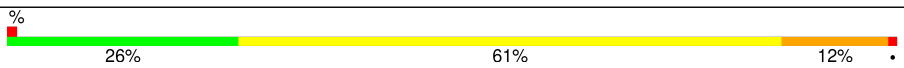
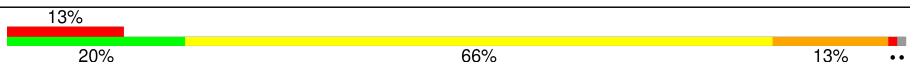
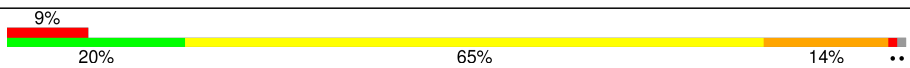
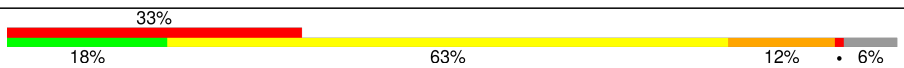
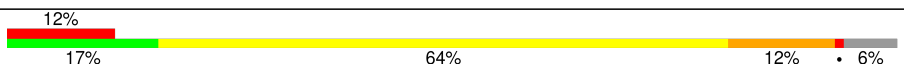
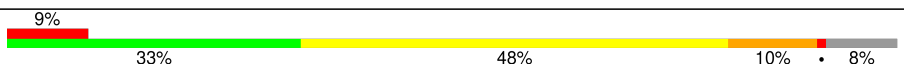
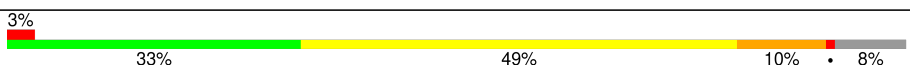
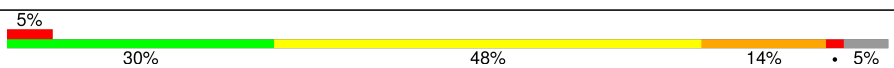
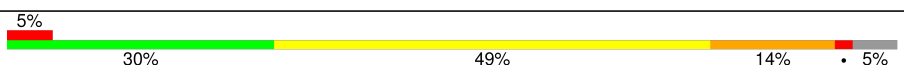
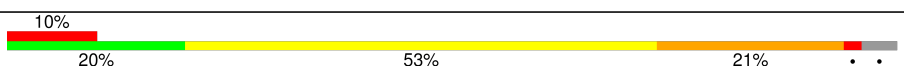
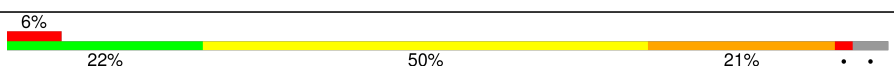
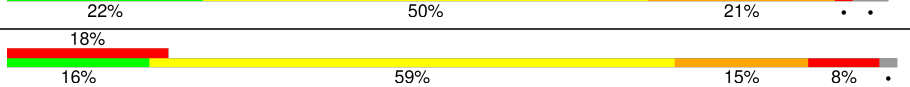
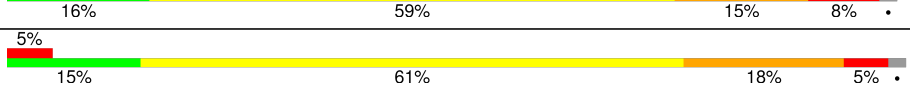
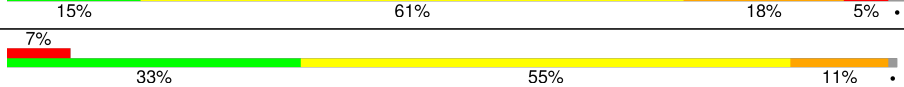
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | QC | 239 |   |
| 3 | XC | 239 |   |
| 4 | QD | 209 |   |
| 4 | XD | 209 |   |
| 5 | QE | 162 |   |
| 5 | XE | 162 |   |
| 6 | QF | 101 |   |
| 6 | XF | 101 |   |
| 7 | QG | 156 |   |
| 7 | XG | 156 |   |
| 8 | QH | 138 |   |
| 8 | XH | 138 |   |
| 9 | QI | 128 |   |
| 9 | XI | 128 |   |
| 10 | QJ | 105 |   |
| 10 | XJ | 105 |   |
| 11 | QK | 129 |   |
| 11 | XK | 129 |   |
| 12 | QL | 132 |   |
| 12 | XL | 132 |   |
| 13 | QM | 126 |   |
| 13 | XM | 126 |   |
| 14 | QN | 61 |   |
| 14 | XN | 61 |   |
| 15 | QO | 89 |   |

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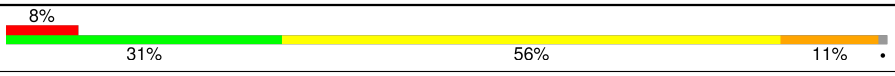
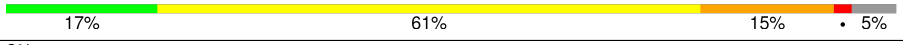
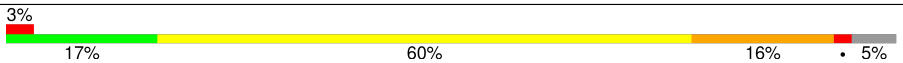
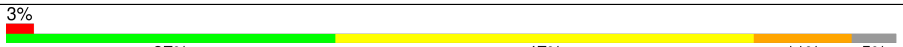
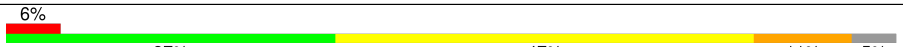
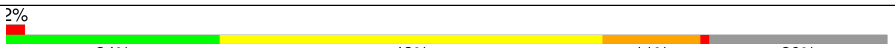
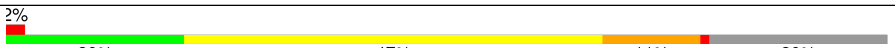
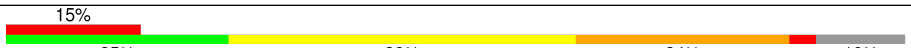
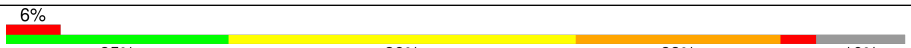
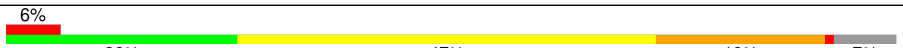
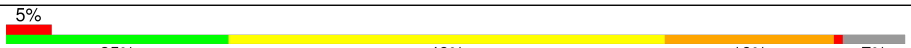
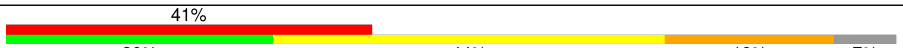
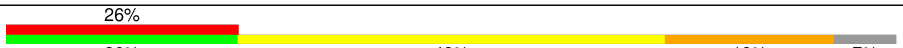
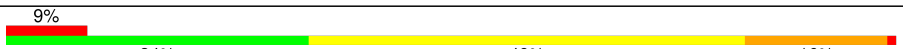
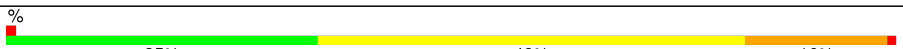
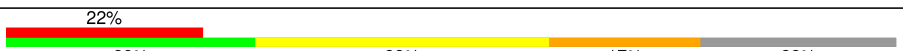
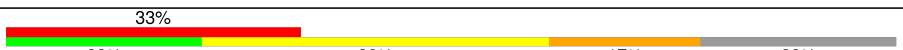
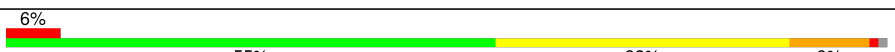
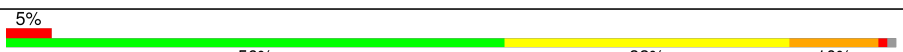
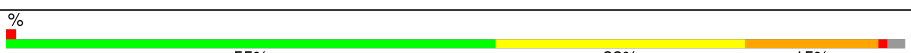
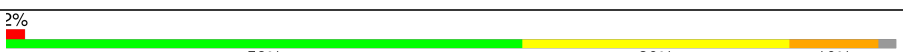
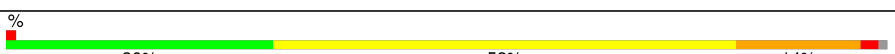
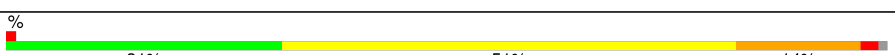
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | XO | 89 |   |
| 16 | QP | 88 |   |
| 16 | XP | 88 |   |
| 17 | QQ | 105 |   |
| 17 | XQ | 105 |   |
| 18 | QR | 88 |   |
| 18 | XR | 88 |   |
| 19 | QS | 93 |   |
| 19 | XS | 93 |   |
| 20 | QT | 106 |   |
| 20 | XT | 106 |   |
| 21 | QU | 27 |   |
| 21 | XU | 27 |   |
| 22 | QV | 77 |   |
| 22 | XV | 77 |   |
| 23 | QX | 25 | |
| 23 | XX | 25 | |
| 24 | QY | 18 |   |
| 24 | XY | 18 |   |
| 25 | RA | 2916 |   |
| 25 | YA | 2916 |   |
| 26 | RB | 122 |   |
| 26 | YB | 122 |   |
| 27 | RD | 276 |   |
| 27 | YD | 276 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | RE | 206 | 3% 22% 48% 24% 5% |
| 28 | YE | 206 | % 24% 47% 24% 5% |
| 29 | RF | 210 | % 35% 47% 13% |
| 29 | YF | 210 | 35% 48% 12% |
| 30 | RG | 182 | 40% 23% 58% 16% |
| 30 | YG | 182 | 8% 23% 58% 16% |
| 31 | RH | 180 | 27% 23% 44% 19% 8% 6% |
| 31 | YH | 180 | 5% 23% 44% 19% 8% 6% |
| 32 | RI | 148 | 13% 39% 43% 16% |
| 32 | YI | 148 | 5% 38% 43% 18% |
| 33 | RN | 140 | 5% 18% 54% 26% |
| 33 | YN | 140 | % 19% 54% 26% |
| 34 | RO | 122 | 36% 53% 9% |
| 34 | YO | 122 | 34% 55% 9% |
| 35 | RP | 150 | 8% 19% 51% 23% 8% |
| 35 | YP | 150 | 3% 19% 51% 23% 7% |
| 36 | RQ | 141 | 6% 32% 50% 16% |
| 36 | YQ | 141 | 4% 30% 51% 16% |
| 37 | RR | 118 | % 32% 49% 16% |
| 37 | YR | 118 | 35% 47% 16% |
| 38 | RS | 112 | 3% 13% 63% 19% 5% |
| 38 | YS | 112 | 3% 13% 62% 20% |
| 39 | RT | 146 | 9% 21% 51% 19% 6% |
| 39 | YT | 146 | 5% 21% 51% 19% 6% |
| 40 | RU | 118 | 3% 34% 52% 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | YU | 118 | 2% 32% 53% 13% |
| 41 | RV | 101 | 3% 27% 52% 21% |
| 41 | YV | 101 | 2% 27% 52% 21% |
| 42 | RW | 113 | 3% 28% 50% 19% |
| 42 | YW | 113 | % 29% 50% 19% |
| 43 | RX | 96 | 5% 40% 42% 15% |
| 43 | YX | 96 | 38% 44% 15% |
| 44 | RY | 110 | 19% 15% 45% 28% 7% |
| 44 | YY | 110 | 5% 19% 42% 28% 7% |
| 45 | RZ | 206 | 11% 44% 32% 12% 11% |
| 45 | YZ | 206 | 8% 46% 32% 10% 11% |
| 46 | R0 | 85 | % 67% 24% 6% |
| 46 | Y0 | 85 | 73% 19% 5% |
| 47 | R1 | 98 | 11% 30% 48% 18% |
| 47 | Y1 | 98 | 6% 29% 49% 18% |
| 48 | R2 | 72 | % 22% 54% 18% |
| 48 | Y2 | 72 | 4% 22% 54% 18% |
| 49 | R3 | 60 | 12% 33% 50% 15% |
| 49 | Y3 | 60 | 5% 33% 50% 13% |
| 50 | R4 | 71 | 39% 7% 42% 39% 11% |
| 50 | Y4 | 71 | 25% 7% 42% 39% 11% |
| 51 | R5 | 60 | 20% 23% 47% 22% 7% |
| 51 | Y5 | 60 | 13% 25% 45% 22% 7% |
| 52 | R6 | 54 | 43% 9% 44% 31% 6% 9% |
| 52 | Y6 | 54 | 44% 9% 44% 31% 6% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | R7 | 49 | 8% 35% 57% 8% |
| 53 | Y7 | 49 | 6% 37% 55% 8% |
| 54 | R8 | 65 | 9% 20% 46% 26% 6% |
| 54 | Y8 | 65 | 3% 22% 43% 28% 6% |
| 55 | R9 | 37 | 76% 51% 46% |
| 55 | Y9 | 37 | 51% 62% 32% 5% |
| 56 | Z6 | 3 | 33% 67% |
| 56 | Z8 | 3 | 33% 67% |

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 |
|---|---|---|---|---|---|---|---|
| 57 | MG | QA | 1604 | - | - | - | X |
| 57 | MG | QA | 1611 | - | - | - | X |
| 57 | MG | QA | 1613 | - | - | - | X |
| 57 | MG | QA | 1614 | - | - | - | X |
| 57 | MG | QA | 1615 | - | - | - | X |
| 57 | MG | QA | 1618 | - | - | - | X |
| 57 | MG | QA | 1620 | - | - | - | X |
| 57 | MG | QA | 1647 | - | - | - | X |
| 57 | MG | QA | 1650 | - | - | - | X |
| 57 | MG | QA | 1655 | - | - | - | X |
| 57 | MG | QA | 1658 | - | - | - | X |
| 57 | MG | QA | 1660 | - | - | - | X |
| 57 | MG | QV | 101 | - | - | - | X |
| 57 | MG | RA | 3002 | - | - | - | X |
| 57 | MG | RA | 3004 | - | - | - | X |
| 57 | MG | RA | 3005 | - | - | - | X |
| 57 | MG | RA | 3006 | - | - | - | X |
| 57 | MG | RA | 3008 | - | - | - | X |
| 57 | MG | RA | 3012 | - | - | - | X |
| 57 | MG | RA | 3015 | - | - | - | X |
| 57 | MG | RA | 3019 | - | - | - | X |
| 57 | MG | RA | 3020 | - | - | - | X |
| 57 | MG | RA | 3021 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3022 | - | - | - | X |
| 57 | MG | RA | 3026 | - | - | - | X |
| 57 | MG | RA | 3031 | - | - | - | X |
| 57 | MG | RA | 3033 | - | - | - | X |
| 57 | MG | RA | 3034 | - | - | - | X |
| 57 | MG | RA | 3035 | - | - | - | X |
| 57 | MG | RA | 3036 | - | - | - | X |
| 57 | MG | RA | 3038 | - | - | - | X |
| 57 | MG | RA | 3040 | - | - | - | X |
| 57 | MG | RA | 3042 | - | - | - | X |
| 57 | MG | RA | 3049 | - | - | - | X |
| 57 | MG | RA | 3050 | - | - | - | X |
| 57 | MG | RA | 3052 | - | - | - | X |
| 57 | MG | RA | 3056 | - | - | - | X |
| 57 | MG | RA | 3058 | - | - | - | X |
| 57 | MG | RA | 3059 | - | - | - | X |
| 57 | MG | RA | 3062 | - | - | - | X |
| 57 | MG | RA | 3063 | - | - | - | X |
| 57 | MG | RA | 3064 | - | - | - | X |
| 57 | MG | RA | 3065 | - | - | - | X |
| 57 | MG | RA | 3068 | - | - | - | X |
| 57 | MG | RA | 3077 | - | - | - | X |
| 57 | MG | RA | 3079 | - | - | - | X |
| 57 | MG | RA | 3081 | - | - | - | X |
| 57 | MG | RA | 3085 | - | - | - | X |
| 57 | MG | RA | 3086 | - | - | - | X |
| 57 | MG | RA | 3087 | - | - | - | X |
| 57 | MG | RA | 3088 | - | - | - | X |
| 57 | MG | RA | 3094 | - | - | - | X |
| 57 | MG | RA | 3095 | - | - | - | X |
| 57 | MG | RA | 3097 | - | - | - | X |
| 57 | MG | RA | 3098 | - | - | - | X |
| 57 | MG | RA | 3105 | - | - | - | X |
| 57 | MG | RA | 3106 | - | - | - | X |
| 57 | MG | RA | 3107 | - | - | - | X |
| 57 | MG | RA | 3119 | - | - | - | X |
| 57 | MG | RA | 3120 | - | - | - | X |
| 57 | MG | RA | 3121 | - | - | - | X |
| 57 | MG | RA | 3123 | - | - | - | X |
| 57 | MG | RA | 3124 | - | - | - | X |
| 57 | MG | RA | 3130 | - | - | - | X |
| 57 | MG | RA | 3131 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3136 | - | - | - | X |
| 57 | MG | RA | 3141 | - | - | - | X |
| 57 | MG | RA | 3143 | - | - | - | X |
| 57 | MG | RA | 3149 | - | - | - | X |
| 57 | MG | RA | 3153 | - | - | - | X |
| 57 | MG | RA | 3161 | - | - | - | X |
| 57 | MG | RA | 3170 | - | - | - | X |
| 57 | MG | RA | 3174 | - | - | - | X |
| 57 | MG | RA | 3175 | - | - | - | X |
| 57 | MG | RA | 3188 | - | - | - | X |
| 57 | MG | RA | 3191 | - | - | - | X |
| 57 | MG | RA | 3197 | - | - | - | X |
| 57 | MG | RA | 3199 | - | - | - | X |
| 57 | MG | RA | 3205 | - | - | - | X |
| 57 | MG | RA | 3210 | - | - | - | X |
| 57 | MG | RA | 3212 | - | - | - | X |
| 57 | MG | RA | 3214 | - | - | - | X |
| 57 | MG | RA | 3220 | - | - | - | X |
| 57 | MG | RA | 3221 | - | - | - | X |
| 57 | MG | RA | 3222 | - | - | - | X |
| 57 | MG | RA | 3227 | - | - | - | X |
| 57 | MG | RA | 3239 | - | - | - | X |
| 57 | MG | RA | 3240 | - | - | - | X |
| 57 | MG | RP | 201 | - | - | - | X |
| 57 | MG | XA | 1603 | - | - | - | X |
| 57 | MG | XA | 1604 | - | - | - | X |
| 57 | MG | XA | 1610 | - | - | - | X |
| 57 | MG | XA | 1615 | - | - | - | X |
| 57 | MG | XA | 1618 | - | - | - | X |
| 57 | MG | XA | 1619 | - | - | - | X |
| 57 | MG | XA | 1620 | - | - | - | X |
| 57 | MG | XA | 1621 | - | - | - | X |
| 57 | MG | XA | 1626 | - | - | - | X |
| 57 | MG | XA | 1628 | - | - | - | X |
| 57 | MG | XA | 1634 | - | - | - | X |
| 57 | MG | XA | 1635 | - | - | - | X |
| 57 | MG | XA | 1636 | - | - | - | X |
| 57 | MG | XA | 1637 | - | - | - | X |
| 57 | MG | XA | 1638 | - | - | - | X |
| 57 | MG | XA | 1651 | - | - | - | X |
| 57 | MG | XA | 1656 | - | - | - | X |
| 57 | MG | XA | 1659 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 57 | MG | XV | 101 | - | - | - | X |
| 57 | MG | Y7 | 101 | - | - | - | X |
| 57 | MG | YA | 3002 | - | - | - | X |
| 57 | MG | YA | 3004 | - | - | - | X |
| 57 | MG | YA | 3006 | - | - | - | X |
| 57 | MG | YA | 3008 | - | - | - | X |
| 57 | MG | YA | 3009 | - | - | - | X |
| 57 | MG | YA | 3011 | - | - | - | X |
| 57 | MG | YA | 3013 | - | - | - | X |
| 57 | MG | YA | 3014 | - | - | - | X |
| 57 | MG | YA | 3015 | - | - | - | X |
| 57 | MG | YA | 3016 | - | - | - | X |
| 57 | MG | YA | 3017 | - | - | - | X |
| 57 | MG | YA | 3023 | - | - | - | X |
| 57 | MG | YA | 3024 | - | - | - | X |
| 57 | MG | YA | 3026 | - | - | - | X |
| 57 | MG | YA | 3031 | - | - | - | X |
| 57 | MG | YA | 3032 | - | - | - | X |
| 57 | MG | YA | 3033 | - | - | - | X |
| 57 | MG | YA | 3034 | - | - | - | X |
| 57 | MG | YA | 3037 | - | - | - | X |
| 57 | MG | YA | 3041 | - | - | - | X |
| 57 | MG | YA | 3042 | - | - | - | X |
| 57 | MG | YA | 3044 | - | - | - | X |
| 57 | MG | YA | 3047 | - | - | - | X |
| 57 | MG | YA | 3048 | - | - | - | X |
| 57 | MG | YA | 3049 | - | - | - | X |
| 57 | MG | YA | 3050 | - | - | - | X |
| 57 | MG | YA | 3059 | - | - | - | X |
| 57 | MG | YA | 3060 | - | - | - | X |
| 57 | MG | YA | 3069 | - | - | - | X |
| 57 | MG | YA | 3072 | - | - | - | X |
| 57 | MG | YA | 3074 | - | - | - | X |
| 57 | MG | YA | 3080 | - | - | - | X |
| 57 | MG | YA | 3081 | - | - | - | X |
| 57 | MG | YA | 3083 | - | - | - | X |
| 57 | MG | YA | 3088 | - | - | - | X |
| 57 | MG | YA | 3091 | - | - | - | X |
| 57 | MG | YA | 3092 | - | - | - | X |
| 57 | MG | YA | 3096 | - | - | - | X |
| 57 | MG | YA | 3100 | - | - | - | X |
| 57 | MG | YA | 3101 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 57 | MG | YA | 3102 | - | - | - | X |
| 57 | MG | YA | 3105 | - | - | - | X |
| 57 | MG | YA | 3106 | - | - | - | X |
| 57 | MG | YA | 3109 | - | - | - | X |
| 57 | MG | YA | 3110 | - | - | - | X |
| 57 | MG | YA | 3115 | - | - | - | X |
| 57 | MG | YA | 3117 | - | - | - | X |
| 57 | MG | YA | 3118 | - | - | - | X |
| 57 | MG | YA | 3120 | - | - | - | X |
| 57 | MG | YA | 3126 | - | - | - | X |
| 57 | MG | YA | 3138 | - | - | - | X |
| 57 | MG | YA | 3141 | - | - | - | X |
| 57 | MG | YA | 3143 | - | - | - | X |
| 57 | MG | YA | 3145 | - | - | - | X |
| 57 | MG | YA | 3161 | - | - | - | X |
| 57 | MG | YA | 3169 | - | - | - | X |
| 57 | MG | YA | 3173 | - | - | - | X |
| 57 | MG | YA | 3177 | - | - | - | X |
| 57 | MG | YA | 3178 | - | - | - | X |
| 57 | MG | YA | 3182 | - | - | - | X |
| 57 | MG | YA | 3185 | - | - | - | X |
| 57 | MG | YA | 3186 | - | - | - | X |
| 57 | MG | YA | 3200 | - | - | - | X |
| 57 | MG | YA | 3203 | - | - | - | X |
| 57 | MG | YA | 3207 | - | - | - | X |
| 57 | MG | YA | 3210 | - | - | - | X |
| 57 | MG | YA | 3211 | - | - | - | X |
| 57 | MG | YA | 3217 | - | - | - | X |
| 57 | MG | YA | 3221 | - | - | - | X |
| 57 | MG | YA | 3230 | - | - | - | X |
| 57 | MG | YA | 3237 | - | - | - | X |
| 57 | MG | YA | 3245 | - | - | - | X |
| 57 | MG | YA | 3255 | - | - | - | X |
| 57 | MG | YA | 3256 | - | - | - | X |
| 57 | MG | YA | 3259 | - | - | - | X |
| 57 | MG | YA | 3262 | - | - | - | X |
| 57 | MG | YA | 3265 | - | - | - | X |
| 57 | MG | YA | 3266 | - | - | - | X |
| 57 | MG | YE | 302 | - | - | - | X |
| 58 | PAR | QA | 1667 | - | - | - | X |

# 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291957 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 rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | QA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32247 | 14353 | 5981 | 10414 | 1499 | | | |
| 1 | XA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32249 | 14354 | 5984 | 10412 | 1499 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | QB | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |
| 2 | XB | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | QC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | XC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | QD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |
| 4 | XD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | QE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 5 | XE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | QF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |
| 6 | XF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | QG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |
| 7 | XG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | QH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |
| 8 | XH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | QI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |
| 9 | XI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | QJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | XJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | QK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |
| 11 | XK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | QL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |
| 12 | XL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | QM | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 597 | 199 | 166 | 2 | | | |
| 13 | XM | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 597 | 199 | 166 | 2 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | QN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 14 | XN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | QO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | XO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | QP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |
| 16 | XP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | QQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | XQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | QR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |
| 18 | XR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | QS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |
| 19 | XS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | QT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |
| 20 | XT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | QU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | XU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called P-site tRNA fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | QV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |
| 22 | XV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |

- Molecule 23 is a RNA chain called A-site ASL SufA6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | QX | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 167 | 75 | 28 | 56 | 8 | | | |
| 23 | XX | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 167 | 75 | 28 | 56 | 8 | | | |

- Molecule 24 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | QY | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 303 | 135 | 55 | 99 | 14 | | | |
| 24 | XY | 14 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 303 | 135 | 55 | 99 | 14 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | RA | 2882 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62071 | 27627 | 11611 | 19952 | 2881 | | | |
| 25 | YA | 2883 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62091 | 27636 | 11613 | 19960 | 2882 | | | |

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

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

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | YB | 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 | RD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |
| 27 | YD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | RE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |
| 28 | YE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | RF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |
| 29 | YF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | RG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 30 | YG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | RH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |
| 31 | YH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | RI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |
| 32 | YI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | RN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 33 | YN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | RO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 34 | YO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | RP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |
| 35 | YP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | RQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 36 | YQ | 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 | RR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 37 | YR | 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 | RS | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |
| 38 | YS | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | RT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 39 | YT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | RU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |
| 40 | YU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | RV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 41 | YV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | RW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | YW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | RX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |
| 43 | YX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | RY | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |
| 44 | YY | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 45 | RZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |
| 45 | YZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 46 | R0 | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 401 | 138 | 108 | 1 | | | |
| 46 | Y0 | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 401 | 138 | 108 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | R1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |
| 47 | Y1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | R2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |
| 48 | Y2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | R3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 49 | Y3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

- Molecule 50 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | R4 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 364 | 108 | 104 | 5 | | | |
| 50 | Y4 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 364 | 108 | 104 | 5 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | R5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 51 | Y5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | R6 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 424 | 264 | 87 | 69 | 4 | | | |
| 52 | Y6 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 424 | 264 | 87 | 69 | 4 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 53 | R7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |
| 53 | Y7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 54 | R8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 54 | Y8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 55 | R9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 55 | Y9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 56 | Z6 | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 74 | 40 | 13 | 19 | 2 | | | |
| 56 | Z8 | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 74 | 40 | 13 | 19 | 2 | | | |

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 57 | QA | 66 | Total | Mg | 0 | 0 |
| | | | 66 | 66 | | |
| 57 | RP | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | YA | 269 | Total | Mg | 0 | 0 |
| | | | 269 | 269 | | |
| 57 | QM | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | YD | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | XX | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | QV | 2 | Total Mg<br>2 2 | 0 | 0 |
| 57 | XA | 72 | Total Mg<br>72 72 | 0 | 0 |
| 57 | R0 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | XT | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | RU | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | QH | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | R8 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | YX | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | RR | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | RD | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | Y7 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | QF | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | R5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | RA | 241 | Total Mg<br>241 241 | 0 | 0 |
| 57 | Y5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | RE | 2 | Total Mg<br>2 2 | 0 | 0 |
| 57 | YB | 3 | Total Mg<br>3 3 | 0 | 0 |
| 57 | XV | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | RB | 2 | Total Mg<br>2 2 | 0 | 0 |
| 57 | RF | 1 | Total Mg<br>1 1 | 0 | 0 |

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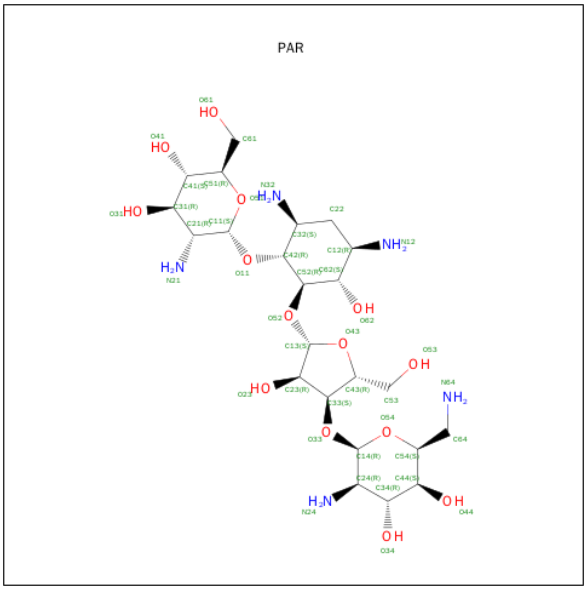
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | XM | 1 | Total Mg<br>1 1 | 0 | 0 |
| 57 | YE | 2 | Total Mg<br>2 2 | 0 | 0 |

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 58 | QA | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 58 | XA | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | Y9 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | QN | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | XN | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | QD | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | XD | 1 | Total Zn<br>1 1 | 0 | 0 |

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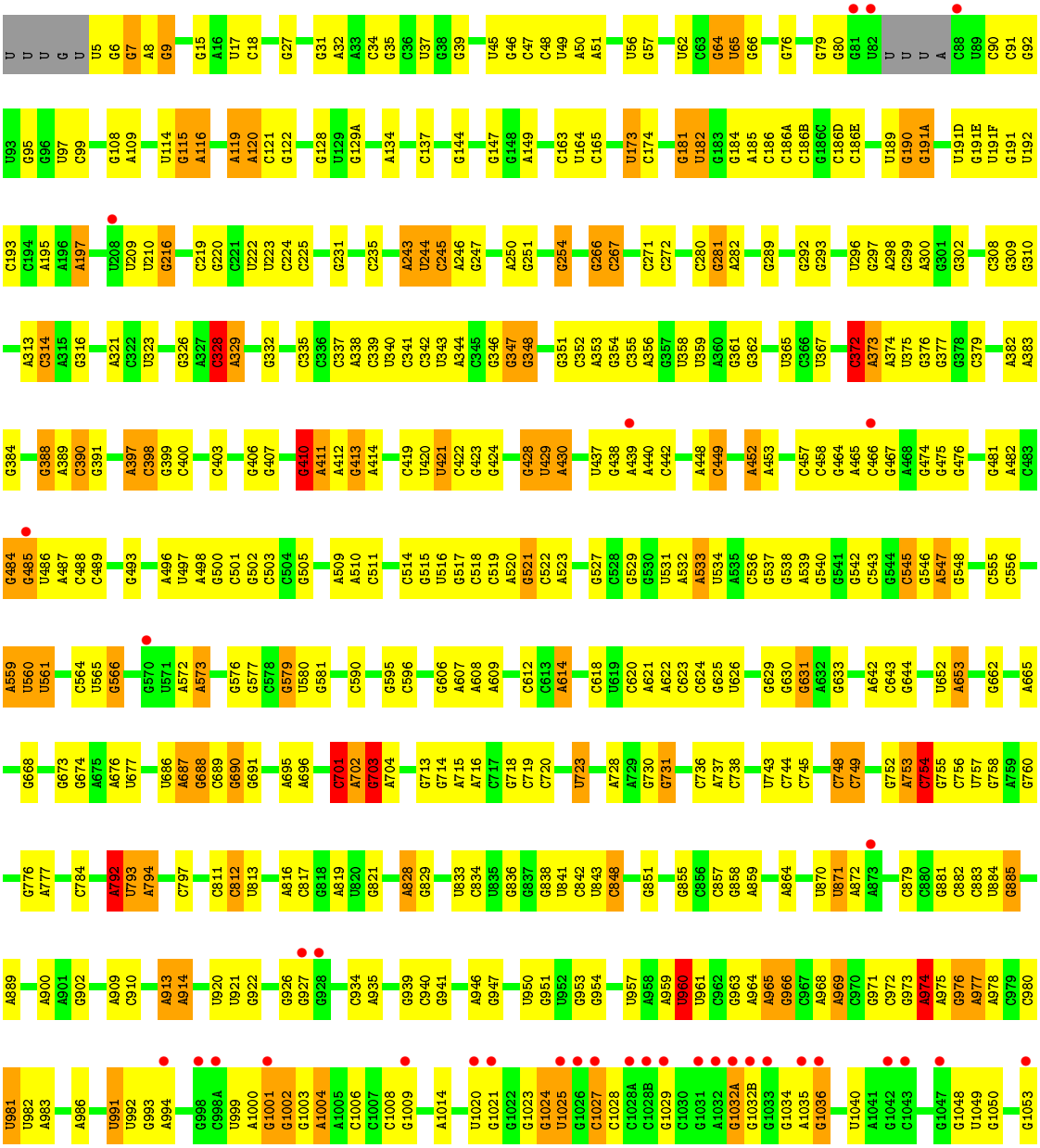
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Zn | | |
| 59 | R9 | 1 | 1 | 1 | 0 | 0 |

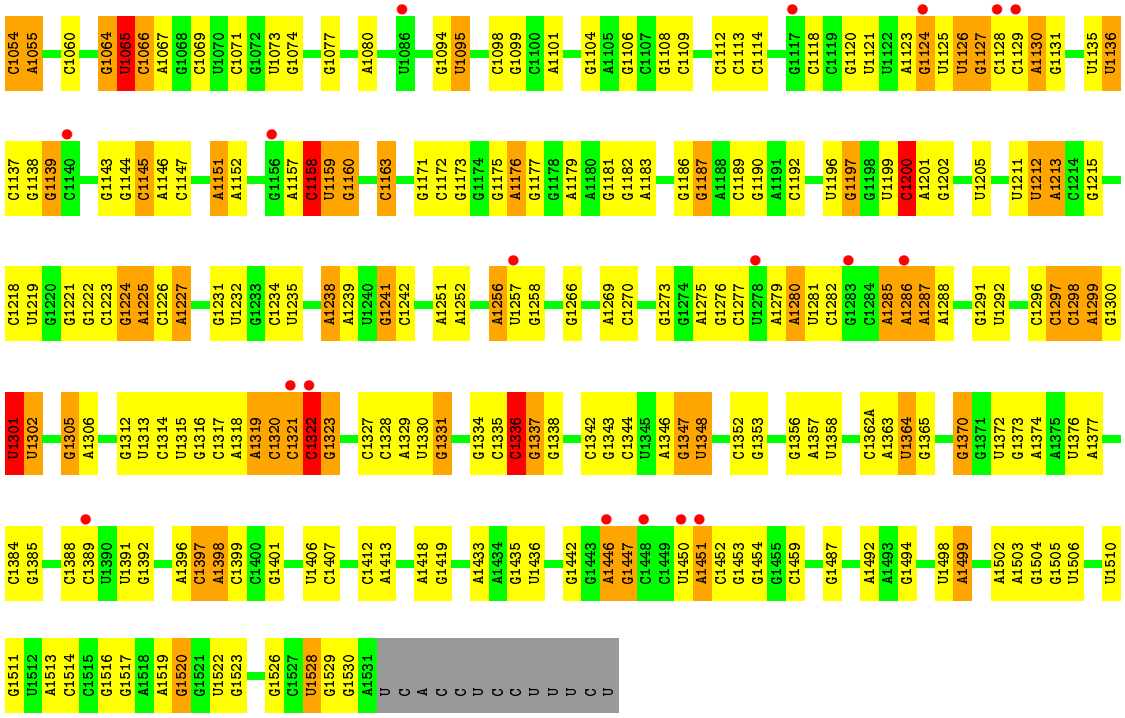
# 3 Residue-property plots (i)

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 rRNA

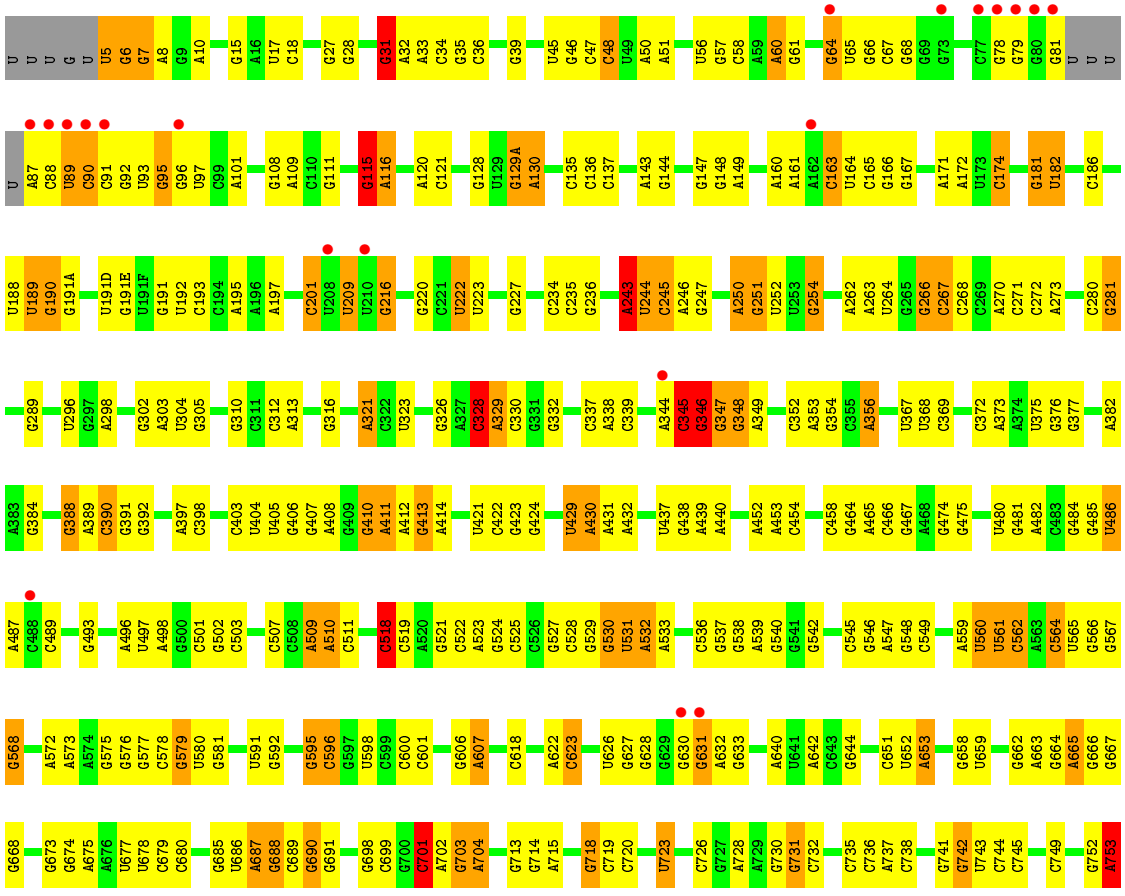
Chain QA:

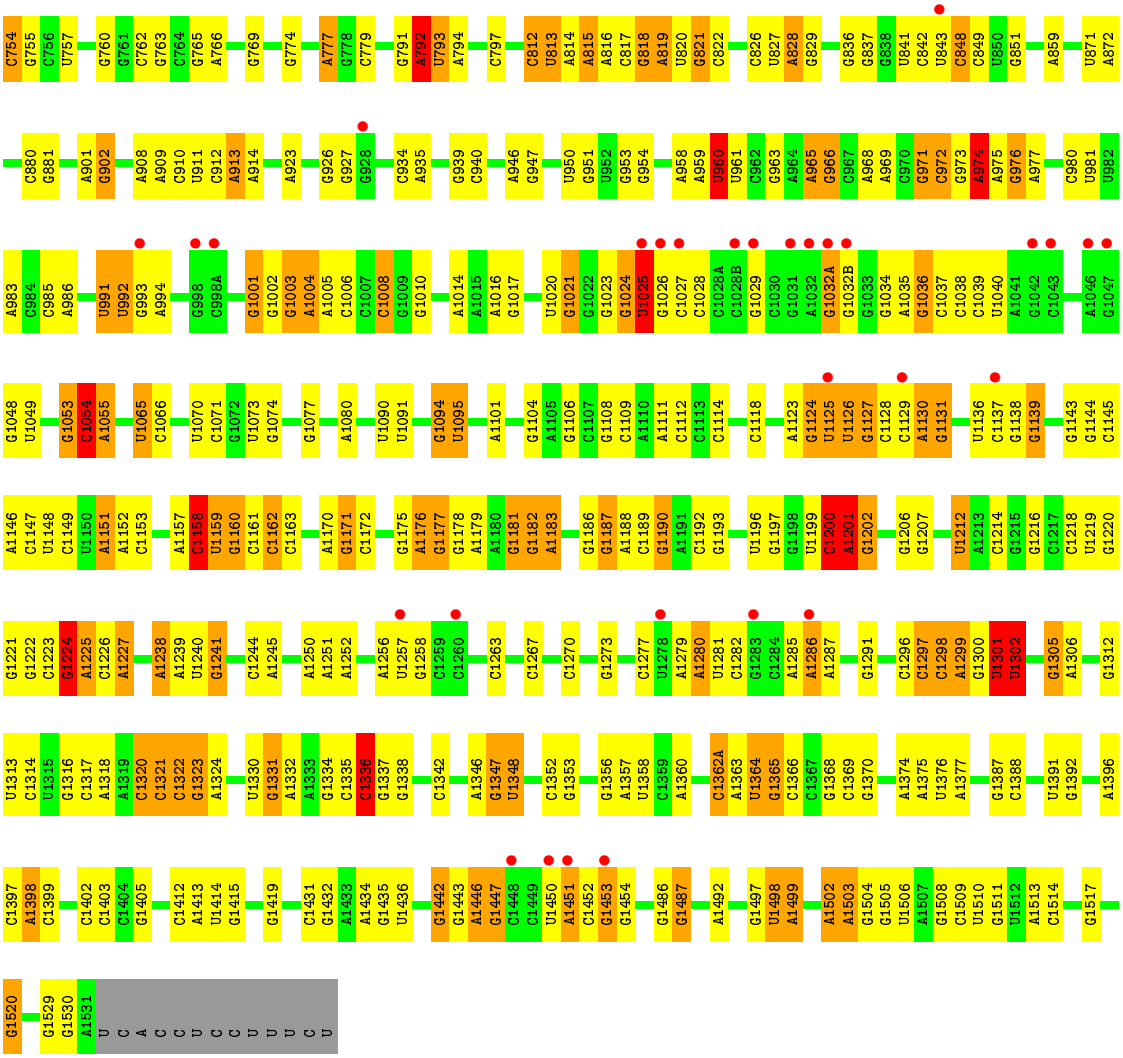





• Molecule 1: 16S rRNA

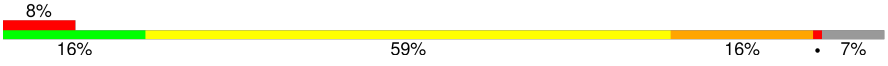
Chain XA:

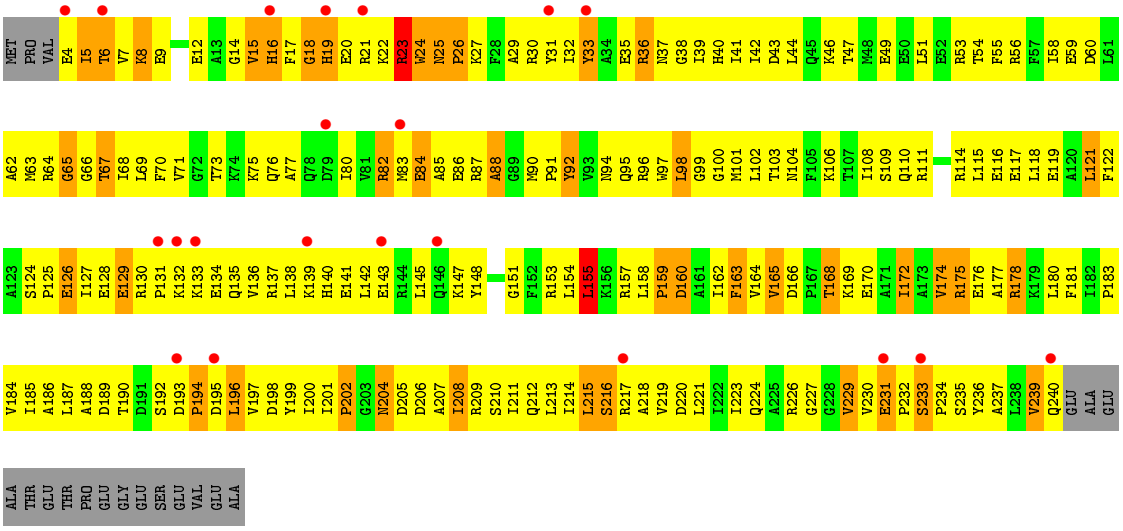




• Molecule 2: 30S ribosomal protein S2

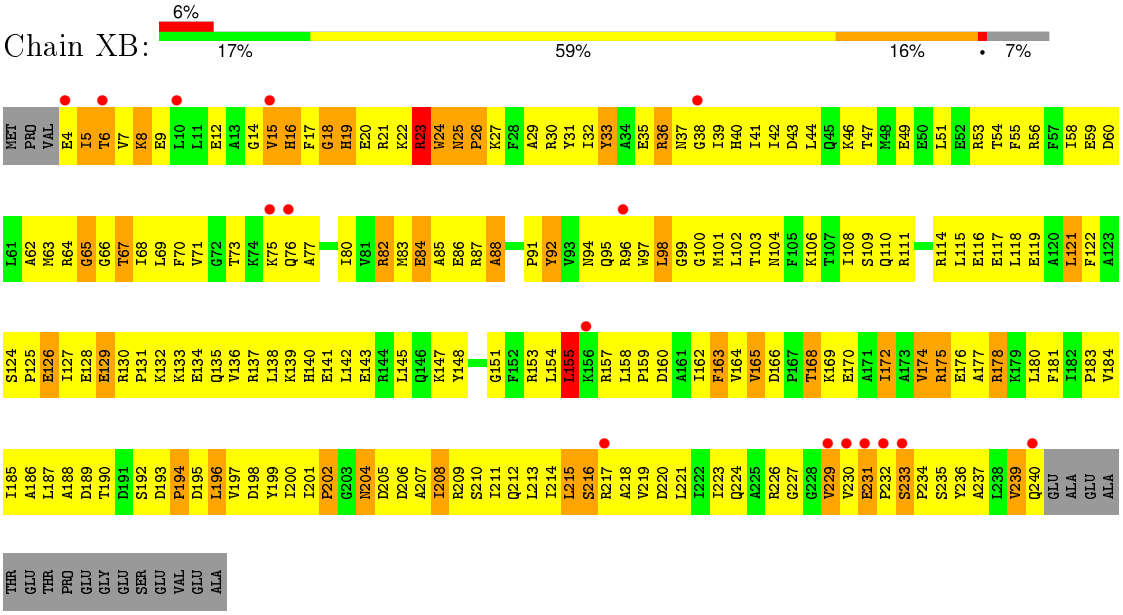
Chain QB:



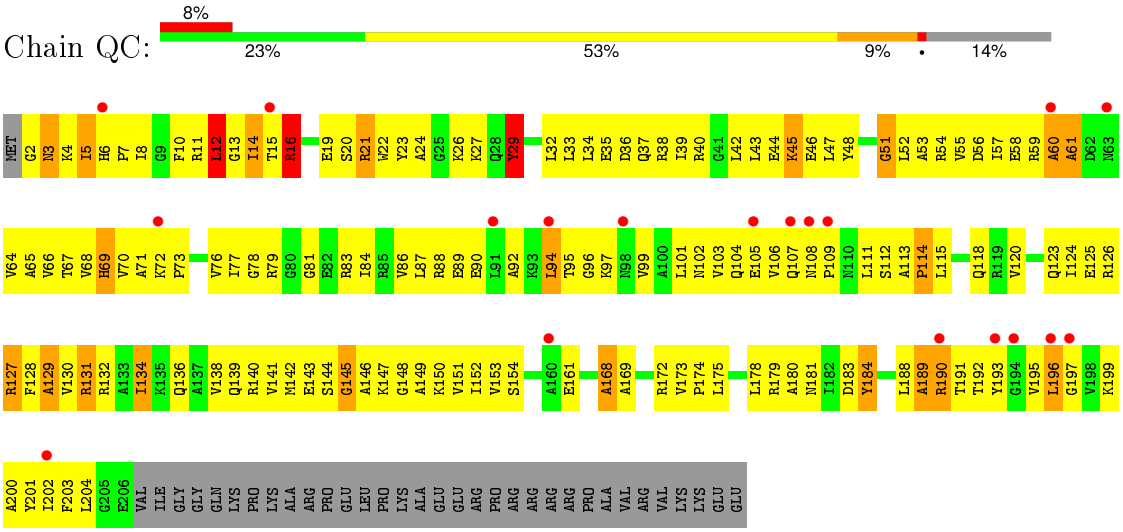
• Molecule 2: 30S ribosomal protein S2

Chain XB:



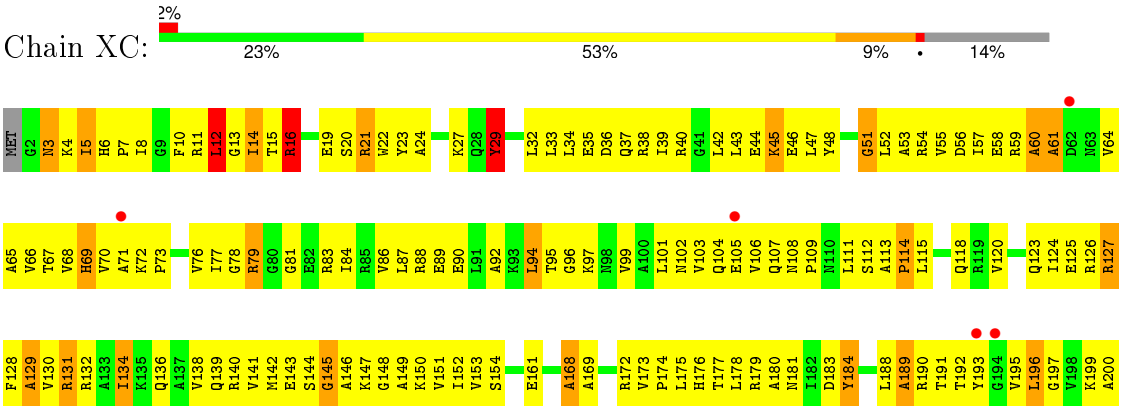

• Molecule 3: 30S ribosomal protein S3

Chain QC:



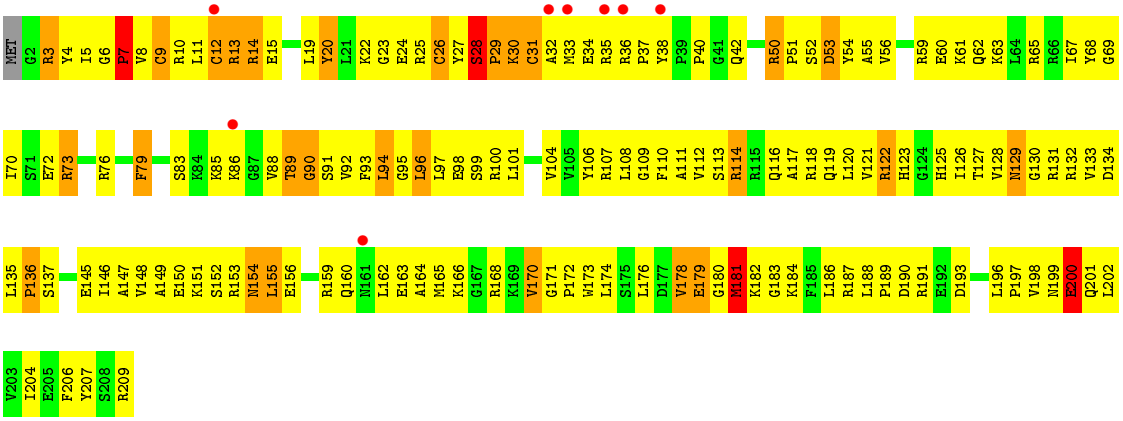

• Molecule 3: 30S ribosomal protein S3

Chain XC:



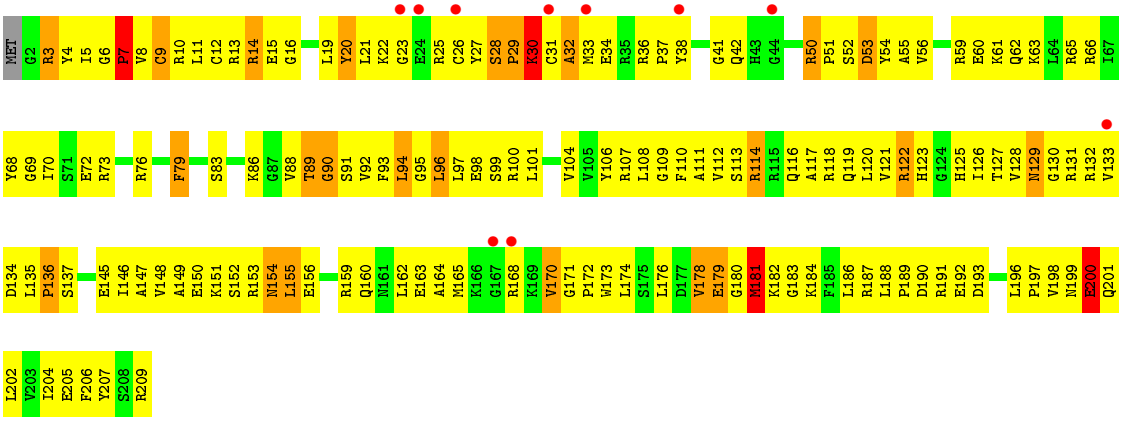
• Molecule 4: 30S ribosomal protein S4

Chain QD:



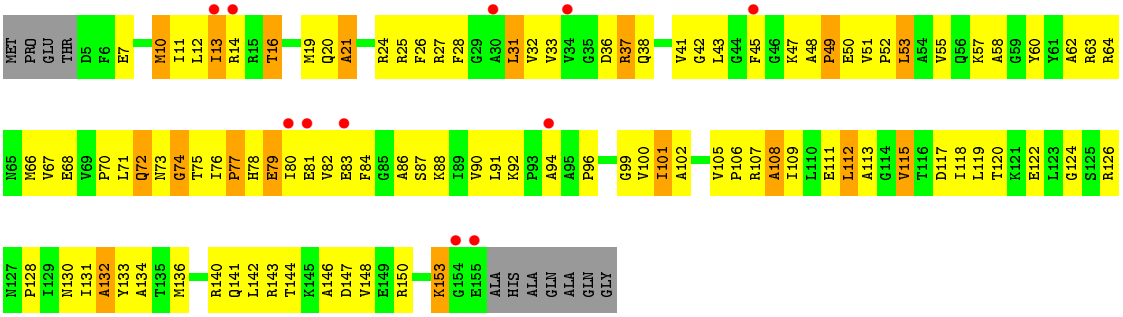

• Molecule 4: 30S ribosomal protein S4

Chain XD:



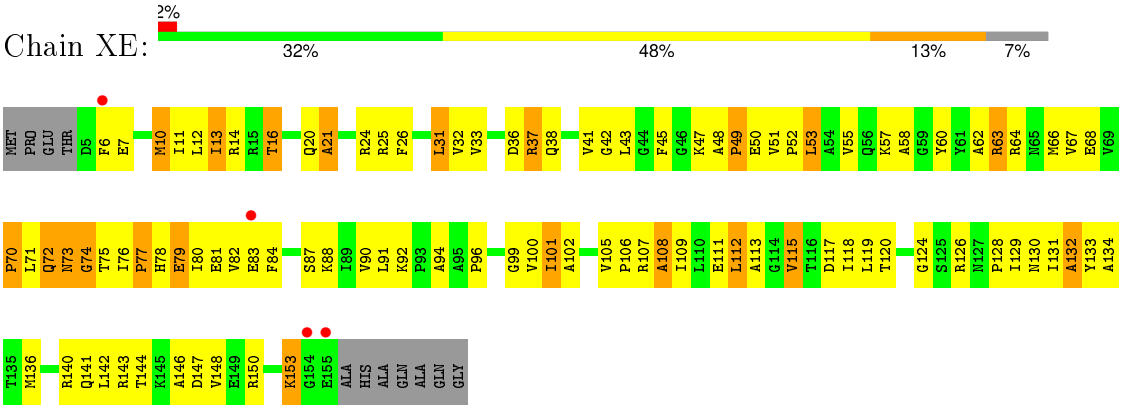

• Molecule 5: 30S ribosomal protein S5

Chain QE:



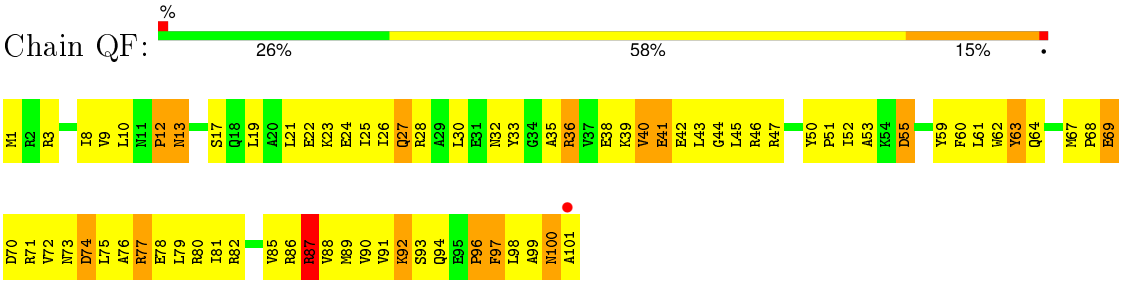
• Molecule 5: 30S ribosomal protein S5

Chain XE:



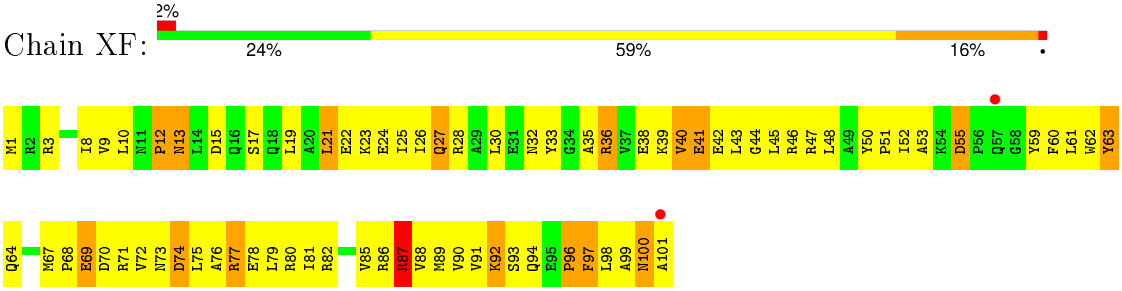

• Molecule 6: 30S ribosomal protein S6

Chain QF:



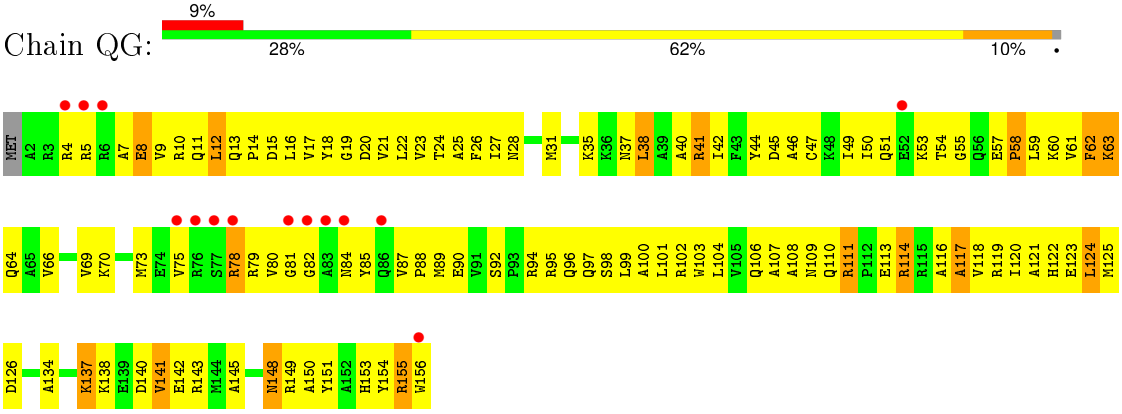

• Molecule 6: 30S ribosomal protein S6

Chain XF:

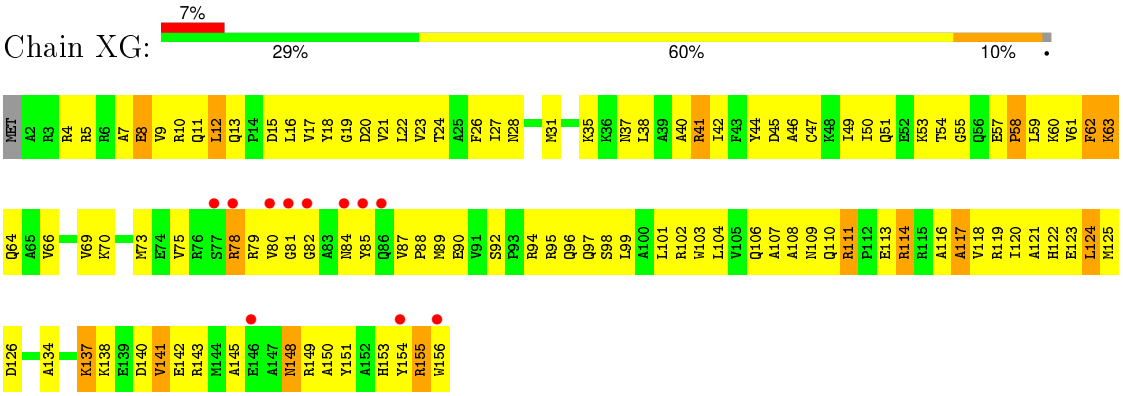



• Molecule 7: 30S ribosomal protein S7

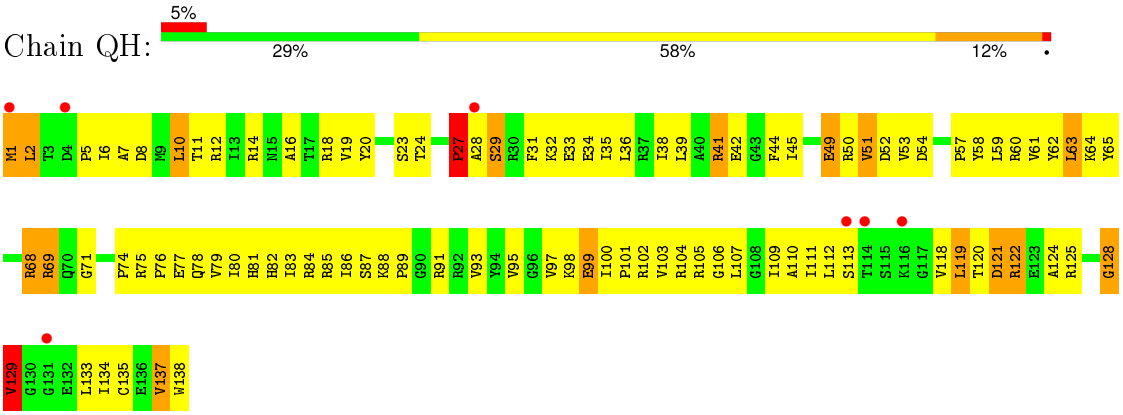
Chain QG:



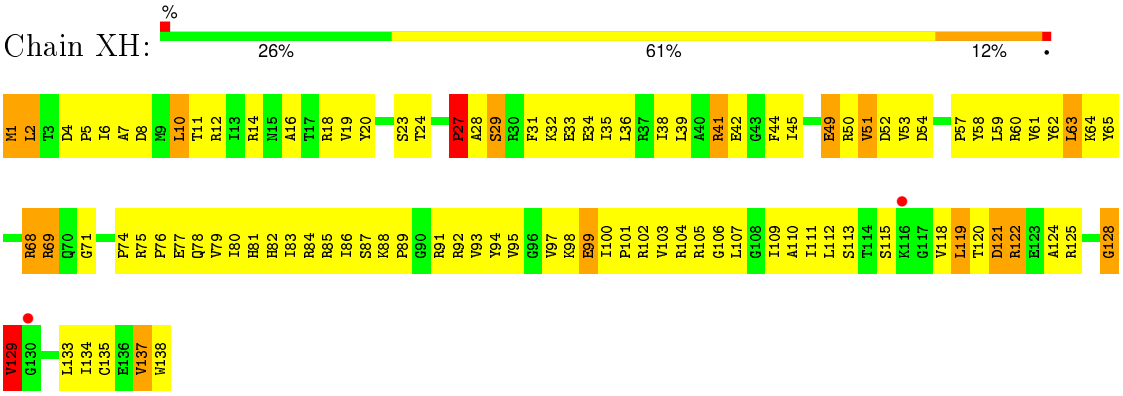

• Molecule 7: 30S ribosomal protein S7



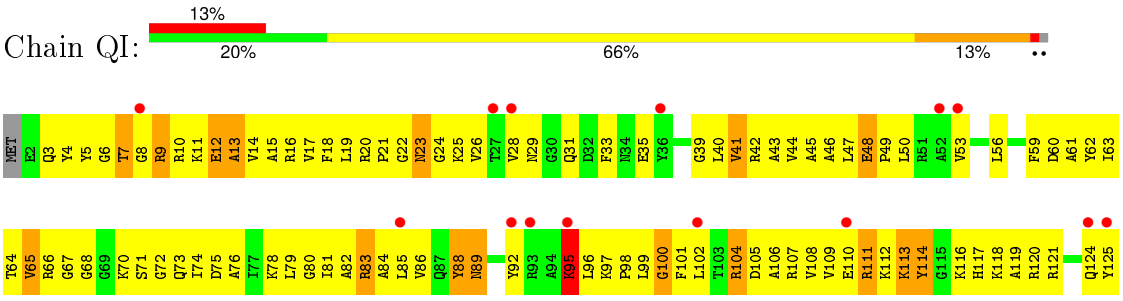

- Molecule 8: 30S ribosomal protein S8




- Molecule 8: 30S ribosomal protein S8

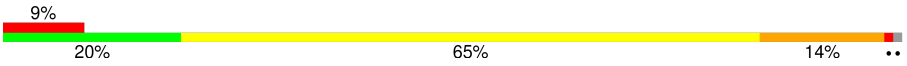


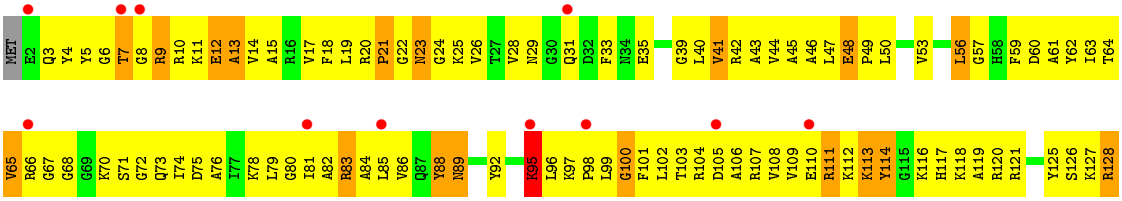

- Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

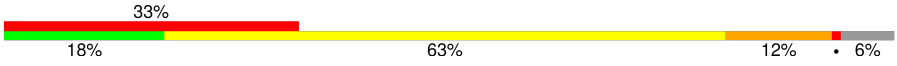
Chain XI:

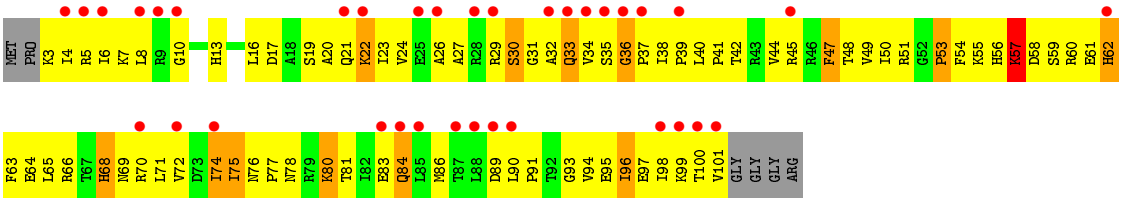


• Molecule 10: 30S ribosomal protein S10

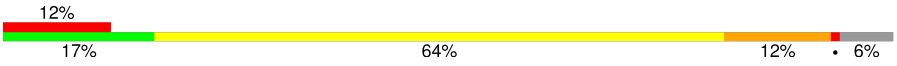
Chain QJ:

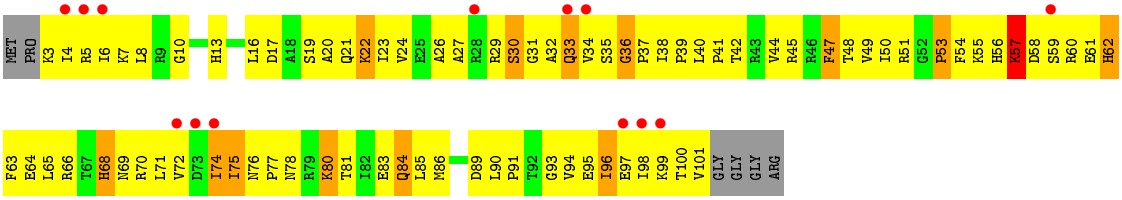


• Molecule 10: 30S ribosomal protein S10

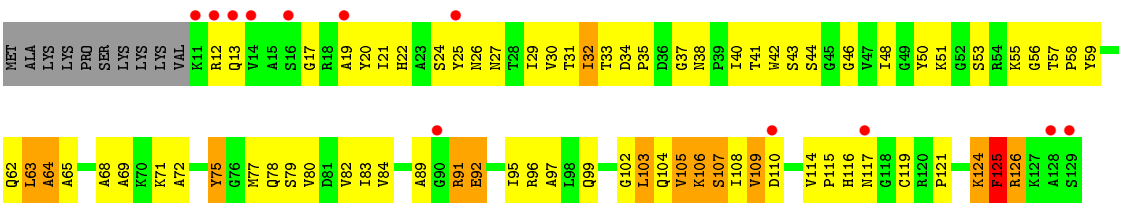
Chain XJ:



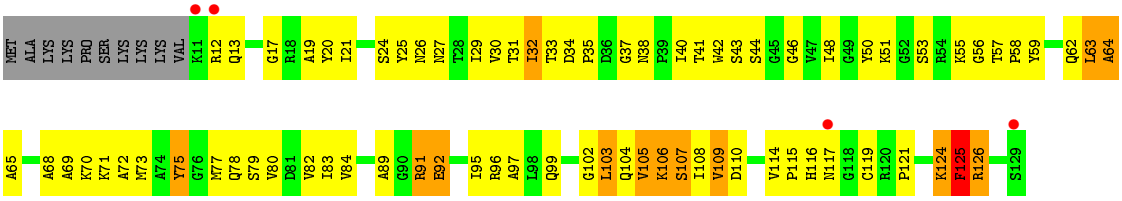
• Molecule 11: 30S ribosomal protein S11

Chain QK:



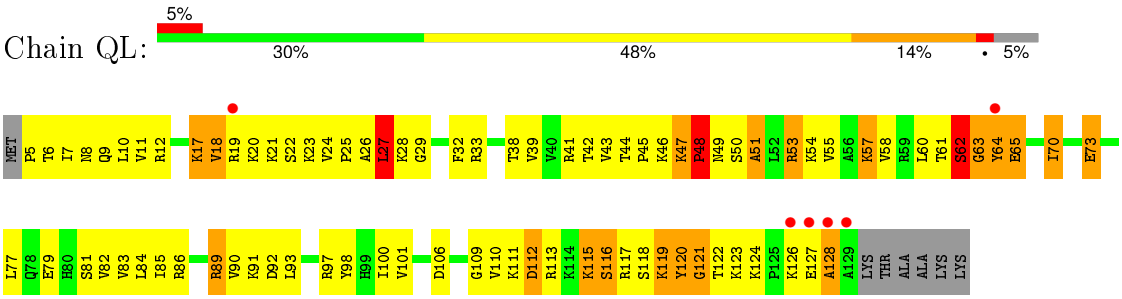
• Molecule 11: 30S ribosomal protein S11

Chain XK:



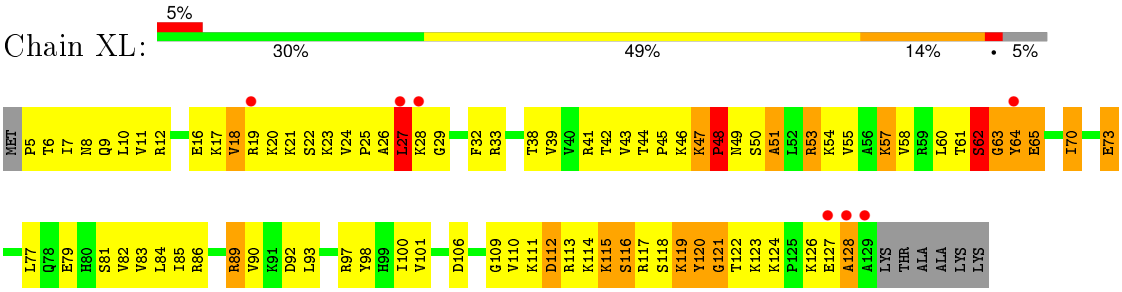
• Molecule 12: 30S ribosomal protein S12

Chain QL:



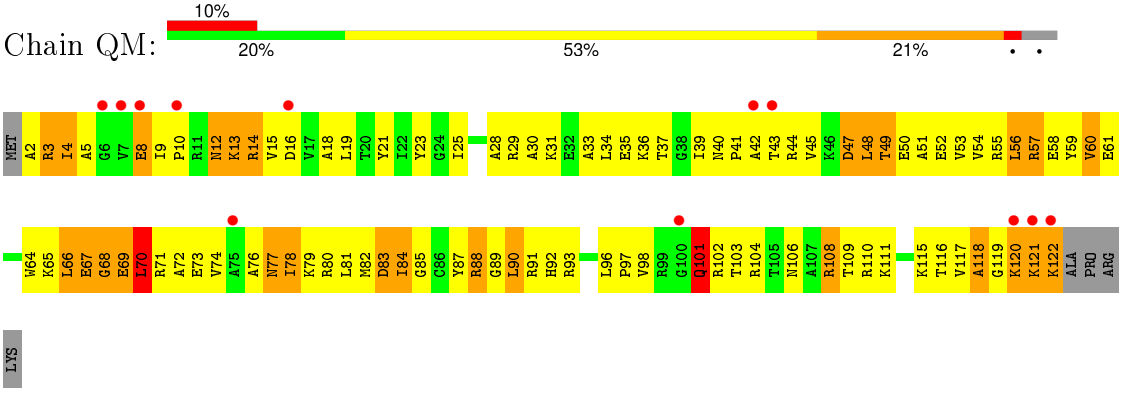
• Molecule 12: 30S ribosomal protein S12

Chain XL:



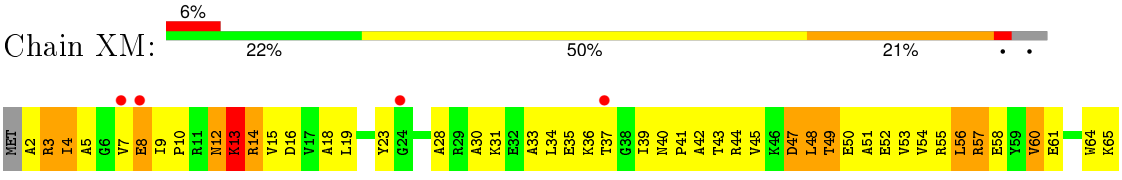
• Molecule 13: 30S ribosomal protein S13

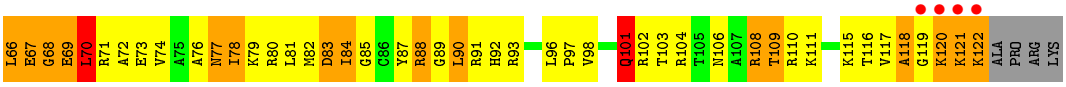
Chain QM:



• Molecule 13: 30S ribosomal protein S13

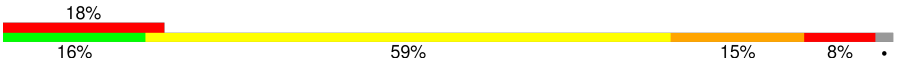
Chain XM:

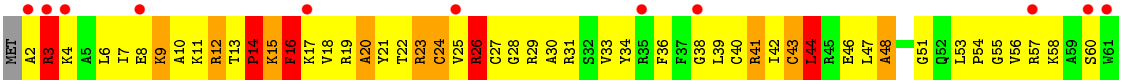





• Molecule 14: 30S ribosomal protein S14

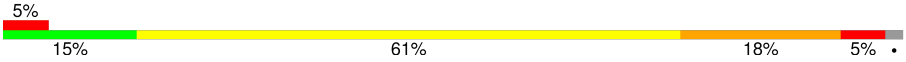
Chain QN:

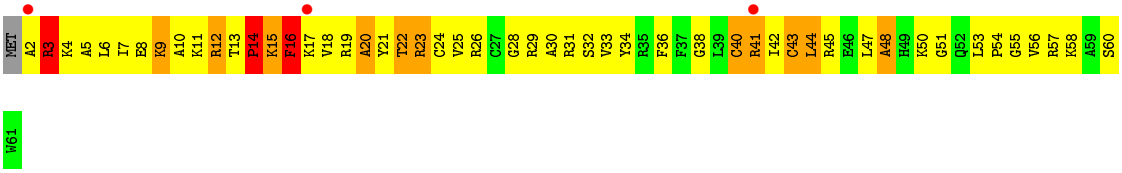



• Molecule 14: 30S ribosomal protein S14

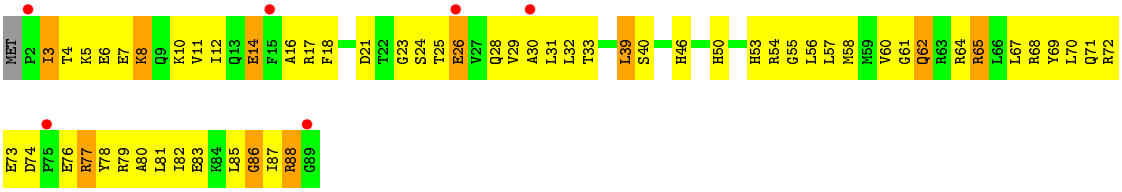
Chain XN:



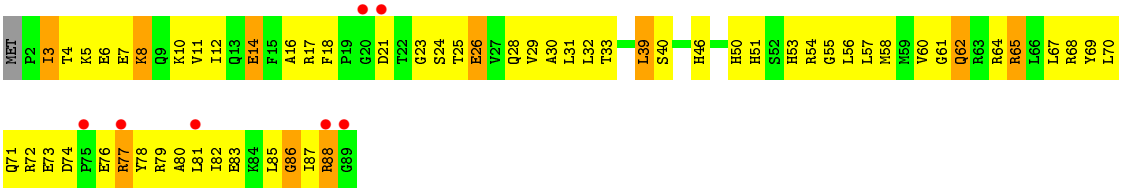

• Molecule 15: 30S ribosomal protein S15

Chain QO:



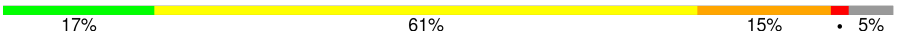

• Molecule 15: 30S ribosomal protein S15

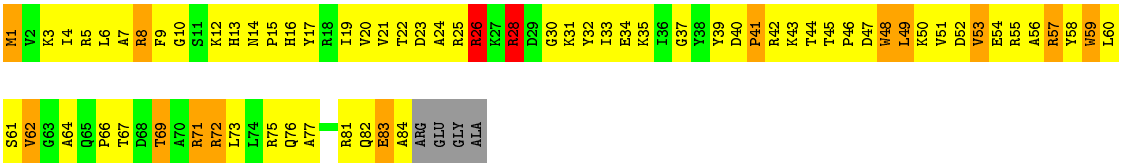
Chain XO:




• Molecule 16: 30S ribosomal protein S16

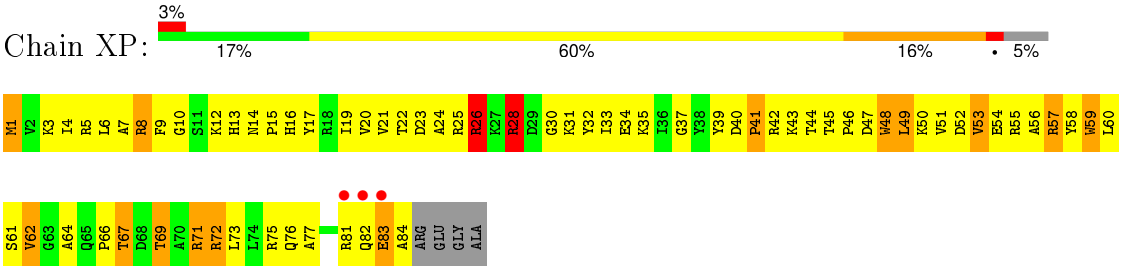
Chain QP:



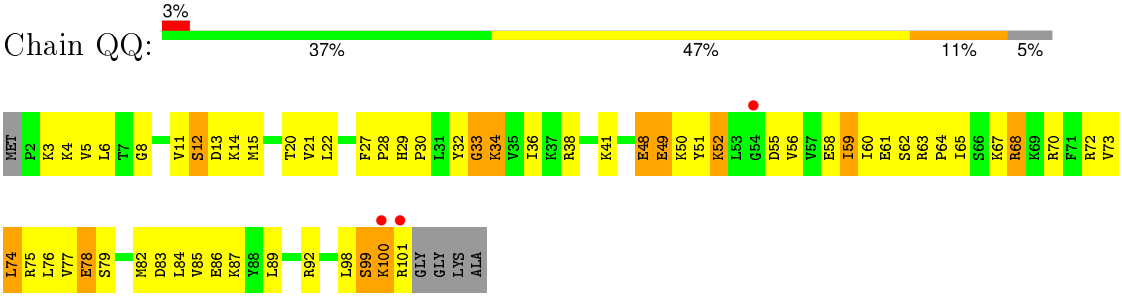
• Molecule 16: 30S ribosomal protein S16

Chain XP:



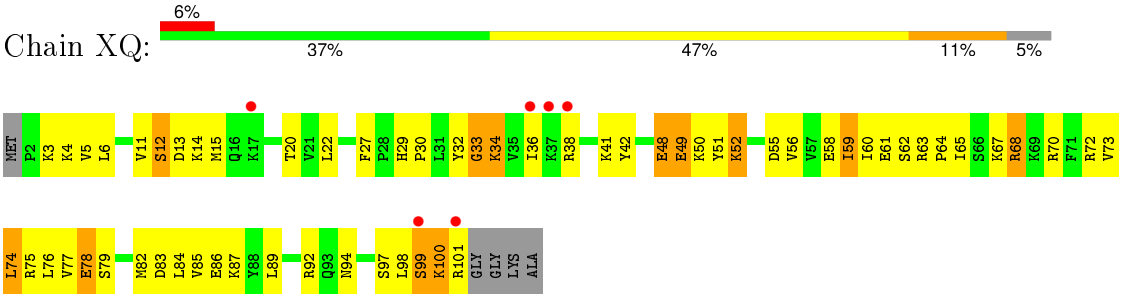

• Molecule 17: 30S ribosomal protein S17

Chain QQ:



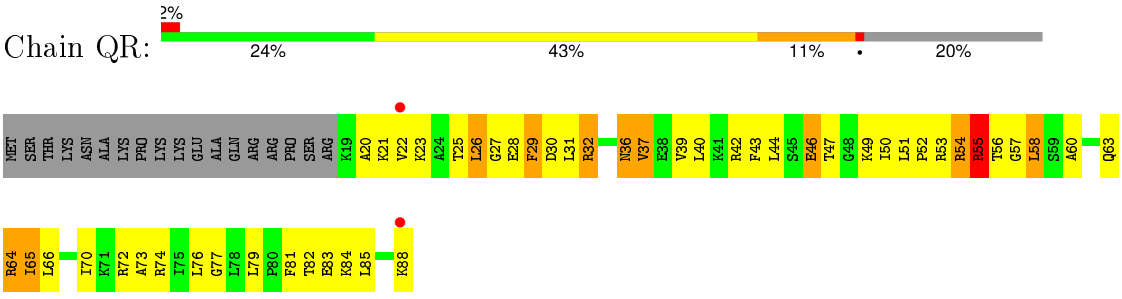

• Molecule 17: 30S ribosomal protein S17

Chain XQ:



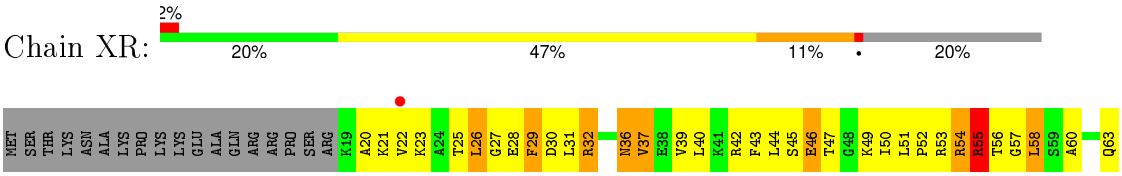

• Molecule 18: 30S ribosomal protein S18

Chain QR:



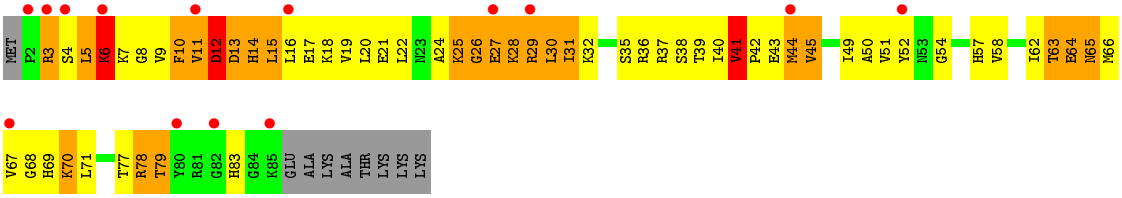

• Molecule 18: 30S ribosomal protein S18

Chain XR:



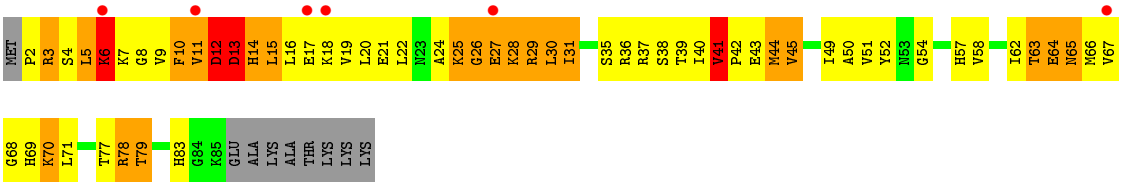
• Molecule 19: 30S ribosomal protein S19

Chain QS:



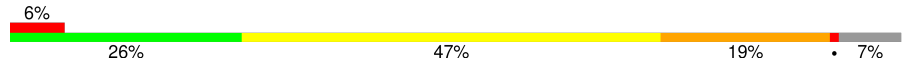

• Molecule 19: 30S ribosomal protein S19

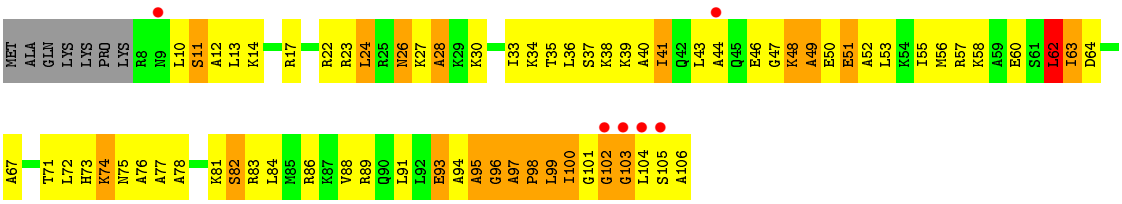
Chain XS:




• Molecule 20: 30S ribosomal protein S20

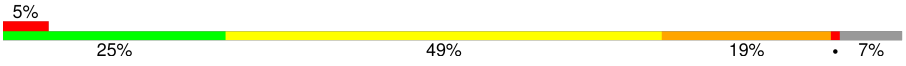
Chain QT:

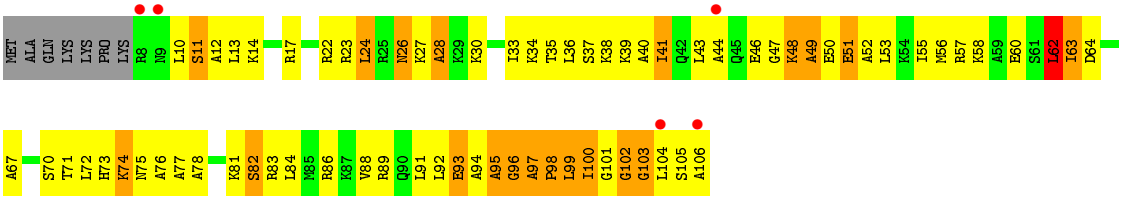



• Molecule 20: 30S ribosomal protein S20

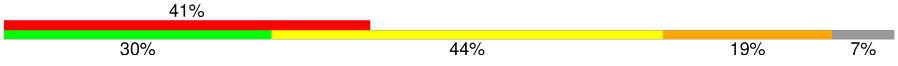
Chain XT:



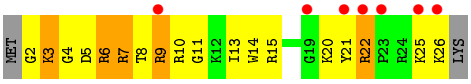




• Molecule 21: 30S ribosomal protein S21

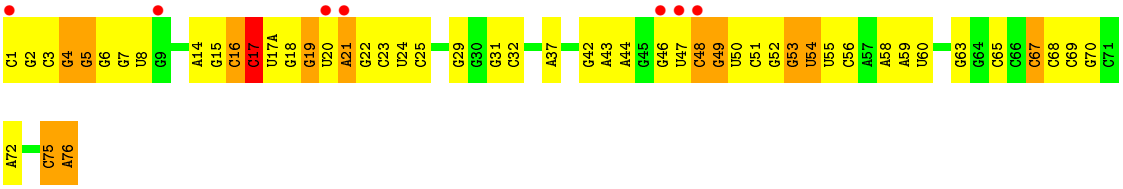
Chain QU:



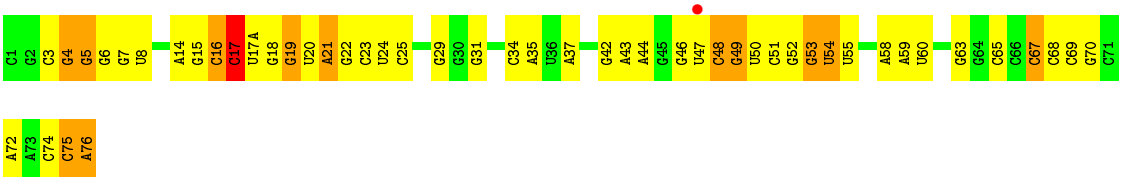
• Molecule 21: 30S ribosomal protein S21




• Molecule 22: P-site tRNA fMet



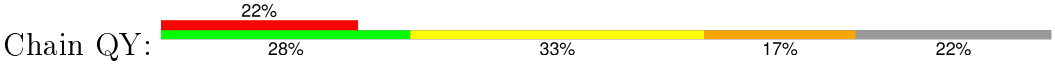

• Molecule 22: P-site tRNA fMet




• Molecule 23: A-site ASL SufA6

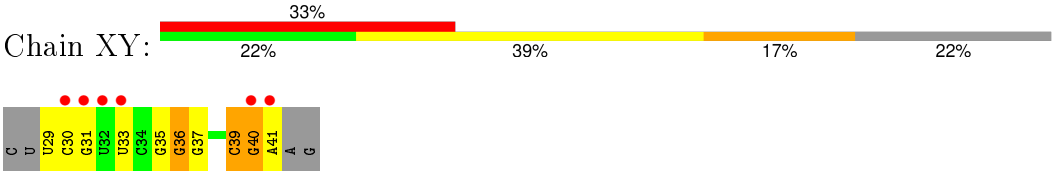
• Molecule 23: A-site ASL SufA6

• Molecule 24: messenger RNA



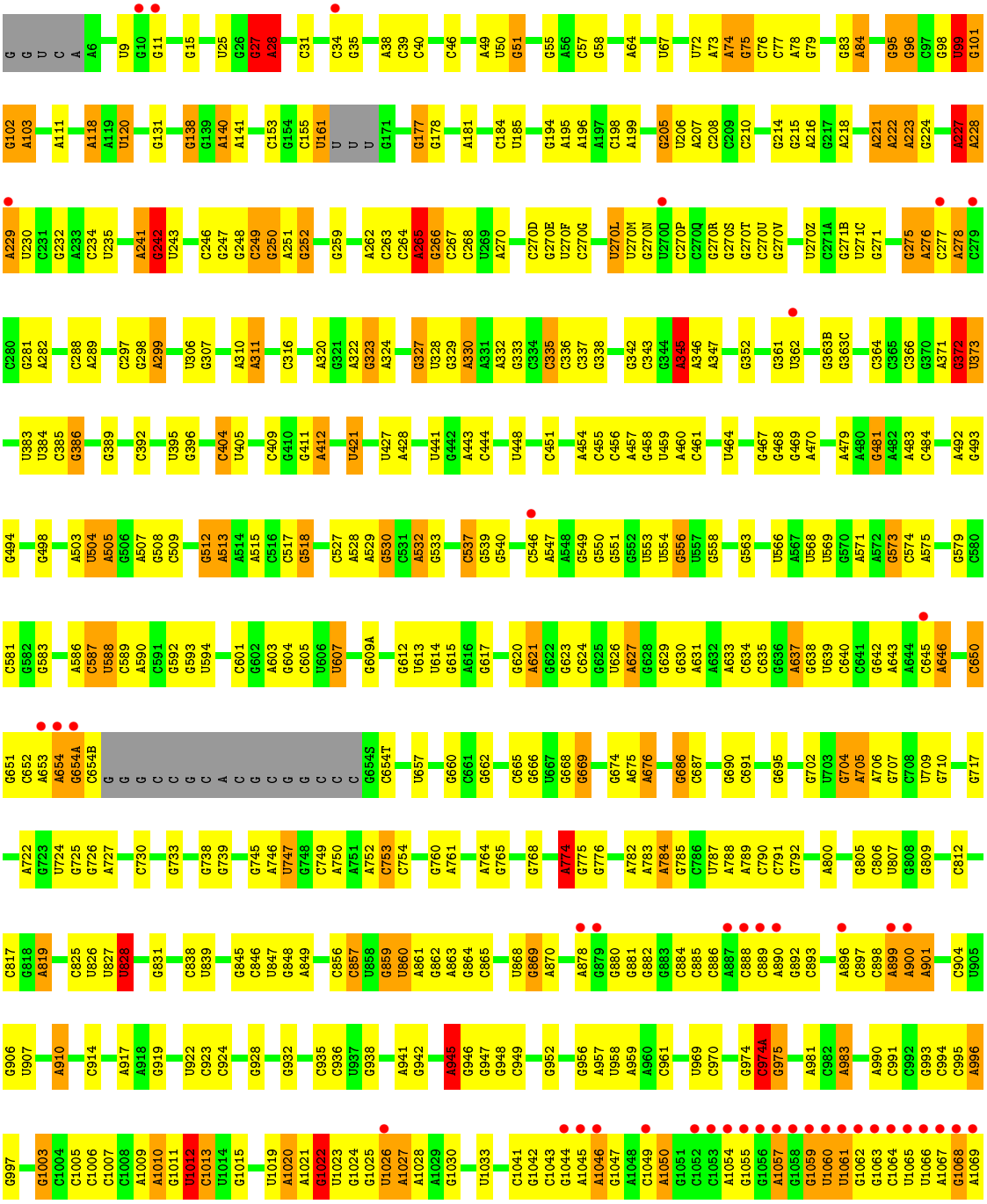
• Molecule 24: messenger RNA

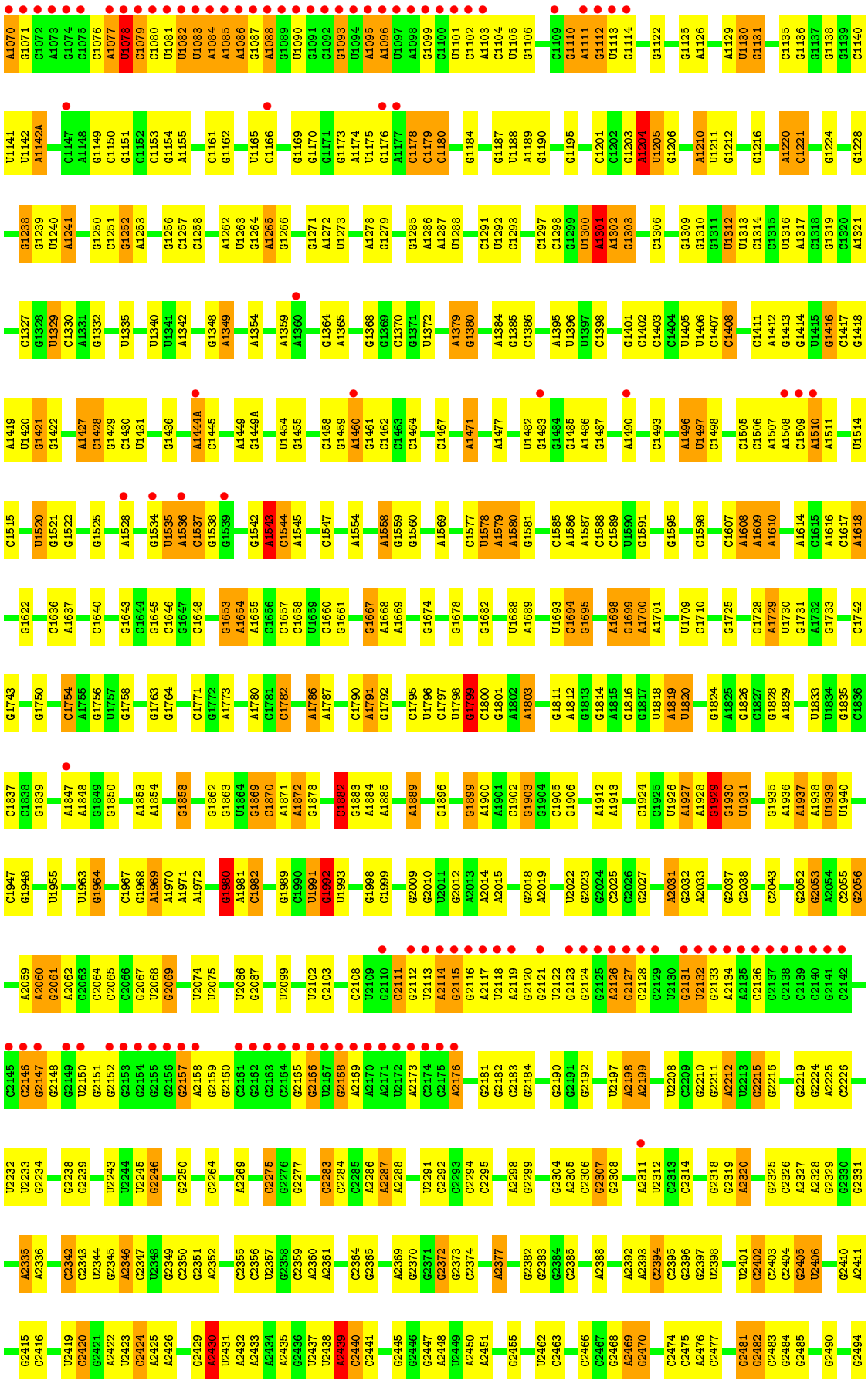
Chain XY:

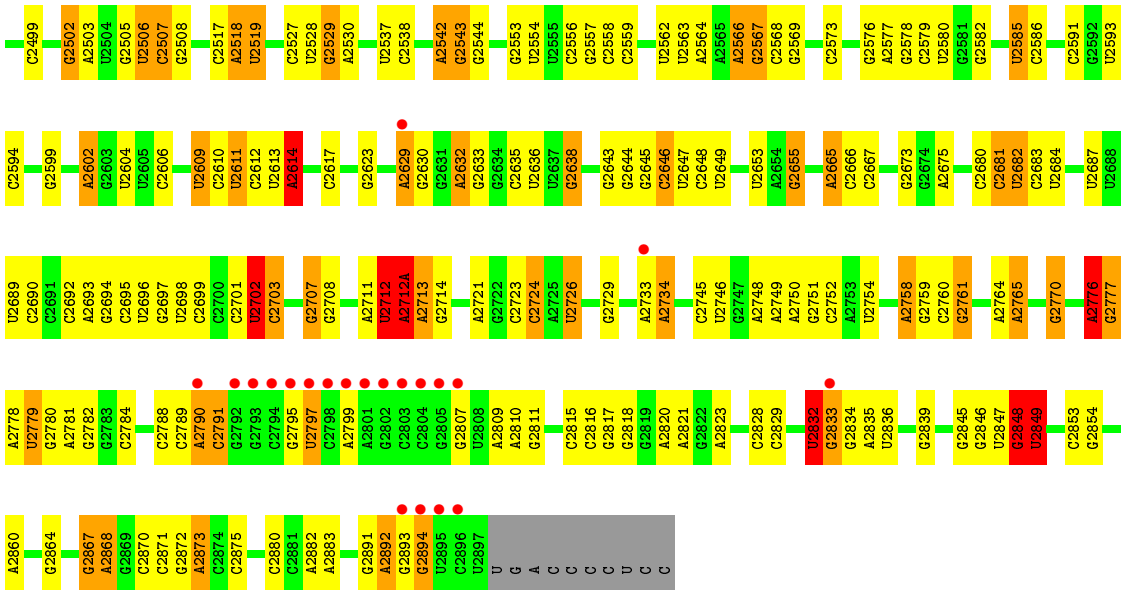



• Molecule 25: 23S rRNA

Chain RA:

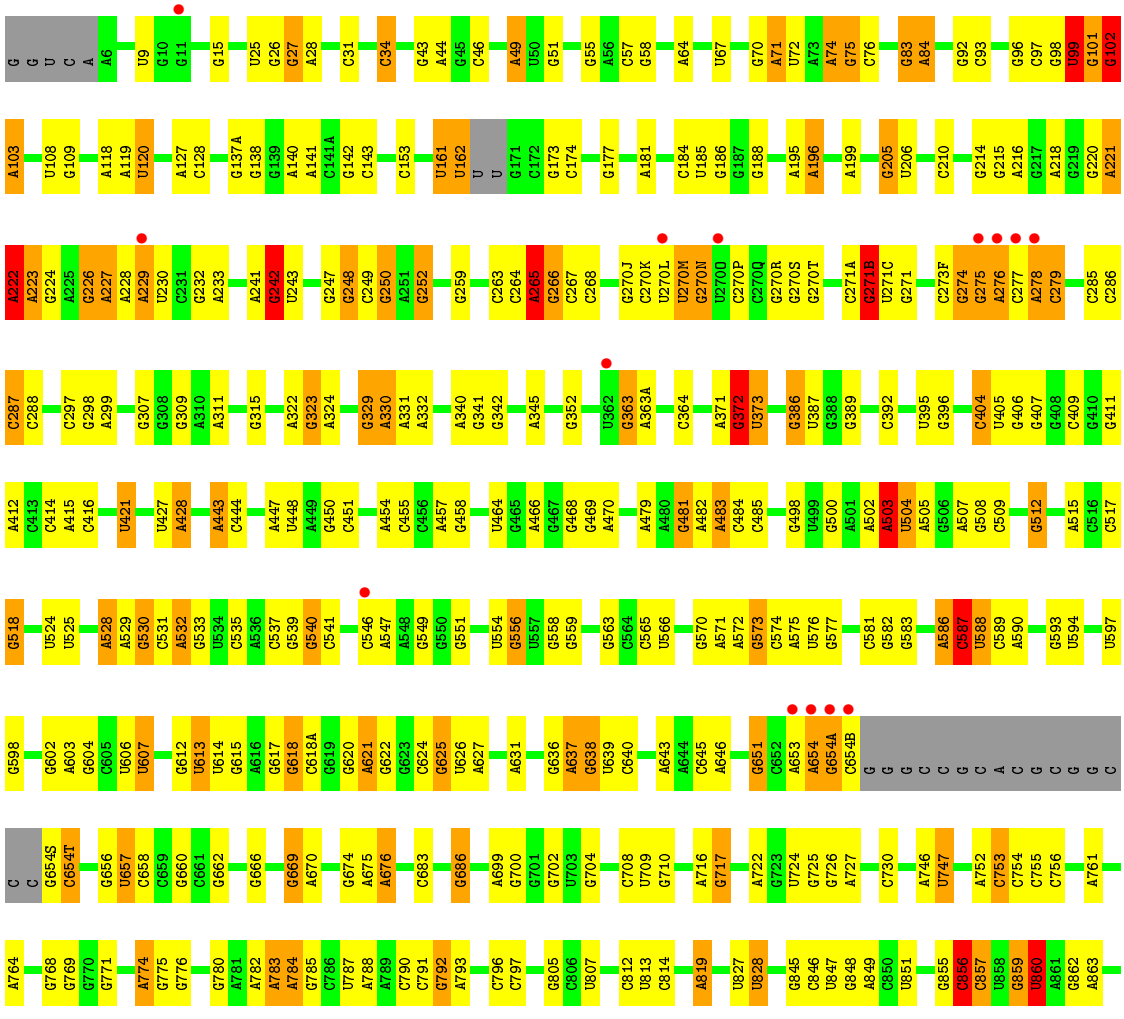






• Molecule 25: 23S rRNA

Chain YA:



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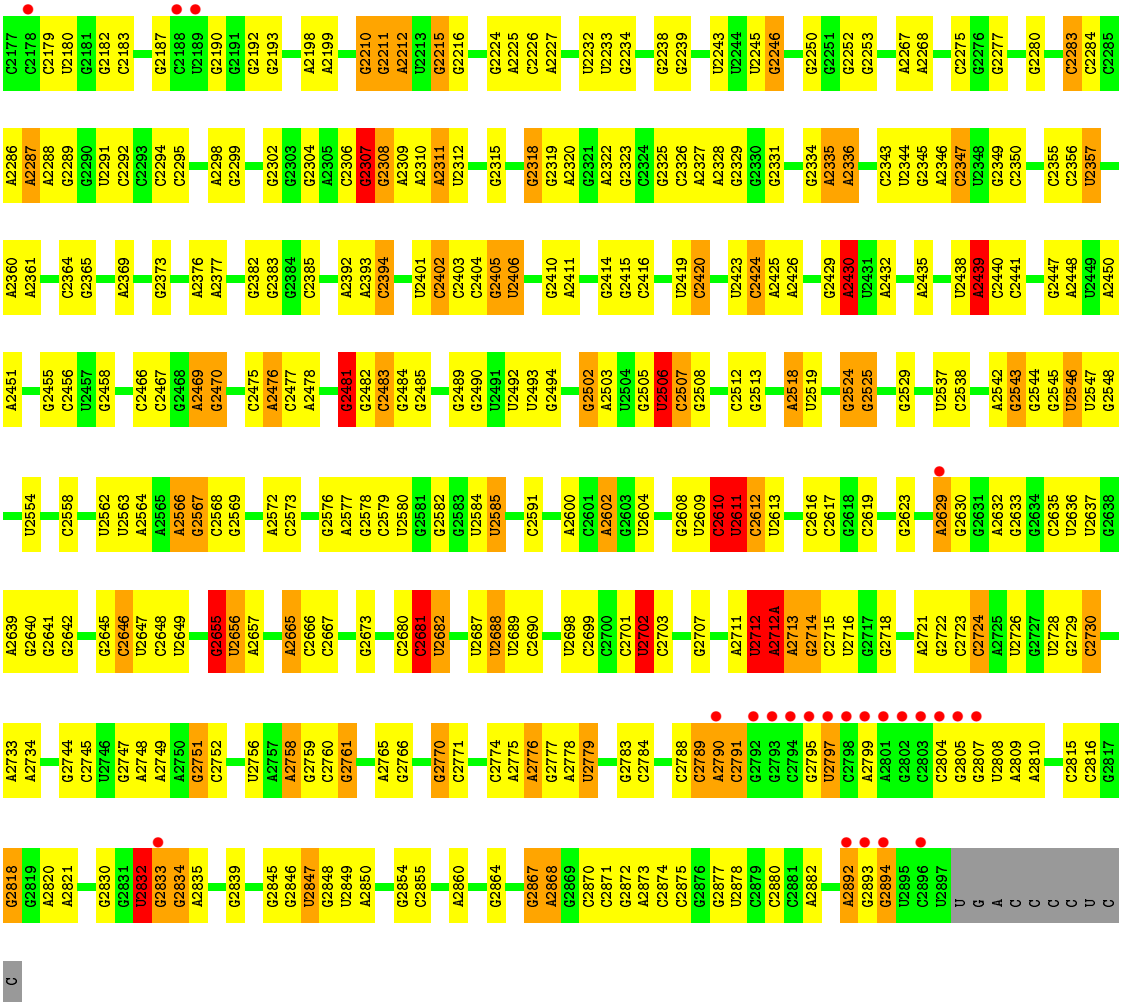
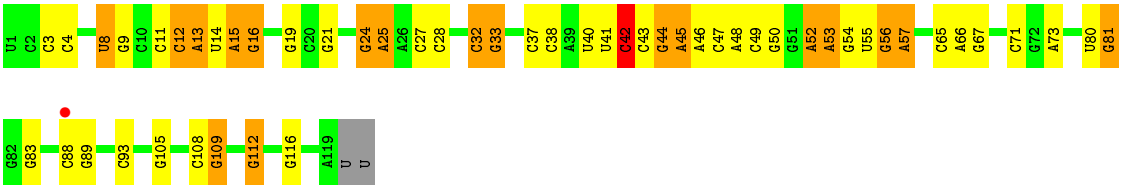
G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176



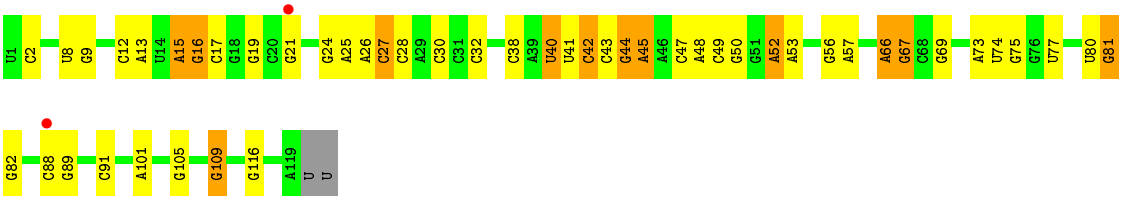
• Molecule 26: 5S rRNA

Chain RB:



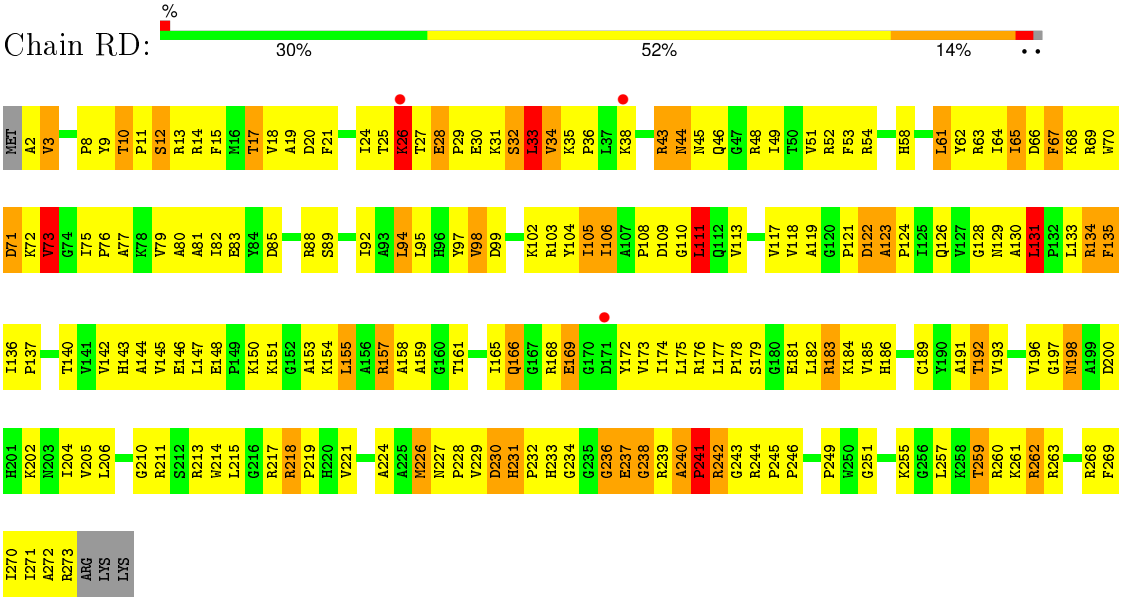
• Molecule 26: 5S rRNA

Chain YB:



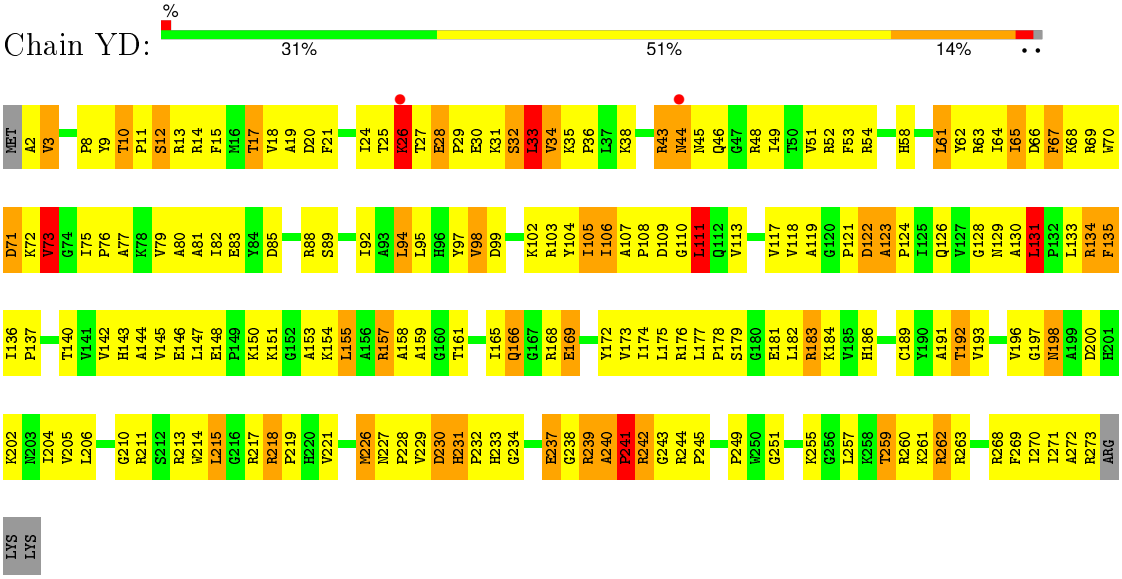
• Molecule 27: 50S ribosomal protein L2

Chain RD:



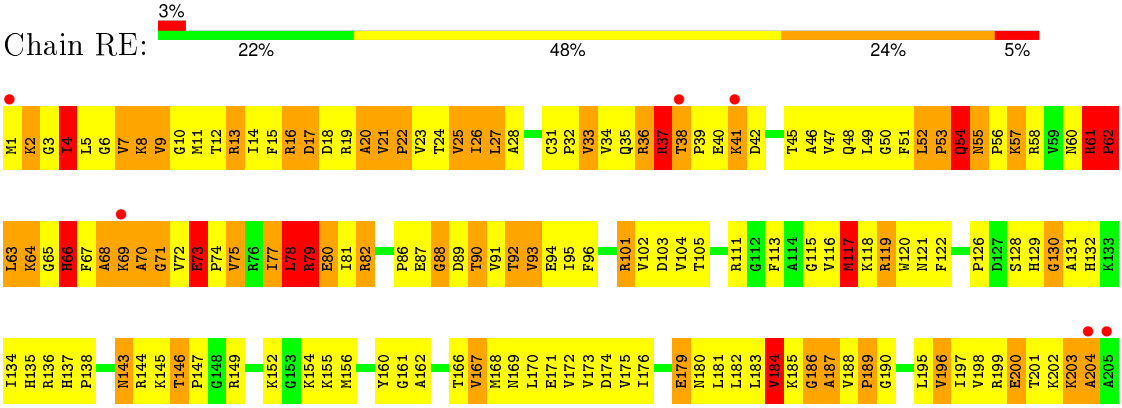

• Molecule 27: 50S ribosomal protein L2

Chain YD:




• Molecule 28: 50S ribosomal protein L3

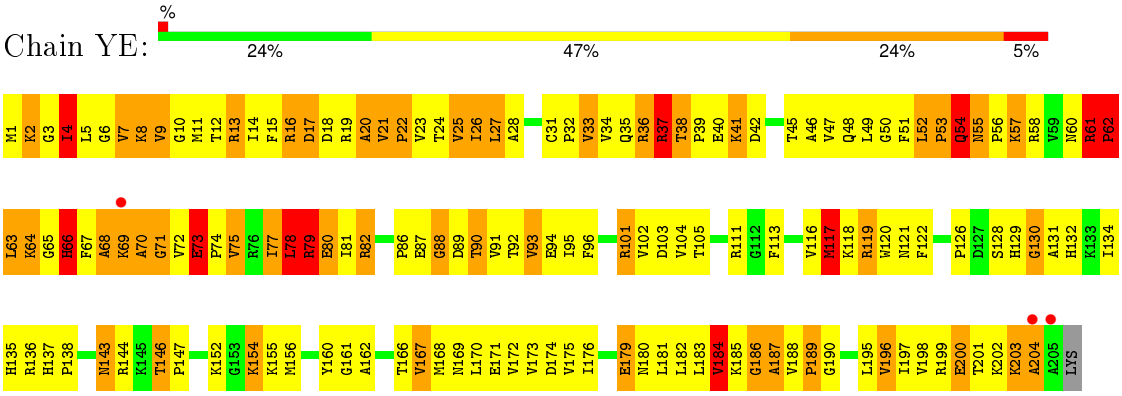
Chain RE:



LYS

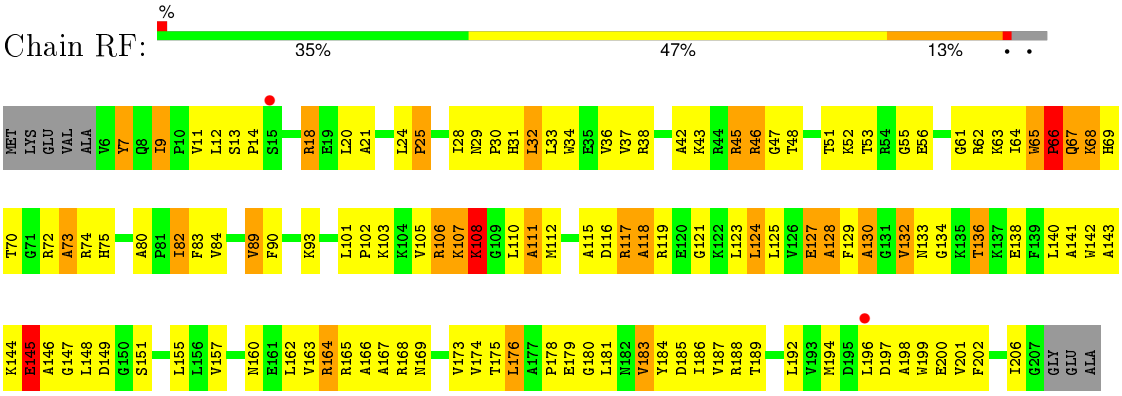
- Molecule 28: 50S ribosomal protein L3

Chain YE:



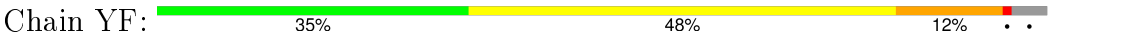

- Molecule 29: 50S ribosomal protein L4

Chain RF:



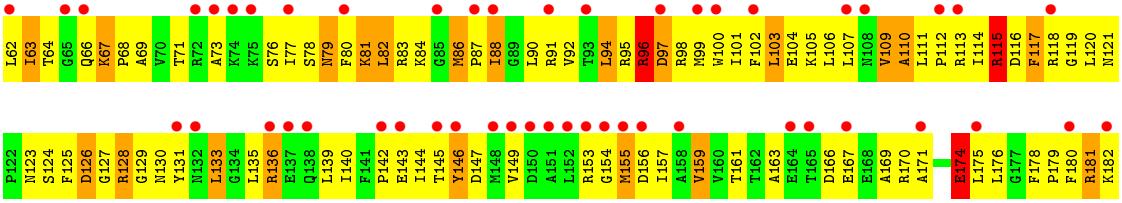

- Molecule 29: 50S ribosomal protein L4

Chain YF:




- Molecule 30: 50S ribosomal protein L5

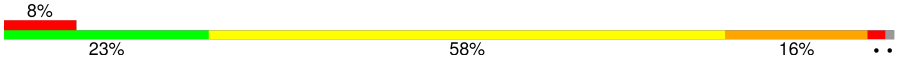
Chain RG:

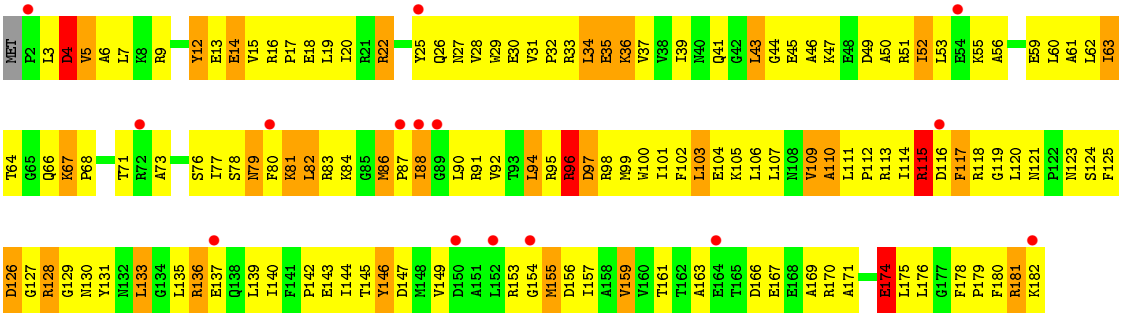




• Molecule 30: 50S ribosomal protein L5

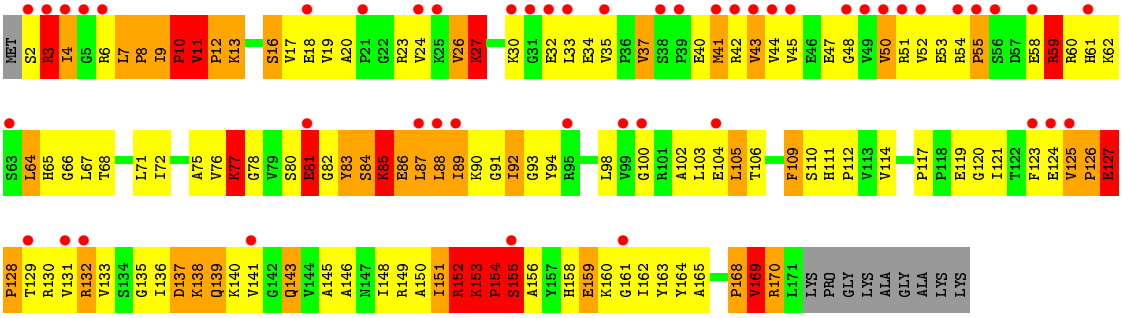
Chain YG:



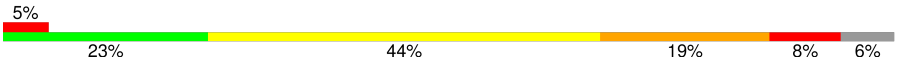
• Molecule 31: 50S ribosomal protein L6

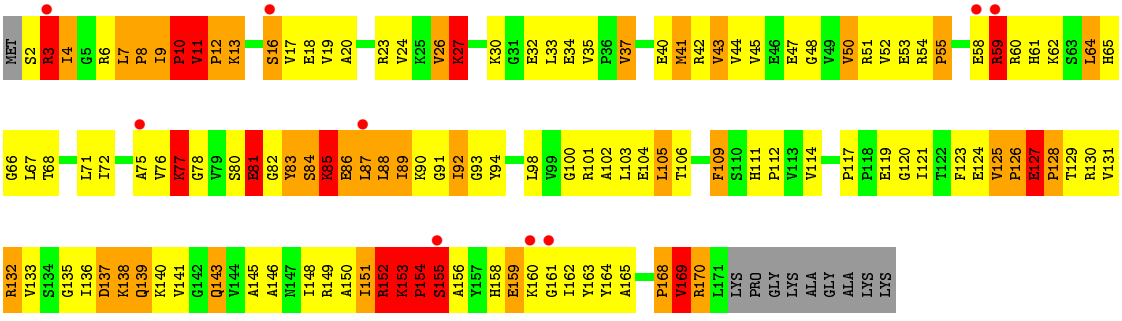
Chain RH:



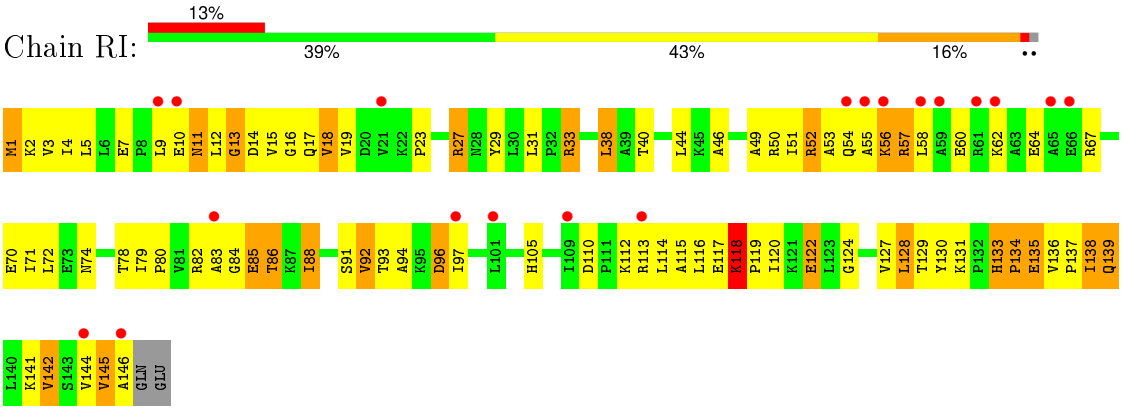
• Molecule 31: 50S ribosomal protein L6

Chain YH:

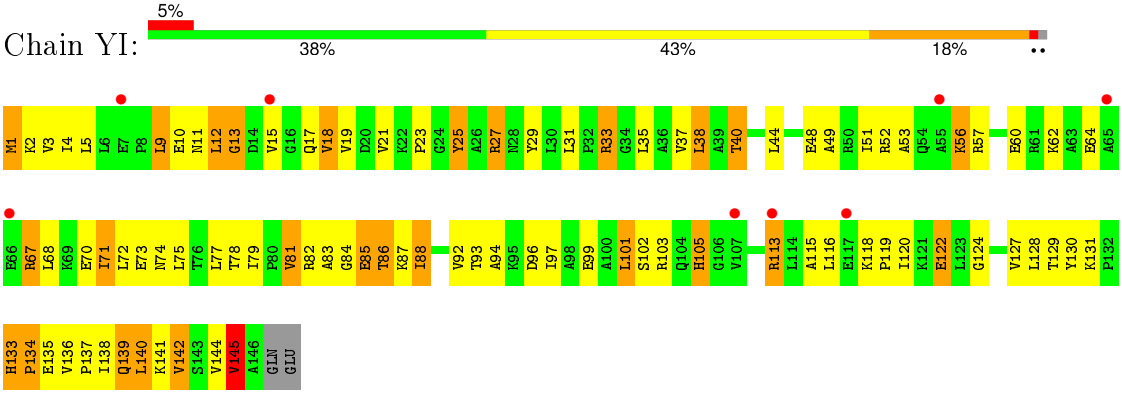


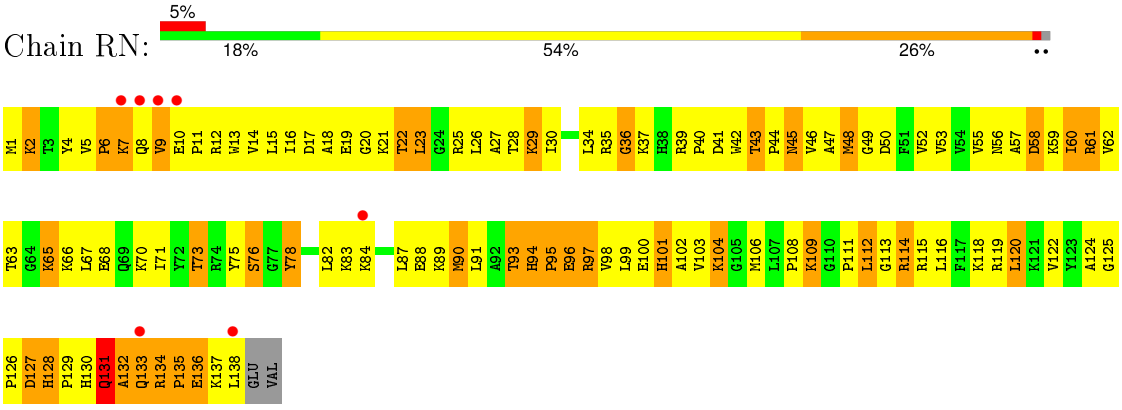
• Molecule 32: 50S ribosomal protein L9



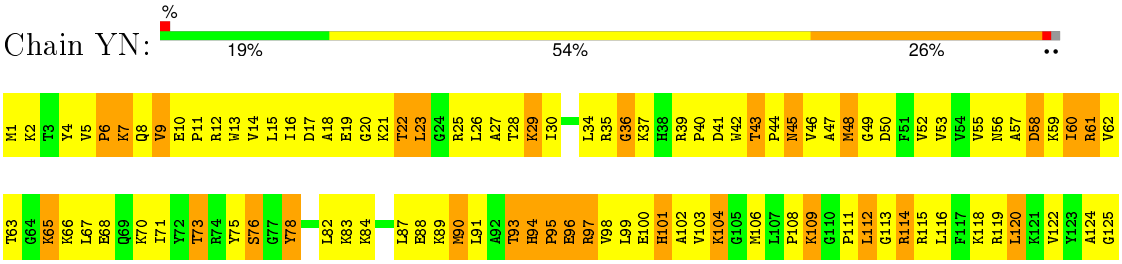

- Molecule 32: 50S ribosomal protein L9




- Molecule 33: 50S ribosomal protein L13

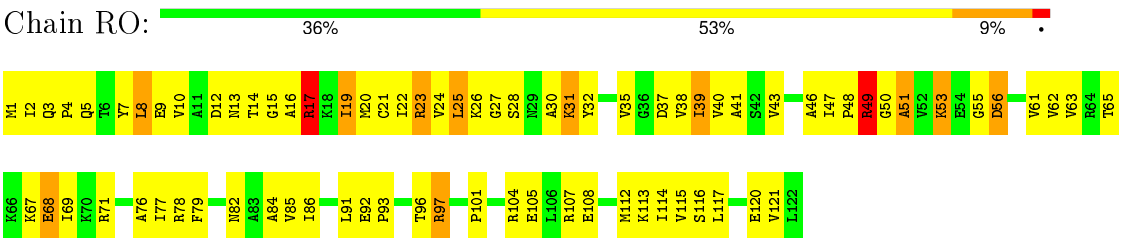



- Molecule 33: 50S ribosomal protein L13



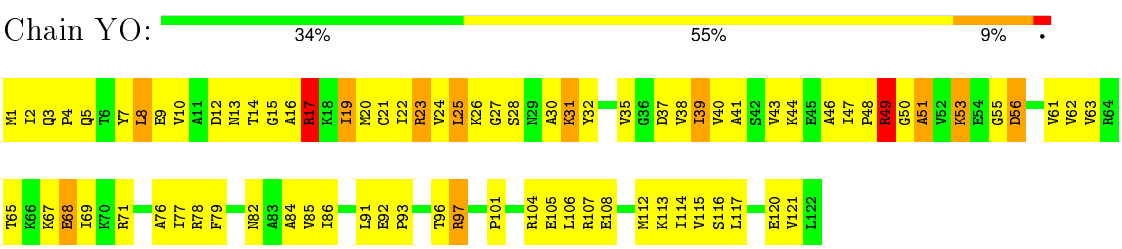
• Molecule 34: 50S ribosomal protein L14

Chain RO:



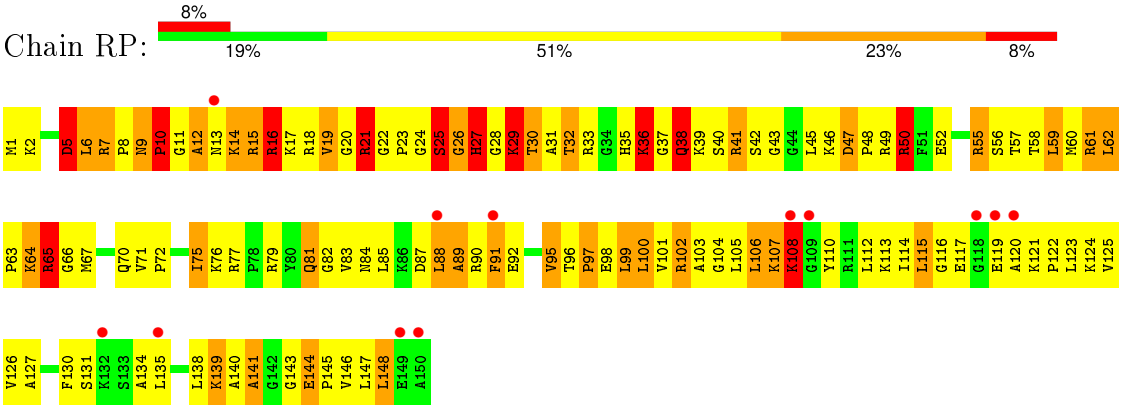

• Molecule 34: 50S ribosomal protein L14

Chain YO:



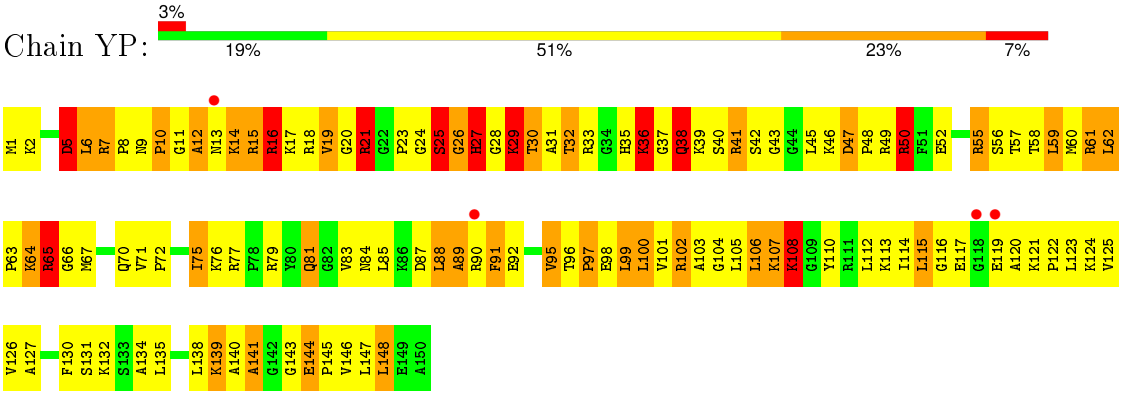

• Molecule 35: 50S ribosomal protein L15

Chain RP:



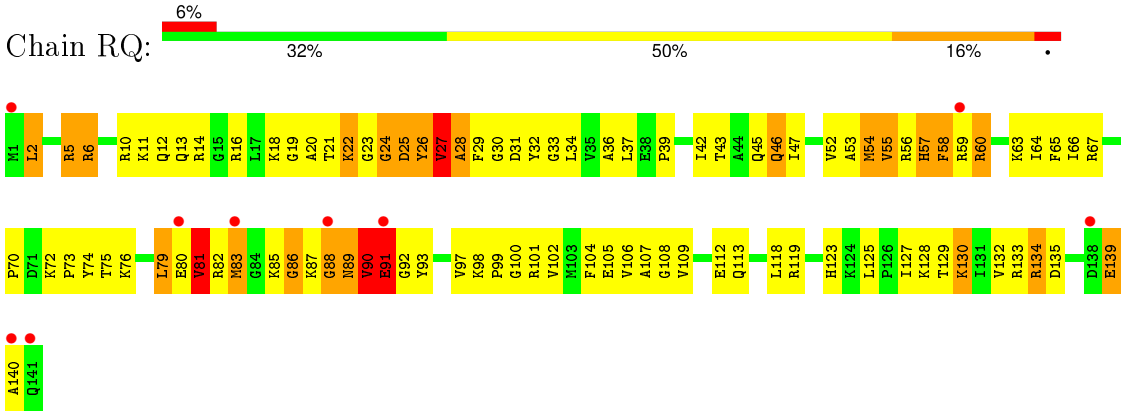

• Molecule 35: 50S ribosomal protein L15

Chain YP:



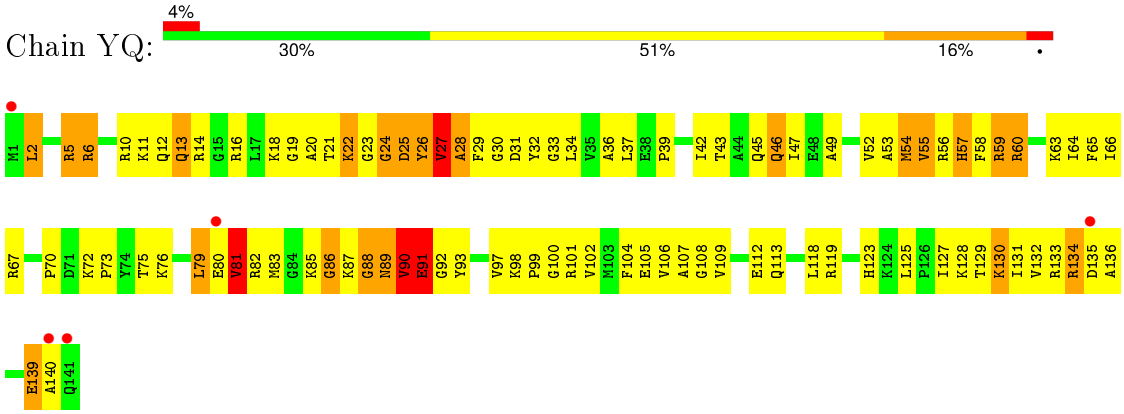
• Molecule 36: 50S ribosomal protein L16

Chain RQ:



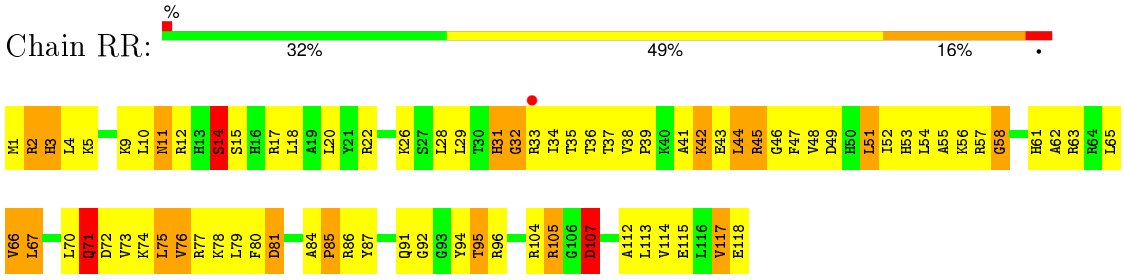

• Molecule 36: 50S ribosomal protein L16

Chain YQ:



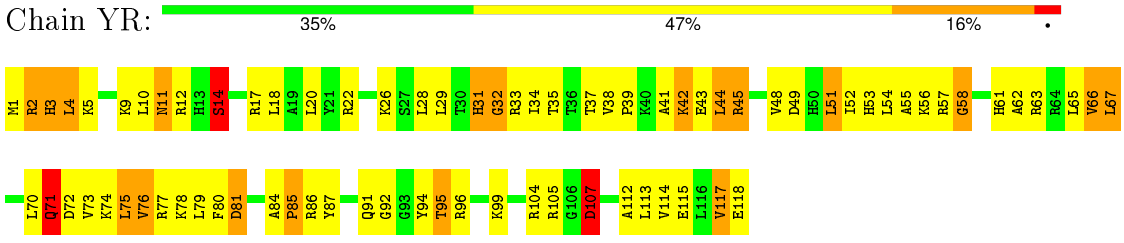

• Molecule 37: 50S ribosomal protein L17

Chain RR:



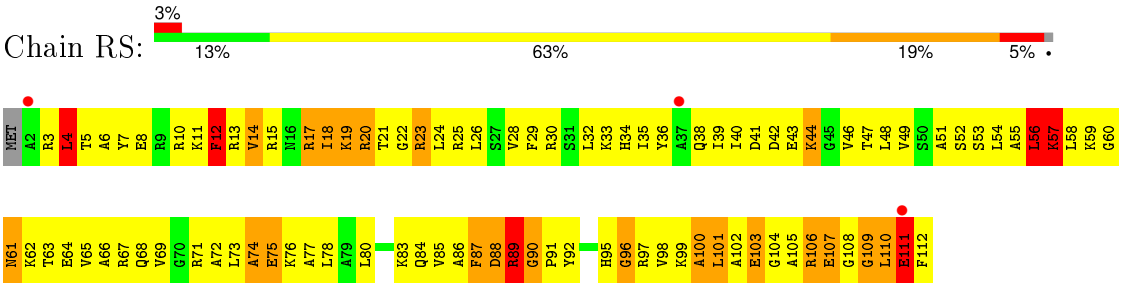

• Molecule 37: 50S ribosomal protein L17

Chain YR:



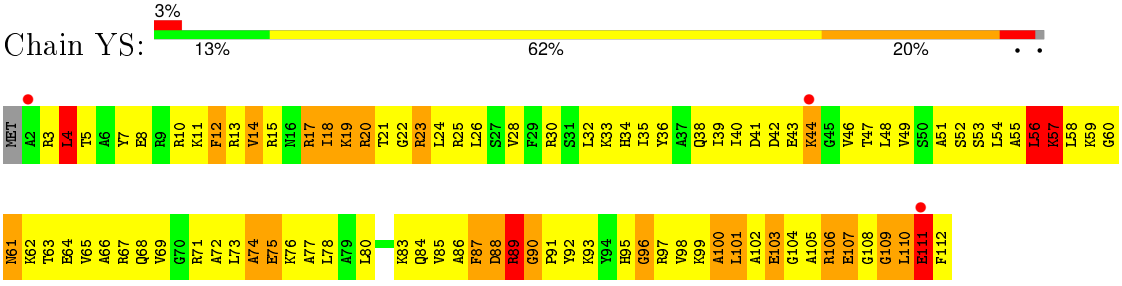

• Molecule 38: 50S ribosomal protein L18

Chain RS:



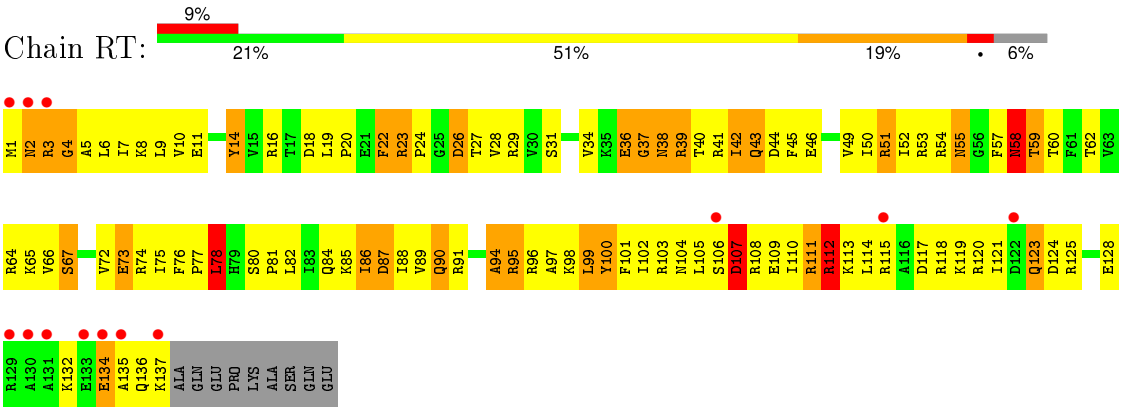

• Molecule 38: 50S ribosomal protein L18

Chain YS:



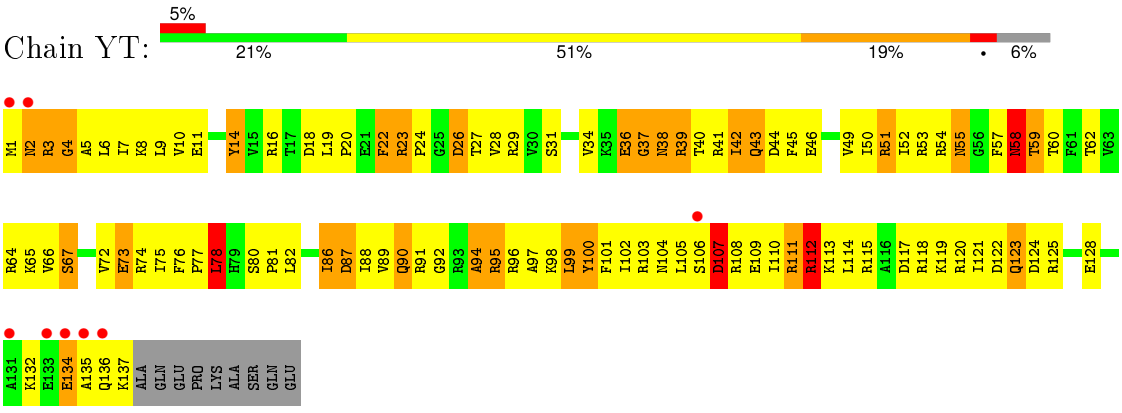

• Molecule 39: 50S ribosomal protein L19

Chain RT:



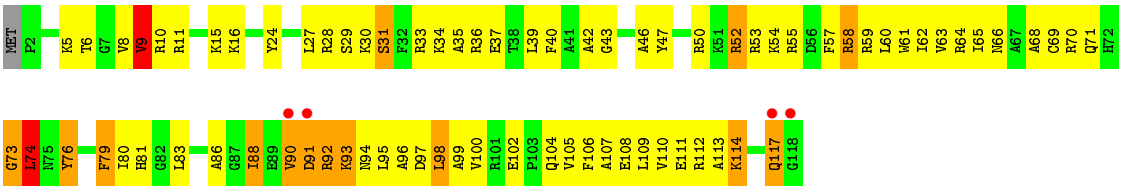

• Molecule 39: 50S ribosomal protein L19

Chain YT:




• Molecule 40: 50S ribosomal protein L20

Chain RU:

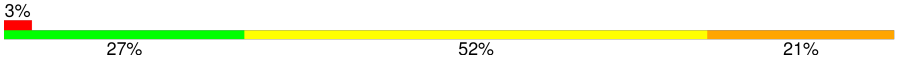


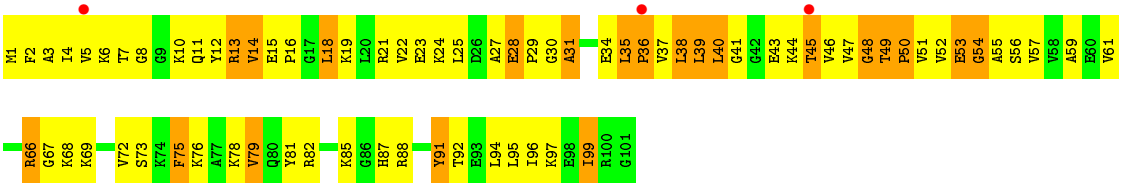
• Molecule 40: 50S ribosomal protein L20

Chain YU:

• Molecule 41: 50S ribosomal protein L21

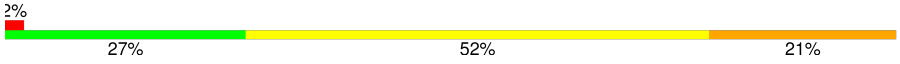
Chain RV:

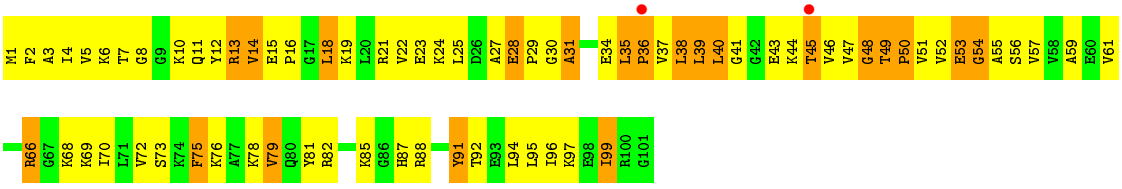


• Molecule 41: 50S ribosomal protein L21

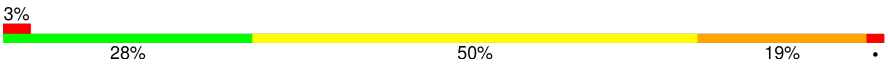
Chain YV:

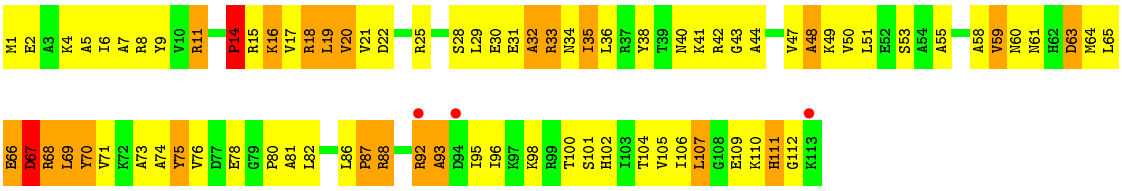


• Molecule 42: 50S ribosomal protein L22

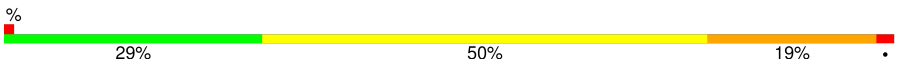
Chain RW:

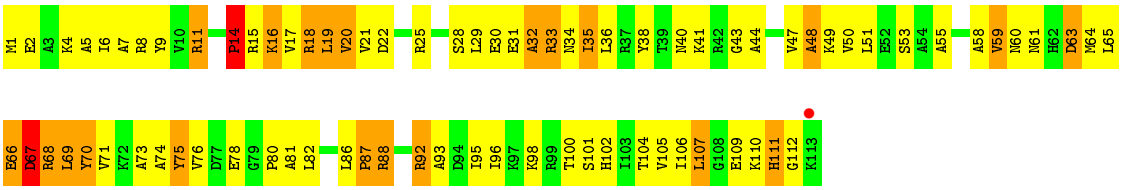


• Molecule 42: 50S ribosomal protein L22

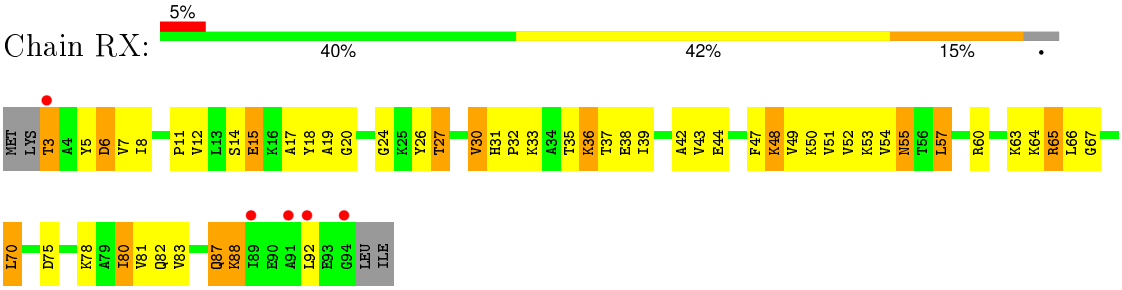
Chain YW:





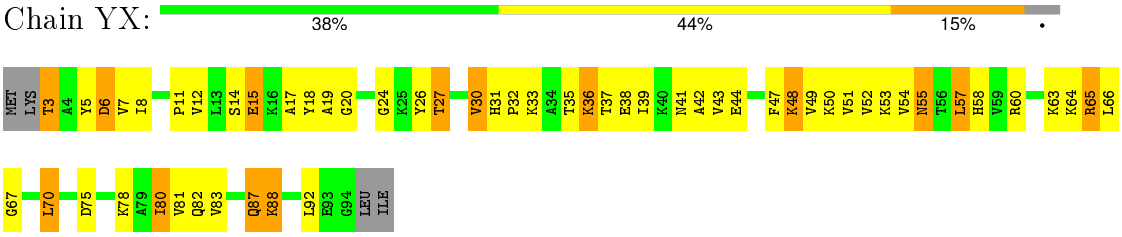
• Molecule 43: 50S ribosomal protein L23

Chain RX:



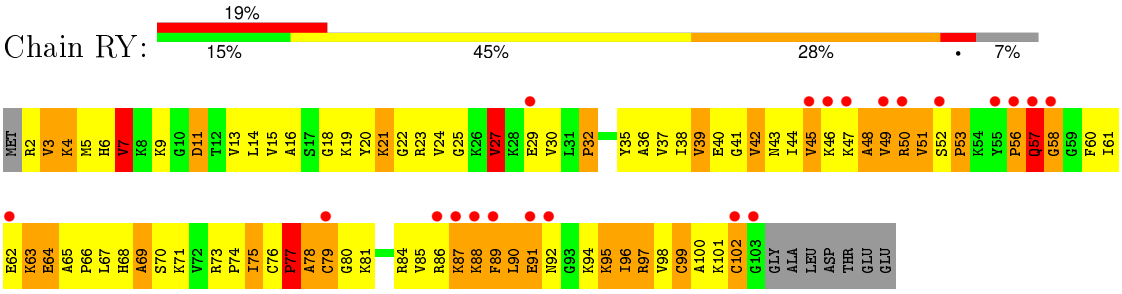
• Molecule 43: 50S ribosomal protein L23

Chain YX:



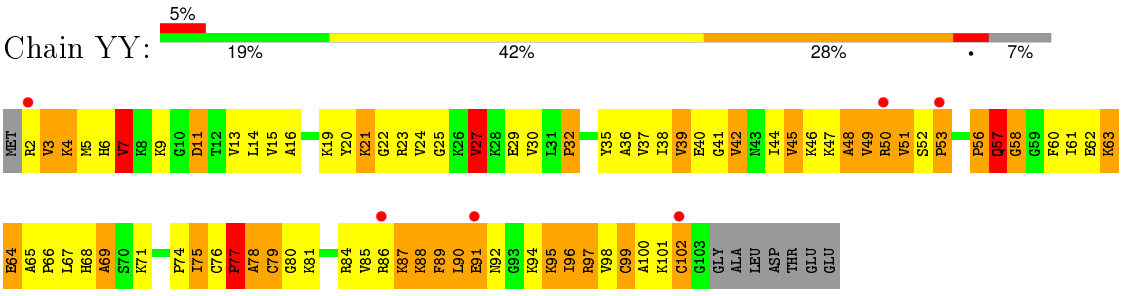
• Molecule 44: 50S ribosomal protein L24

Chain RY:



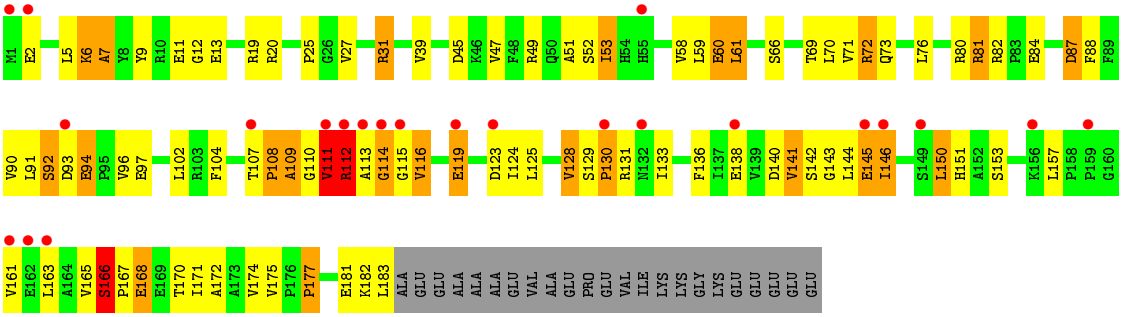
• Molecule 44: 50S ribosomal protein L24

Chain YY:

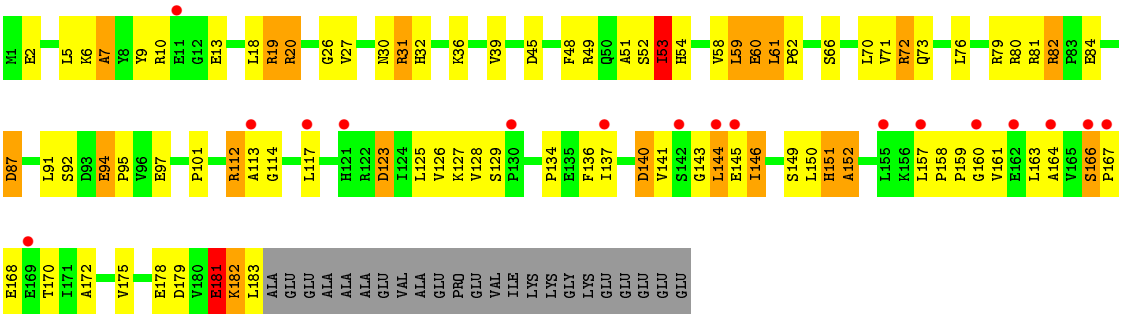


• Molecule 45: 50S ribosomal protein L25

Chain RZ:

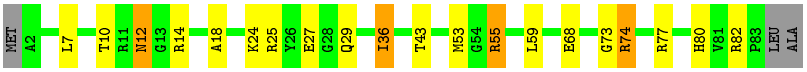



- Molecule 45: 50S ribosomal protein L25

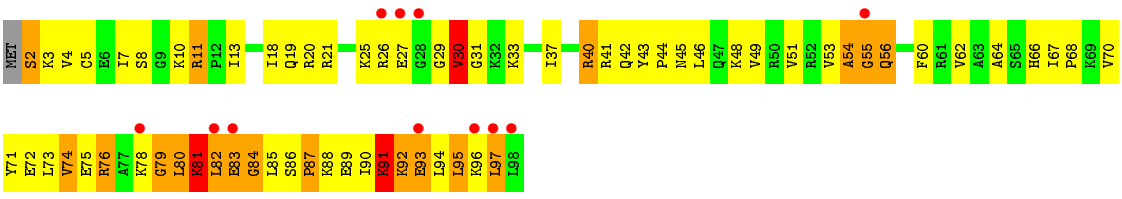



- Molecule 46: 50S ribosomal protein L27

- Molecule 46: 50S ribosomal protein L27

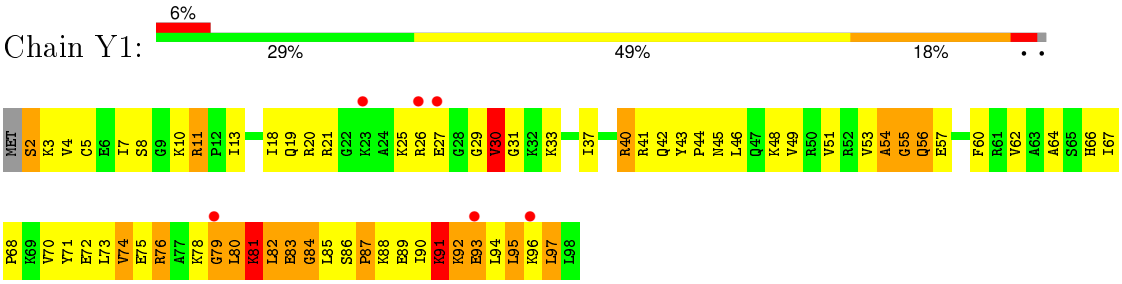



- Molecule 47: 50S ribosomal protein L28



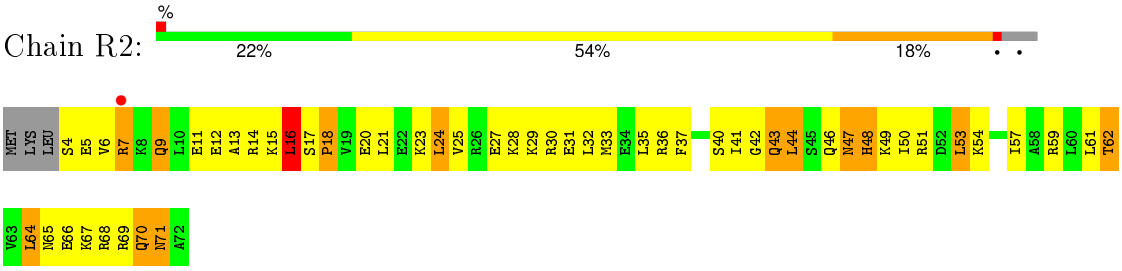

- Molecule 47: 50S ribosomal protein L28

Chain Y1:



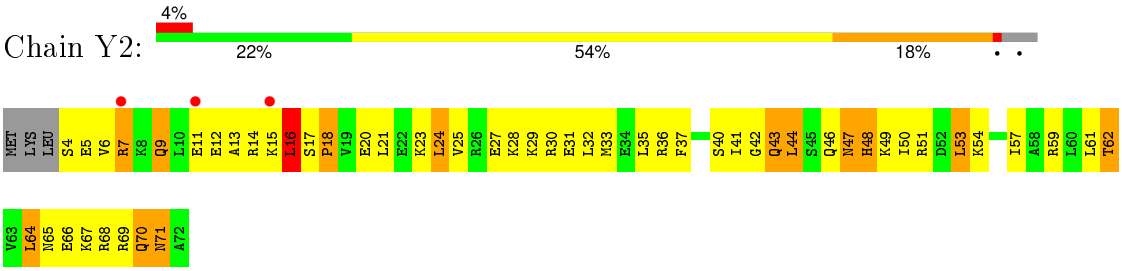

• Molecule 48: 50S ribosomal protein L29

Chain R2:



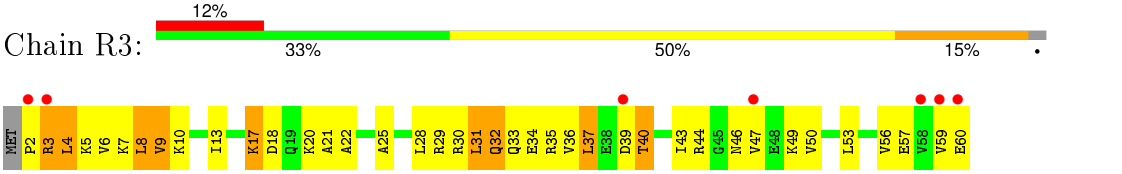

• Molecule 48: 50S ribosomal protein L29

Chain Y2:



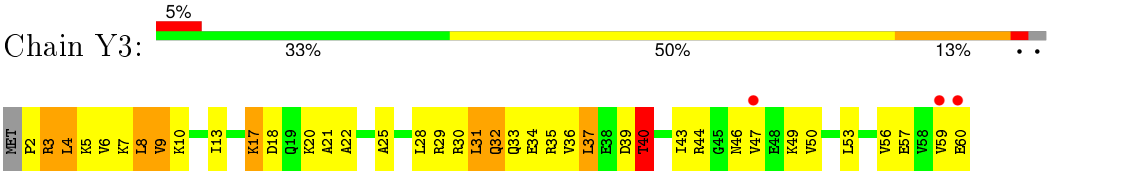

• Molecule 49: 50S ribosomal protein L30

Chain R3:



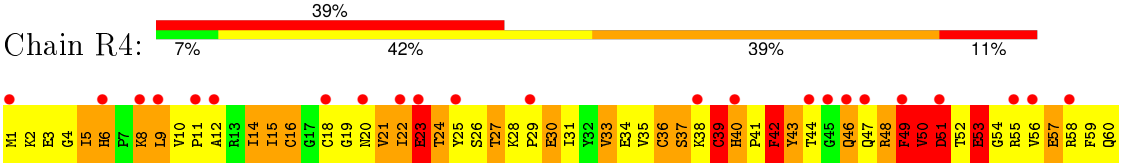

• Molecule 49: 50S ribosomal protein L30

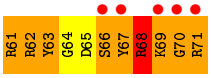
Chain Y3:




• Molecule 50: 50S ribosomal protein L31

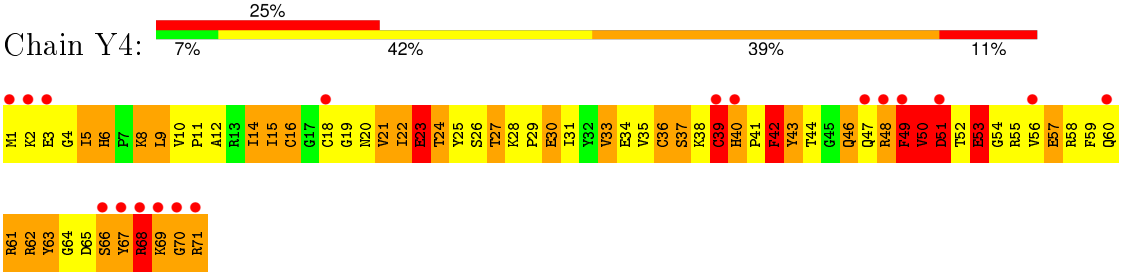
Chain R4:






• Molecule 50: 50S ribosomal protein L31

Chain Y4:

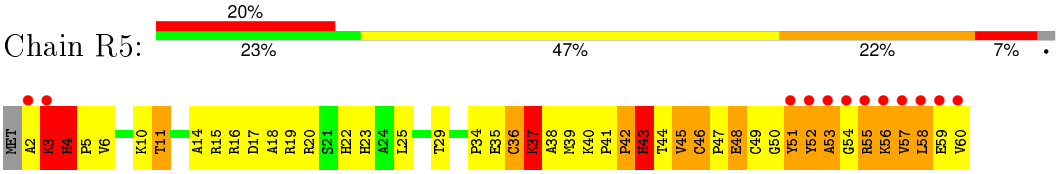






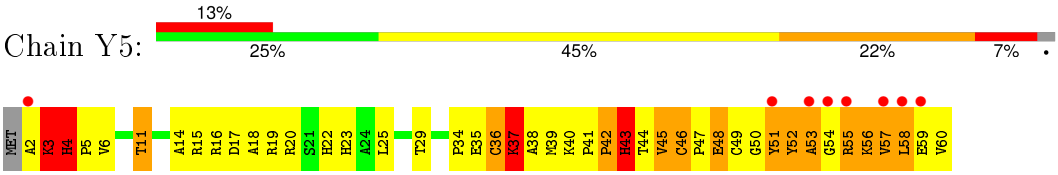
• Molecule 51: 50S ribosomal protein L32

Chain R5:



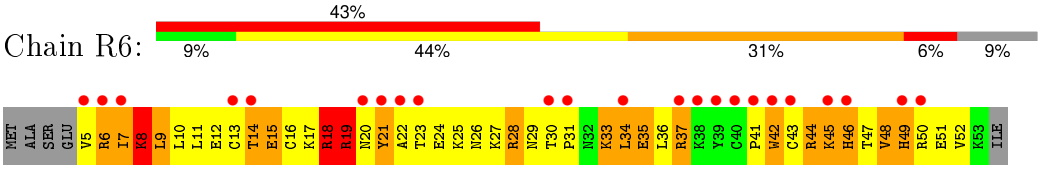

• Molecule 51: 50S ribosomal protein L32

Chain Y5:



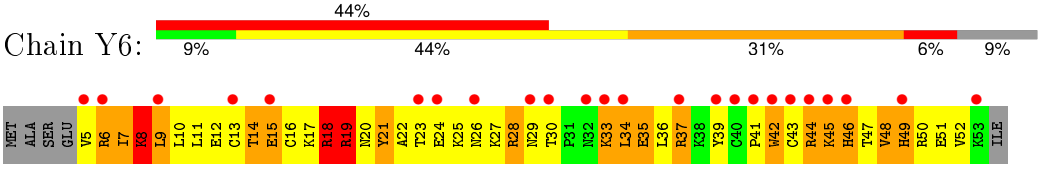

• Molecule 52: 50S ribosomal protein L33

Chain R6:



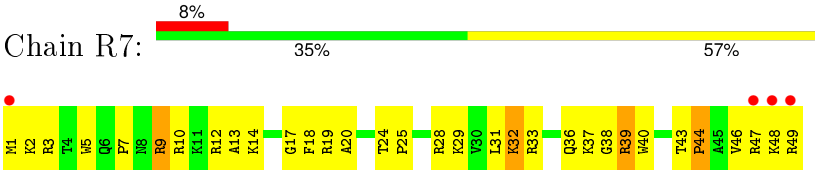

• Molecule 52: 50S ribosomal protein L33

Chain Y6:



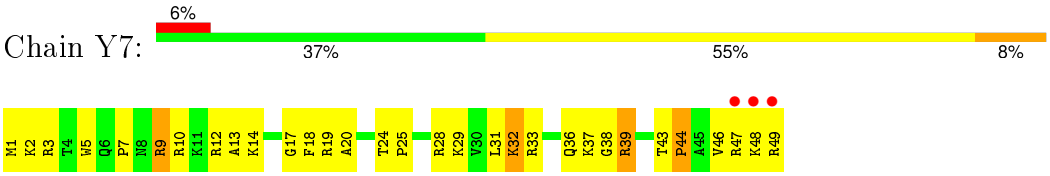

• Molecule 53: 50S ribosomal protein L34

Chain R7:



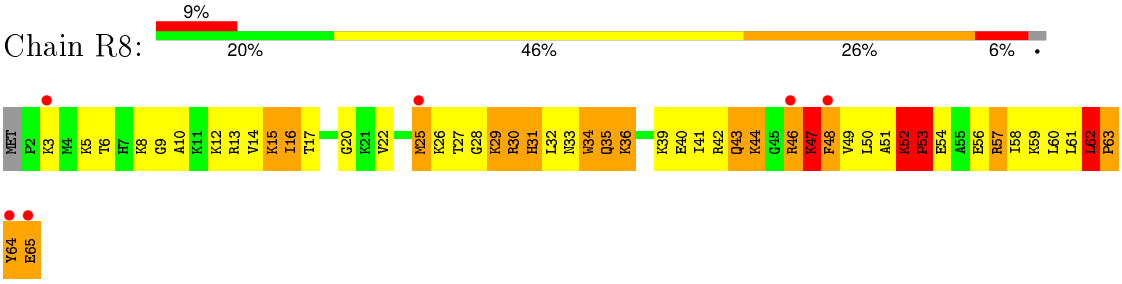

• Molecule 53: 50S ribosomal protein L34

Chain Y7:



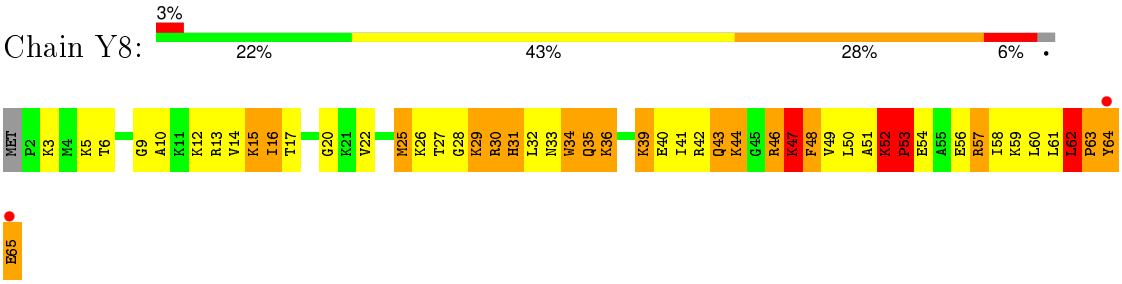

• Molecule 54: 50S ribosomal protein L35

Chain R8:



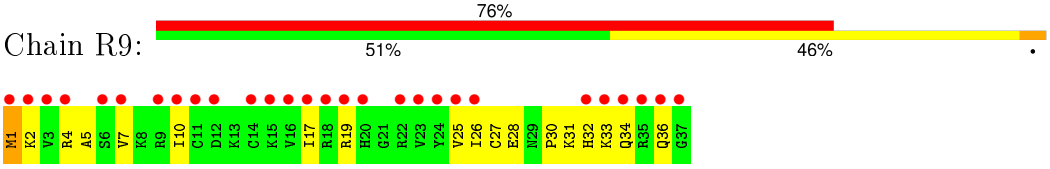

• Molecule 54: 50S ribosomal protein L35

Chain Y8:



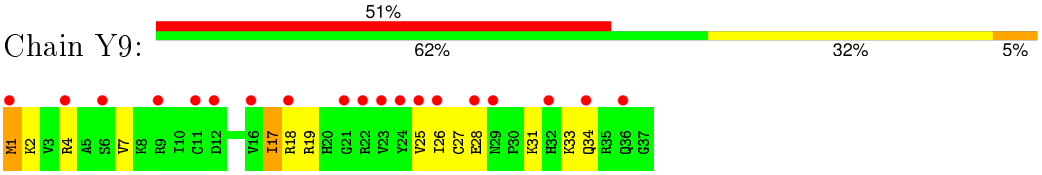

• Molecule 55: 50S ribosomal protein L36

Chain R9:




• Molecule 55: 50S ribosomal protein L36

Chain Y9:




• Molecule 56: tRNA acceptor end mimic

Chain Z6:

• Molecule 56: tRNA acceptor end mimic

Chain Z8:

C74
C75
A76

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 210.20Å 450.23Å 621.74Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 34.97 – 3.22<br>34.97 – 3.18 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.5 (34.97-3.22)<br>98.6 (34.97-3.18) | Depositor<br>EDS |
| $R_{merge}$ | 0.25 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.66 (at 3.18Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.229 , 0.260<br>0.231 , 0.260 | Depositor<br>DCC |
| $R_{free}$ test set | 43406 reflections (4.91%) | DCC |
| Wilson B-factor (Å$^2$) | 67.8 | Xtriage |
| Anisotropy | 0.089 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.27 , 74.9 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.45$, $< L^2 > = 0.27$ | Xtriage |
| Outliers | 0 of 962803 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 291957 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 91.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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, PAR, 1MG, PPU

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 | QA | 0.31 | 0/36098 | 0.86 | 46/56341 (0.1%) |
| 1 | XA | 0.34 | 1/36101 (0.0%) | 0.89 | 66/56346 (0.1%) |
| 2 | QB | 0.35 | 0/1959 | 0.65 | 0/2642 |
| 2 | XB | 0.35 | 0/1959 | 0.65 | 0/2642 |
| 3 | QC | 0.36 | 0/1629 | 0.60 | 0/2195 |
| 3 | XC | 0.36 | 0/1629 | 0.60 | 0/2195 |
| 4 | QD | 0.41 | 0/1733 | 0.68 | 1/2318 (0.0%) |
| 4 | XD | 0.44 | 0/1733 | 0.68 | 1/2318 (0.0%) |
| 5 | QE | 0.38 | 0/1171 | 0.66 | 0/1576 |
| 5 | XE | 0.38 | 0/1171 | 0.66 | 0/1576 |
| 6 | QF | 0.43 | 0/856 | 0.68 | 0/1154 |
| 6 | XF | 0.42 | 0/856 | 0.68 | 0/1154 |
| 7 | QG | 0.37 | 0/1276 | 0.60 | 0/1709 |
| 7 | XG | 0.36 | 0/1276 | 0.60 | 0/1709 |
| 8 | QH | 0.40 | 0/1136 | 0.69 | 0/1527 |
| 8 | XH | 0.40 | 0/1136 | 0.69 | 0/1527 |
| 9 | QI | 0.36 | 0/1029 | 0.67 | 0/1379 |
| 9 | XI | 0.36 | 0/1029 | 0.67 | 0/1379 |
| 10 | QJ | 0.35 | 0/814 | 0.61 | 0/1095 |
| 10 | XJ | 0.36 | 0/814 | 0.61 | 0/1095 |
| 11 | QK | 0.40 | 0/900 | 0.67 | 0/1213 |
| 11 | XK | 0.40 | 0/900 | 0.67 | 0/1213 |
| 12 | QL | 0.45 | 0/991 | 1.00 | 4/1327 (0.3%) |
| 12 | XL | 0.46 | 0/991 | 1.00 | 4/1327 (0.3%) |
| 13 | QM | 0.34 | 0/974 | 0.66 | 0/1303 |
| 13 | XM | 0.34 | 0/974 | 0.66 | 0/1303 |
| 14 | QN | 0.42 | 0/501 | 0.68 | 0/664 |
| 14 | XN | 0.52 | 0/501 | 0.67 | 0/664 |
| 15 | QO | 0.39 | 0/745 | 0.67 | 0/992 |
| 15 | XO | 0.39 | 0/745 | 0.67 | 0/992 |
| 16 | QP | 0.36 | 0/721 | 0.67 | 0/970 |
| 16 | XP | 0.36 | 0/721 | 0.67 | 0/970 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | QQ | 0.37 | 0/847 | 0.68 | 0/1131 |
| 17 | XQ | 0.37 | 0/847 | 0.68 | 0/1131 |
| 18 | QR | 0.39 | 0/579 | 0.72 | 0/768 |
| 18 | XR | 0.39 | 0/579 | 0.72 | 0/768 |
| 19 | QS | 0.36 | 0/689 | 0.84 | 2/926 (0.2%) |
| 19 | XS | 0.36 | 0/689 | 0.84 | 2/926 (0.2%) |
| 20 | QT | 0.33 | 0/765 | 0.69 | 0/1007 |
| 20 | XT | 0.34 | 0/765 | 0.69 | 0/1007 |
| 21 | QU | 0.37 | 0/221 | 0.63 | 0/288 |
| 21 | XU | 0.37 | 0/221 | 0.63 | 0/288 |
| 22 | QV | 0.52 | 0/1836 | 0.99 | 5/2859 (0.2%) |
| 22 | XV | 0.52 | 0/1836 | 0.99 | 6/2859 (0.2%) |
| 23 | QX | 0.39 | 0/185 | 0.72 | 0/285 |
| 23 | XX | 0.86 | 1/185 (0.5%) | 1.12 | 1/285 (0.4%) |
| 24 | QY | 0.52 | 0/311 | 0.88 | 0/483 |
| 24 | XY | 0.53 | 0/311 | 0.89 | 0/483 |
| 25 | RA | 0.39 | 1/69521 (0.0%) | 0.91 | 95/108529 (0.1%) |
| 25 | YA | 0.44 | 3/69543 (0.0%) | 0.94 | 121/108563 (0.1%) |
| 26 | RB | 0.34 | 0/2878 | 0.89 | 3/4490 (0.1%) |
| 26 | YB | 0.35 | 0/2878 | 0.89 | 0/4490 |
| 27 | RD | 0.59 | 2/2165 (0.1%) | 0.90 | 4/2919 (0.1%) |
| 27 | YD | 0.56 | 1/2165 (0.0%) | 0.90 | 4/2919 (0.1%) |
| 28 | RE | 0.52 | 0/1601 | 0.91 | 2/2160 (0.1%) |
| 28 | YE | 0.52 | 0/1601 | 0.91 | 2/2160 (0.1%) |
| 29 | RF | 0.50 | 0/1620 | 0.76 | 0/2194 |
| 29 | YF | 0.50 | 0/1620 | 0.76 | 0/2194 |
| 30 | RG | 0.40 | 0/1499 | 0.66 | 0/2016 |
| 30 | YG | 0.40 | 0/1499 | 0.66 | 0/2016 |
| 31 | RH | 0.45 | 0/1332 | 0.85 | 3/1802 (0.2%) |
| 31 | YH | 0.45 | 0/1332 | 0.85 | 4/1802 (0.2%) |
| 32 | RI | 0.29 | 0/1151 | 0.63 | 0/1558 |
| 32 | YI | 0.30 | 0/1151 | 0.63 | 0/1558 |
| 33 | RN | 0.46 | 0/1131 | 0.78 | 1/1525 (0.1%) |
| 33 | YN | 0.46 | 0/1131 | 0.78 | 1/1525 (0.1%) |
| 34 | RO | 0.53 | 0/943 | 0.71 | 0/1269 |
| 34 | YO | 0.53 | 0/943 | 0.71 | 0/1269 |
| 35 | RP | 0.50 | 0/1162 | 0.94 | 3/1544 (0.2%) |
| 35 | YP | 0.49 | 0/1162 | 0.95 | 3/1544 (0.2%) |
| 36 | RQ | 0.54 | 0/1143 | 0.90 | 3/1527 (0.2%) |
| 36 | YQ | 0.54 | 0/1143 | 0.89 | 3/1527 (0.2%) |
| 37 | RR | 0.45 | 0/982 | 0.80 | 1/1312 (0.1%) |
| 37 | YR | 0.45 | 0/982 | 0.80 | 1/1312 (0.1%) |
| 38 | RS | 0.46 | 0/892 | 0.82 | 1/1187 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | YS | 0.45 | 0/892 | 0.82 | 1/1187 (0.1%) |
| 39 | RT | 0.47 | 0/1155 | 0.73 | 2/1542 (0.1%) |
| 39 | YT | 0.46 | 0/1155 | 0.73 | 2/1542 (0.1%) |
| 40 | RU | 0.48 | 0/982 | 0.78 | 0/1306 |
| 40 | YU | 0.48 | 0/982 | 0.77 | 0/1306 |
| 41 | RV | 0.47 | 0/790 | 0.82 | 0/1057 |
| 41 | YV | 0.47 | 0/790 | 0.82 | 0/1057 |
| 42 | RW | 0.45 | 0/911 | 0.75 | 0/1220 |
| 42 | YW | 0.45 | 0/911 | 0.75 | 0/1220 |
| 43 | RX | 0.56 | 0/739 | 0.77 | 0/993 |
| 43 | YX | 0.56 | 0/739 | 0.77 | 0/993 |
| 44 | RY | 0.52 | 0/798 | 0.80 | 0/1064 |
| 44 | YY | 0.52 | 0/798 | 0.80 | 0/1064 |
| 45 | RZ | 0.32 | 0/1493 | 0.60 | 0/2026 |
| 45 | YZ | 0.33 | 0/1493 | 0.63 | 0/2026 |
| 46 | R0 | 0.30 | 0/657 | 0.56 | 0/874 |
| 46 | Y0 | 0.31 | 0/657 | 0.53 | 0/874 |
| 47 | R1 | 0.49 | 0/770 | 0.85 | 1/1022 (0.1%) |
| 47 | Y1 | 0.49 | 0/770 | 0.85 | 1/1022 (0.1%) |
| 48 | R2 | 0.51 | 0/583 | 0.83 | 1/771 (0.1%) |
| 48 | Y2 | 0.50 | 0/583 | 0.83 | 1/771 (0.1%) |
| 49 | R3 | 0.47 | 0/474 | 0.72 | 0/635 |
| 49 | Y3 | 0.43 | 0/474 | 0.71 | 0/635 |
| 50 | R4 | 0.38 | 0/594 | 0.78 | 1/795 (0.1%) |
| 50 | Y4 | 0.38 | 0/594 | 0.78 | 1/795 (0.1%) |
| 51 | R5 | 0.51 | 0/473 | 0.74 | 0/639 |
| 51 | Y5 | 0.51 | 0/473 | 0.74 | 0/639 |
| 52 | R6 | 0.42 | 0/431 | 0.76 | 0/575 |
| 52 | Y6 | 0.42 | 0/431 | 0.76 | 0/575 |
| 53 | R7 | 0.56 | 0/438 | 0.76 | 0/575 |
| 53 | Y7 | 0.56 | 0/438 | 0.76 | 0/575 |
| 54 | R8 | 0.62 | 0/525 | 0.93 | 1/691 (0.1%) |
| 54 | Y8 | 0.62 | 0/525 | 0.93 | 1/691 (0.1%) |
| 55 | R9 | 0.35 | 0/310 | 0.59 | 0/407 |
| 55 | Y9 | 0.37 | 0/310 | 0.61 | 0/407 |
| 56 | Z6 | 0.79 | 0/40 | 1.79 | 1/60 (1.7%) |
| 56 | Z8 | 0.78 | 0/40 | 1.81 | 1/60 (1.7%) |
| All | All | 0.41 | 9/316323 (0.0%) | 0.87 | 408/472911 (0.1%) |

The worst 5 of 9 bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | RD | 236 | GLY | C-N | 8.55 | 1.53 | 1.34 |
| 25 | YA | 1762 | A | N9-C4 | 6.24 | 1.41 | 1.37 |
| 23 | XX | 8 | A | C6-N6 | 6.10 | 1.38 | 1.33 |
| 25 | RA | 654(T) | C | C1'-N1 | 5.71 | 1.57 | 1.48 |
| 1 | XA | 518 | C | N3-C4 | -5.32 | 1.30 | 1.33 |

The worst 5 of 408 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | QL | 47 | LYS | C-N-CD | -20.48 | 75.56 | 120.60 |
| 12 | XL | 47 | LYS | C-N-CD | -20.46 | 75.59 | 120.60 |
| 1 | XA | 518 | C | C5-C4-N4 | 15.43 | 131.00 | 120.20 |
| 1 | XA | 518 | C | C6-N1-C1' | 12.95 | 136.34 | 120.80 |
| 1 | XA | 518 | C | C2-N1-C1' | -11.78 | 105.84 | 118.80 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | QA | 32247 | 0 | 16278 | 492 | 0 |
| 1 | XA | 32249 | 0 | 16279 | 531 | 1 |
| 2 | QB | 1924 | 0 | 1975 | 287 | 0 |
| 2 | XB | 1924 | 0 | 1975 | 289 | 0 |
| 3 | QC | 1605 | 0 | 1668 | 207 | 0 |
| 3 | XC | 1605 | 0 | 1668 | 207 | 1 |
| 4 | QD | 1703 | 0 | 1764 | 253 | 0 |
| 4 | XD | 1703 | 0 | 1765 | 215 | 0 |
| 5 | QE | 1155 | 0 | 1213 | 136 | 0 |
| 5 | XE | 1155 | 0 | 1213 | 131 | 0 |
| 6 | QF | 843 | 0 | 857 | 94 | 0 |
| 6 | XF | 843 | 0 | 857 | 100 | 0 |
| 7 | QG | 1257 | 0 | 1296 | 145 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 7 | XG | 1257 | 0 | 1296 | 141 | 0 |
| 8 | QH | 1116 | 0 | 1175 | 140 | 0 |
| 8 | XH | 1116 | 0 | 1177 | 144 | 0 |
| 9 | QI | 1010 | 0 | 1037 | 141 | 0 |
| 9 | XI | 1010 | 0 | 1037 | 153 | 0 |
| 10 | QJ | 801 | 0 | 849 | 149 | 0 |
| 10 | XJ | 801 | 0 | 849 | 135 | 0 |
| 11 | QK | 885 | 0 | 904 | 100 | 1 |
| 11 | XK | 885 | 0 | 904 | 103 | 0 |
| 12 | QL | 975 | 0 | 1062 | 104 | 0 |
| 12 | XL | 975 | 0 | 1062 | 108 | 0 |
| 13 | QM | 964 | 0 | 1034 | 161 | 0 |
| 13 | XM | 964 | 0 | 1034 | 161 | 0 |
| 14 | QN | 492 | 0 | 530 | 98 | 0 |
| 14 | XN | 492 | 0 | 529 | 100 | 0 |
| 15 | QO | 734 | 0 | 771 | 75 | 0 |
| 15 | XO | 734 | 0 | 771 | 72 | 0 |
| 16 | QP | 705 | 0 | 725 | 112 | 0 |
| 16 | XP | 705 | 0 | 725 | 110 | 0 |
| 17 | QQ | 834 | 0 | 904 | 83 | 0 |
| 17 | XQ | 834 | 0 | 904 | 75 | 0 |
| 18 | QR | 574 | 0 | 644 | 66 | 0 |
| 18 | XR | 574 | 0 | 644 | 69 | 0 |
| 19 | QS | 674 | 0 | 699 | 113 | 0 |
| 19 | XS | 674 | 0 | 699 | 152 | 0 |
| 20 | QT | 763 | 0 | 860 | 105 | 0 |
| 20 | XT | 763 | 0 | 861 | 101 | 0 |
| 21 | QU | 217 | 0 | 234 | 26 | 0 |
| 21 | XU | 217 | 0 | 234 | 26 | 0 |
| 22 | QV | 1644 | 0 | 836 | 25 | 0 |
| 22 | XV | 1644 | 0 | 836 | 28 | 0 |
| 23 | QX | 167 | 0 | 87 | 12 | 0 |
| 23 | XX | 167 | 0 | 87 | 13 | 0 |
| 24 | QY | 303 | 0 | 154 | 11 | 0 |
| 24 | XY | 303 | 0 | 154 | 11 | 0 |
| 25 | RA | 62071 | 0 | 31285 | 855 | 0 |
| 25 | YA | 62091 | 0 | 31296 | 839 | 0 |
| 26 | RB | 2573 | 0 | 1306 | 58 | 0 |
| 26 | YB | 2573 | 0 | 1306 | 35 | 0 |
| 27 | RD | 2115 | 0 | 2195 | 317 | 0 |
| 27 | YD | 2115 | 0 | 2195 | 320 | 0 |
| 28 | RE | 1568 | 0 | 1634 | 271 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 28 | YE | 1568 | 0 | 1634 | 264 | 0 |
| 29 | RF | 1585 | 0 | 1632 | 177 | 0 |
| 29 | YF | 1585 | 0 | 1632 | 174 | 0 |
| 30 | RG | 1474 | 0 | 1535 | 205 | 0 |
| 30 | YG | 1474 | 0 | 1535 | 183 | 0 |
| 31 | RH | 1307 | 0 | 1382 | 226 | 0 |
| 31 | YH | 1307 | 0 | 1382 | 226 | 0 |
| 32 | RI | 1136 | 0 | 1223 | 69 | 1 |
| 32 | YI | 1136 | 0 | 1223 | 50 | 0 |
| 33 | RN | 1104 | 0 | 1180 | 194 | 0 |
| 33 | YN | 1104 | 0 | 1180 | 189 | 0 |
| 34 | RO | 933 | 0 | 996 | 122 | 0 |
| 34 | YO | 933 | 0 | 996 | 123 | 0 |
| 35 | RP | 1145 | 0 | 1227 | 245 | 0 |
| 35 | YP | 1145 | 0 | 1228 | 242 | 0 |
| 36 | RQ | 1122 | 0 | 1179 | 158 | 0 |
| 36 | YQ | 1122 | 0 | 1179 | 154 | 0 |
| 37 | RR | 968 | 0 | 1033 | 112 | 0 |
| 37 | YR | 968 | 0 | 1033 | 111 | 0 |
| 38 | RS | 882 | 0 | 943 | 160 | 0 |
| 38 | YS | 882 | 0 | 943 | 154 | 0 |
| 39 | RT | 1141 | 0 | 1202 | 150 | 0 |
| 39 | YT | 1141 | 0 | 1202 | 157 | 0 |
| 40 | RU | 964 | 0 | 1022 | 129 | 0 |
| 40 | YU | 964 | 0 | 1022 | 135 | 0 |
| 41 | RV | 779 | 0 | 852 | 129 | 0 |
| 41 | YV | 779 | 0 | 852 | 135 | 1 |
| 42 | RW | 900 | 0 | 964 | 98 | 0 |
| 42 | YW | 900 | 0 | 964 | 98 | 0 |
| 43 | RX | 725 | 0 | 778 | 67 | 0 |
| 43 | YX | 725 | 0 | 778 | 68 | 0 |
| 44 | RY | 785 | 0 | 878 | 168 | 0 |
| 44 | YY | 785 | 0 | 878 | 152 | 0 |
| 45 | RZ | 1461 | 0 | 1493 | 77 | 0 |
| 45 | YZ | 1461 | 0 | 1493 | 59 | 0 |
| 46 | R0 | 648 | 0 | 672 | 27 | 0 |
| 46 | Y0 | 648 | 0 | 672 | 20 | 0 |
| 47 | R1 | 763 | 0 | 848 | 138 | 0 |
| 47 | Y1 | 763 | 0 | 848 | 140 | 0 |
| 48 | R2 | 581 | 0 | 629 | 81 | 0 |
| 48 | Y2 | 581 | 0 | 629 | 76 | 0 |
| 49 | R3 | 469 | 0 | 518 | 39 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 49 | Y3 | 469 | 0 | 518 | 42 | 0 |
| 50 | R4 | 581 | 0 | 574 | 155 | 0 |
| 50 | Y4 | 581 | 0 | 574 | 188 | 0 |
| 51 | R5 | 459 | 0 | 480 | 74 | 0 |
| 51 | Y5 | 459 | 0 | 480 | 75 | 1 |
| 52 | R6 | 424 | 0 | 450 | 92 | 0 |
| 52 | Y6 | 424 | 0 | 450 | 88 | 0 |
| 53 | R7 | 430 | 0 | 480 | 43 | 0 |
| 53 | Y7 | 430 | 0 | 480 | 41 | 0 |
| 54 | R8 | 517 | 0 | 582 | 103 | 0 |
| 54 | Y8 | 517 | 0 | 582 | 103 | 0 |
| 55 | R9 | 307 | 0 | 335 | 18 | 0 |
| 55 | Y9 | 307 | 0 | 336 | 16 | 0 |
| 56 | Z6 | 74 | 0 | 51 | 4 | 0 |
| 56 | Z8 | 74 | 0 | 51 | 6 | 0 |
| 57 | QA | 66 | 0 | 0 | 0 | 0 |
| 57 | QF | 1 | 0 | 0 | 0 | 0 |
| 57 | QH | 1 | 0 | 0 | 0 | 0 |
| 57 | QM | 1 | 0 | 0 | 0 | 0 |
| 57 | QV | 2 | 0 | 0 | 0 | 0 |
| 57 | R0 | 1 | 0 | 0 | 0 | 0 |
| 57 | R5 | 1 | 0 | 0 | 0 | 0 |
| 57 | R8 | 1 | 0 | 0 | 0 | 0 |
| 57 | RA | 241 | 0 | 0 | 0 | 0 |
| 57 | RB | 2 | 0 | 0 | 0 | 0 |
| 57 | RD | 1 | 0 | 0 | 0 | 0 |
| 57 | RE | 2 | 0 | 0 | 0 | 0 |
| 57 | RF | 1 | 0 | 0 | 0 | 0 |
| 57 | RP | 2 | 0 | 0 | 0 | 0 |
| 57 | RR | 1 | 0 | 0 | 0 | 0 |
| 57 | RU | 1 | 0 | 0 | 0 | 0 |
| 57 | XA | 72 | 0 | 0 | 0 | 0 |
| 57 | XM | 1 | 0 | 0 | 0 | 0 |
| 57 | XT | 1 | 0 | 0 | 0 | 0 |
| 57 | XV | 1 | 0 | 0 | 0 | 0 |
| 57 | XX | 1 | 0 | 0 | 0 | 0 |
| 57 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y7 | 1 | 0 | 0 | 0 | 0 |
| 57 | YA | 269 | 0 | 0 | 0 | 0 |
| 57 | YB | 3 | 0 | 0 | 0 | 0 |
| 57 | YD | 1 | 0 | 0 | 0 | 0 |
| 57 | YE | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 57 | YX | 1 | 0 | 0 | 0 | 0 |
| 58 | QA | 42 | 0 | 45 | 1 | 0 |
| 58 | XA | 42 | 0 | 45 | 1 | 0 |
| 59 | QD | 1 | 0 | 0 | 0 | 0 |
| 59 | QN | 1 | 0 | 0 | 0 | 0 |
| 59 | R9 | 1 | 0 | 0 | 0 | 0 |
| 59 | XD | 1 | 0 | 0 | 0 | 0 |
| 59 | XN | 1 | 0 | 0 | 0 | 0 |
| 59 | Y9 | 1 | 0 | 0 | 0 | 0 |
| All | All | 291957 | 0 | 198335 | 14232 | 3 |

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 29.

The worst 5 of 14232 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) |
|---|---|---|---|
| 14:XN:32:SER:CB | 14:XN:41:ARG:HB3 | 1.23 | 1.55 |
| 14:XN:32:SER:HB3 | 14:XN:41:ARG:CB | 1.28 | 1.54 |
| 31:RH:127:GLU:CG | 31:RH:128:PRO:HD3 | 1.36 | 1.53 |
| 31:YH:127:GLU:CG | 31:YH:128:PRO:HD3 | 1.36 | 1.52 |
| 4:XD:22:LYS:CG | 4:XD:26:CYS:SG | 2.01 | 1.49 |

All (3) 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) |
|---|---|---|---|
| 41:YV:51:VAL:N | 51:Y5:60:VAL:O[4_445] | 2.16 | 0.04 |
| 32:RI:91:SER:OG | 1:XA:368:U:OP1[4_555] | 2.17 | 0.03 |
| 11:QK:99:GLN:NE2 | 3:XC:79:ARG:NH2[4_555] | 2.19 | 0.01 |

## 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 | QB | 235/256 (92%) | 153 (65%) | 52 (22%) | 30 (13%) | 0 2 |
| 2 | XB | 235/256 (92%) | 153 (65%) | 52 (22%) | 30 (13%) | 0 2 |
| 3 | QC | 203/239 (85%) | 128 (63%) | 56 (28%) | 19 (9%) | 1 5 |
| 3 | XC | 203/239 (85%) | 129 (64%) | 55 (27%) | 19 (9%) | 1 5 |
| 4 | QD | 206/209 (99%) | 136 (66%) | 50 (24%) | 20 (10%) | 1 4 |
| 4 | XD | 206/209 (99%) | 135 (66%) | 49 (24%) | 22 (11%) | 0 3 |
| 5 | QE | 149/162 (92%) | 103 (69%) | 31 (21%) | 15 (10%) | 1 4 |
| 5 | XE | 149/162 (92%) | 103 (69%) | 30 (20%) | 16 (11%) | 0 3 |
| 6 | QF | 99/101 (98%) | 66 (67%) | 24 (24%) | 9 (9%) | 1 5 |
| 6 | XF | 99/101 (98%) | 66 (67%) | 24 (24%) | 9 (9%) | 1 5 |
| 7 | QG | 153/156 (98%) | 102 (67%) | 36 (24%) | 15 (10%) | 1 4 |
| 7 | XG | 153/156 (98%) | 103 (67%) | 36 (24%) | 14 (9%) | 1 5 |
| 8 | QH | 136/138 (99%) | 92 (68%) | 29 (21%) | 15 (11%) | 0 3 |
| 8 | XH | 136/138 (99%) | 92 (68%) | 29 (21%) | 15 (11%) | 0 3 |
| 9 | QI | 125/128 (98%) | 77 (62%) | 32 (26%) | 16 (13%) | 0 2 |
| 9 | XI | 125/128 (98%) | 77 (62%) | 32 (26%) | 16 (13%) | 0 2 |
| 10 | QJ | 97/105 (92%) | 68 (70%) | 20 (21%) | 9 (9%) | 1 5 |
| 10 | XJ | 97/105 (92%) | 68 (70%) | 19 (20%) | 10 (10%) | 1 4 |
| 11 | QK | 117/129 (91%) | 87 (74%) | 21 (18%) | 9 (8%) | 1 8 |
| 11 | XK | 117/129 (91%) | 87 (74%) | 21 (18%) | 9 (8%) | 1 8 |
| 12 | QL | 123/132 (93%) | 85 (69%) | 24 (20%) | 14 (11%) | 0 3 |
| 12 | XL | 123/132 (93%) | 85 (69%) | 24 (20%) | 14 (11%) | 0 3 |
| 13 | QM | 119/126 (94%) | 71 (60%) | 28 (24%) | 20 (17%) | 0 1 |
| 13 | XM | 119/126 (94%) | 71 (60%) | 26 (22%) | 22 (18%) | 0 0 |
| 14 | QN | 58/61 (95%) | 31 (53%) | 15 (26%) | 12 (21%) | 0 0 |
| 14 | XN | 58/61 (95%) | 32 (55%) | 14 (24%) | 12 (21%) | 0 0 |
| 15 | QO | 86/89 (97%) | 61 (71%) | 19 (22%) | 6 (7%) | 1 10 |
| 15 | XO | 86/89 (97%) | 60 (70%) | 20 (23%) | 6 (7%) | 1 10 |
| 16 | QP | 82/88 (93%) | 48 (58%) | 23 (28%) | 11 (13%) | 0 1 |
| 16 | XP | 82/88 (93%) | 48 (58%) | 23 (28%) | 11 (13%) | 0 1 |
| 17 | QQ | 98/105 (93%) | 75 (76%) | 15 (15%) | 8 (8%) | 1 7 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 17 | XQ | 98/105 (93%) | 75 (76%) | 15 (15%) | 8 (8%) | 1 7 |
| 18 | QR | 68/88 (77%) | 46 (68%) | 14 (21%) | 8 (12%) | 0 3 |
| 18 | XR | 68/88 (77%) | 46 (68%) | 14 (21%) | 8 (12%) | 0 3 |
| 19 | QS | 82/93 (88%) | 47 (57%) | 17 (21%) | 18 (22%) | 0 0 |
| 19 | XS | 82/93 (88%) | 46 (56%) | 18 (22%) | 18 (22%) | 0 0 |
| 20 | QT | 97/106 (92%) | 63 (65%) | 16 (16%) | 18 (19%) | 0 0 |
| 20 | XT | 97/106 (92%) | 63 (65%) | 15 (16%) | 19 (20%) | 0 0 |
| 21 | QU | 23/27 (85%) | 15 (65%) | 4 (17%) | 4 (17%) | 0 1 |
| 21 | XU | 23/27 (85%) | 15 (65%) | 4 (17%) | 4 (17%) | 0 1 |
| 27 | RD | 270/276 (98%) | 203 (75%) | 48 (18%) | 19 (7%) | 1 10 |
| 27 | YD | 270/276 (98%) | 204 (76%) | 47 (17%) | 19 (7%) | 1 10 |
| 28 | RE | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0 0 |
| 28 | YE | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0 0 |
| 29 | RF | 200/210 (95%) | 144 (72%) | 36 (18%) | 20 (10%) | 1 4 |
| 29 | YF | 200/210 (95%) | 144 (72%) | 36 (18%) | 20 (10%) | 1 4 |
| 30 | RG | 179/182 (98%) | 119 (66%) | 39 (22%) | 21 (12%) | 0 3 |
| 30 | YG | 179/182 (98%) | 119 (66%) | 39 (22%) | 21 (12%) | 0 3 |
| 31 | RH | 168/180 (93%) | 94 (56%) | 36 (21%) | 38 (23%) | 0 0 |
| 31 | YH | 168/180 (93%) | 94 (56%) | 36 (21%) | 38 (23%) | 0 0 |
| 32 | RI | 144/148 (97%) | 101 (70%) | 26 (18%) | 17 (12%) | 0 3 |
| 32 | YI | 144/148 (97%) | 103 (72%) | 24 (17%) | 17 (12%) | 0 3 |
| 33 | RN | 136/140 (97%) | 84 (62%) | 30 (22%) | 22 (16%) | 0 1 |
| 33 | YN | 136/140 (97%) | 84 (62%) | 30 (22%) | 22 (16%) | 0 1 |
| 34 | RO | 120/122 (98%) | 90 (75%) | 21 (18%) | 9 (8%) | 1 9 |
| 34 | YO | 120/122 (98%) | 90 (75%) | 21 (18%) | 9 (8%) | 1 9 |
| 35 | RP | 148/150 (99%) | 97 (66%) | 19 (13%) | 32 (22%) | 0 0 |
| 35 | YP | 148/150 (99%) | 97 (66%) | 19 (13%) | 32 (22%) | 0 0 |
| 36 | RQ | 139/141 (99%) | 95 (68%) | 30 (22%) | 14 (10%) | 1 4 |
| 36 | YQ | 139/141 (99%) | 97 (70%) | 28 (20%) | 14 (10%) | 1 4 |
| 37 | RR | 116/118 (98%) | 82 (71%) | 20 (17%) | 14 (12%) | 0 2 |
| 37 | YR | 116/118 (98%) | 82 (71%) | 20 (17%) | 14 (12%) | 0 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 38 | RS | 109/112 (97%) | 62 (57%) | 28 (26%) | 19 (17%) | 0 1 |
| 38 | YS | 109/112 (97%) | 62 (57%) | 28 (26%) | 19 (17%) | 0 1 |
| 39 | RT | 135/146 (92%) | 83 (62%) | 32 (24%) | 20 (15%) | 0 1 |
| 39 | YT | 135/146 (92%) | 83 (62%) | 32 (24%) | 20 (15%) | 0 1 |
| 40 | RU | 115/118 (98%) | 86 (75%) | 20 (17%) | 9 (8%) | 1 8 |
| 40 | YU | 115/118 (98%) | 86 (75%) | 20 (17%) | 9 (8%) | 1 8 |
| 41 | RV | 99/101 (98%) | 73 (74%) | 16 (16%) | 10 (10%) | 1 4 |
| 41 | YV | 99/101 (98%) | 73 (74%) | 16 (16%) | 10 (10%) | 1 4 |
| 42 | RW | 111/113 (98%) | 75 (68%) | 22 (20%) | 14 (13%) | 0 2 |
| 42 | YW | 111/113 (98%) | 75 (68%) | 22 (20%) | 14 (13%) | 0 2 |
| 43 | RX | 90/96 (94%) | 77 (86%) | 8 (9%) | 5 (6%) | 2 18 |
| 43 | YX | 90/96 (94%) | 77 (86%) | 8 (9%) | 5 (6%) | 2 18 |
| 44 | RY | 100/110 (91%) | 58 (58%) | 16 (16%) | 26 (26%) | 0 0 |
| 44 | YY | 100/110 (91%) | 57 (57%) | 17 (17%) | 26 (26%) | 0 0 |
| 45 | RZ | 181/206 (88%) | 118 (65%) | 39 (22%) | 24 (13%) | 0 2 |
| 45 | YZ | 181/206 (88%) | 130 (72%) | 34 (19%) | 17 (9%) | 1 5 |
| 46 | R0 | 80/85 (94%) | 69 (86%) | 8 (10%) | 3 (4%) | 4 28 |
| 46 | Y0 | 80/85 (94%) | 70 (88%) | 9 (11%) | 1 (1%) | 15 58 |
| 47 | R1 | 95/98 (97%) | 64 (67%) | 20 (21%) | 11 (12%) | 0 3 |
| 47 | Y1 | 95/98 (97%) | 64 (67%) | 20 (21%) | 11 (12%) | 0 3 |
| 48 | R2 | 67/72 (93%) | 47 (70%) | 11 (16%) | 9 (13%) | 0 1 |
| 48 | Y2 | 67/72 (93%) | 47 (70%) | 11 (16%) | 9 (13%) | 0 1 |
| 49 | R3 | 57/60 (95%) | 45 (79%) | 9 (16%) | 3 (5%) | 2 19 |
| 49 | Y3 | 57/60 (95%) | 45 (79%) | 9 (16%) | 3 (5%) | 2 19 |
| 50 | R4 | 69/71 (97%) | 23 (33%) | 20 (29%) | 26 (38%) | 0 0 |
| 50 | Y4 | 69/71 (97%) | 23 (33%) | 20 (29%) | 26 (38%) | 0 0 |
| 51 | R5 | 57/60 (95%) | 33 (58%) | 9 (16%) | 15 (26%) | 0 0 |
| 51 | Y5 | 57/60 (95%) | 33 (58%) | 9 (16%) | 15 (26%) | 0 0 |
| 52 | R6 | 47/54 (87%) | 15 (32%) | 18 (38%) | 14 (30%) | 0 0 |
| 52 | Y6 | 47/54 (87%) | 15 (32%) | 18 (38%) | 14 (30%) | 0 0 |
| 53 | R7 | 47/49 (96%) | 37 (79%) | 7 (15%) | 3 (6%) | 2 13 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 53 | Y7 | 47/49 (96%) | 37 (79%) | 7 (15%) | 3 (6%) | 2 13 |
| 54 | R8 | 62/65 (95%) | 36 (58%) | 15 (24%) | 11 (18%) | 0 0 |
| 54 | Y8 | 62/65 (95%) | 36 (58%) | 15 (24%) | 11 (18%) | 0 0 |
| 55 | R9 | 35/37 (95%) | 31 (89%) | 4 (11%) | 0 | 100 100 |
| 55 | Y9 | 35/37 (95%) | 31 (89%) | 4 (11%) | 0 | 100 100 |
| All | All | 11470/12128 (95%) | 7647 (67%) | 2334 (20%) | 1489 (13%) | 0 2 |

5 of 1489 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | QB | 6 | THR |
| 2 | QB | 15 | VAL |
| 2 | QB | 26 | PRO |
| 2 | QB | 84 | GLU |
| 2 | QB | 88 | ALA |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | QB | 205/220 (93%) | 181 (88%) | 24 (12%) | 7 30 |
| 2 | XB | 205/220 (93%) | 181 (88%) | 24 (12%) | 7 30 |
| 3 | QC | 159/188 (85%) | 143 (90%) | 16 (10%) | 9 37 |
| 3 | XC | 159/188 (85%) | 143 (90%) | 16 (10%) | 9 37 |
| 4 | QD | 180/181 (99%) | 160 (89%) | 20 (11%) | 8 32 |
| 4 | XD | 180/181 (99%) | 165 (92%) | 15 (8%) | 14 49 |
| 5 | QE | 116/123 (94%) | 108 (93%) | 8 (7%) | 19 59 |
| 5 | XE | 116/123 (94%) | 107 (92%) | 9 (8%) | 16 53 |
| 6 | QF | 90/90 (100%) | 76 (84%) | 14 (16%) | 3 15 |
| 6 | XF | 90/90 (100%) | 76 (84%) | 14 (16%) | 3 15 |
| 7 | QG | 126/127 (99%) | 114 (90%) | 12 (10%) | 11 40 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 7 | XG | 126/127 (99%) | 115 (91%) | 11 (9%) | 13 45 |
| 8 | QH | 119/119 (100%) | 106 (89%) | 13 (11%) | 8 33 |
| 8 | XH | 119/119 (100%) | 106 (89%) | 13 (11%) | 8 33 |
| 9 | QI | 98/99 (99%) | 87 (89%) | 11 (11%) | 7 32 |
| 9 | XI | 98/99 (99%) | 87 (89%) | 11 (11%) | 7 32 |
| 10 | QJ | 89/92 (97%) | 81 (91%) | 8 (9%) | 12 43 |
| 10 | XJ | 89/92 (97%) | 81 (91%) | 8 (9%) | 12 43 |
| 11 | QK | 90/99 (91%) | 81 (90%) | 9 (10%) | 9 37 |
| 11 | XK | 90/99 (91%) | 81 (90%) | 9 (10%) | 9 37 |
| 12 | QL | 104/109 (95%) | 90 (86%) | 14 (14%) | 5 22 |
| 12 | XL | 104/109 (95%) | 90 (86%) | 14 (14%) | 5 22 |
| 13 | QM | 97/101 (96%) | 81 (84%) | 16 (16%) | 3 13 |
| 13 | XM | 97/101 (96%) | 81 (84%) | 16 (16%) | 3 13 |
| 14 | QN | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 11 |
| 14 | XN | 49/50 (98%) | 44 (90%) | 5 (10%) | 9 36 |
| 15 | QO | 79/80 (99%) | 73 (92%) | 6 (8%) | 16 55 |
| 15 | XO | 79/80 (99%) | 73 (92%) | 6 (8%) | 16 55 |
| 16 | QP | 72/74 (97%) | 63 (88%) | 9 (12%) | 6 26 |
| 16 | XP | 72/74 (97%) | 63 (88%) | 9 (12%) | 6 26 |
| 17 | QQ | 95/97 (98%) | 89 (94%) | 6 (6%) | 22 63 |
| 17 | XQ | 95/97 (98%) | 89 (94%) | 6 (6%) | 22 63 |
| 18 | QR | 61/77 (79%) | 54 (88%) | 7 (12%) | 7 31 |
| 18 | XR | 61/77 (79%) | 54 (88%) | 7 (12%) | 7 31 |
| 19 | QS | 73/80 (91%) | 62 (85%) | 11 (15%) | 3 17 |
| 19 | XS | 73/80 (91%) | 62 (85%) | 11 (15%) | 3 17 |
| 20 | QT | 76/82 (93%) | 68 (90%) | 8 (10%) | 8 35 |
| 20 | XT | 76/82 (93%) | 68 (90%) | 8 (10%) | 8 35 |
| 21 | QU | 20/22 (91%) | 19 (95%) | 1 (5%) | 30 71 |
| 21 | XU | 20/22 (91%) | 19 (95%) | 1 (5%) | 30 71 |
| 27 | RD | 214/218 (98%) | 177 (83%) | 37 (17%) | 2 12 |
| 27 | YD | 214/218 (98%) | 177 (83%) | 37 (17%) | 2 12 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 28 | RE | 165/166 (99%) | 127 (77%) | 38 (23%) | 1 5 |
| 28 | YE | 165/166 (99%) | 127 (77%) | 38 (23%) | 1 5 |
| 29 | RF | 161/166 (97%) | 140 (87%) | 21 (13%) | 5 24 |
| 29 | YF | 161/166 (97%) | 140 (87%) | 21 (13%) | 5 24 |
| 30 | RG | 155/156 (99%) | 130 (84%) | 25 (16%) | 3 14 |
| 30 | YG | 155/156 (99%) | 130 (84%) | 25 (16%) | 3 14 |
| 31 | RH | 142/148 (96%) | 114 (80%) | 28 (20%) | 1 8 |
| 31 | YH | 142/148 (96%) | 114 (80%) | 28 (20%) | 1 8 |
| 32 | RI | 122/124 (98%) | 94 (77%) | 28 (23%) | 1 5 |
| 32 | YI | 122/124 (98%) | 93 (76%) | 29 (24%) | 1 4 |
| 33 | RN | 117/119 (98%) | 98 (84%) | 19 (16%) | 3 14 |
| 33 | YN | 117/119 (98%) | 98 (84%) | 19 (16%) | 3 14 |
| 34 | RO | 100/100 (100%) | 90 (90%) | 10 (10%) | 9 37 |
| 34 | YO | 100/100 (100%) | 90 (90%) | 10 (10%) | 9 37 |
| 35 | RP | 116/116 (100%) | 89 (77%) | 27 (23%) | 1 4 |
| 35 | YP | 116/116 (100%) | 89 (77%) | 27 (23%) | 1 4 |
| 36 | RQ | 111/111 (100%) | 93 (84%) | 18 (16%) | 3 14 |
| 36 | YQ | 111/111 (100%) | 93 (84%) | 18 (16%) | 3 14 |
| 37 | RR | 101/101 (100%) | 84 (83%) | 17 (17%) | 2 13 |
| 37 | YR | 101/101 (100%) | 84 (83%) | 17 (17%) | 2 13 |
| 38 | RS | 87/88 (99%) | 74 (85%) | 13 (15%) | 4 17 |
| 38 | YS | 87/88 (99%) | 74 (85%) | 13 (15%) | 4 17 |
| 39 | RT | 120/127 (94%) | 97 (81%) | 23 (19%) | 2 10 |
| 39 | YT | 120/127 (94%) | 97 (81%) | 23 (19%) | 2 10 |
| 40 | RU | 93/94 (99%) | 80 (86%) | 13 (14%) | 4 20 |
| 40 | YU | 93/94 (99%) | 80 (86%) | 13 (14%) | 4 20 |
| 41 | RV | 82/82 (100%) | 71 (87%) | 11 (13%) | 5 23 |
| 41 | YV | 82/82 (100%) | 71 (87%) | 11 (13%) | 5 23 |
| 42 | RW | 92/92 (100%) | 77 (84%) | 15 (16%) | 3 14 |
| 42 | YW | 92/92 (100%) | 77 (84%) | 15 (16%) | 3 14 |
| 43 | RX | 74/78 (95%) | 63 (85%) | 11 (15%) | 4 17 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 43 | YX | 74/78 (95%) | 63 (85%) | 11 (15%) | 4 17 |
| 44 | RY | 85/91 (93%) | 70 (82%) | 15 (18%) | 2 12 |
| 44 | YY | 85/91 (93%) | 70 (82%) | 15 (18%) | 2 12 |
| 45 | RZ | 162/179 (90%) | 140 (86%) | 22 (14%) | 5 22 |
| 45 | YZ | 162/179 (90%) | 140 (86%) | 22 (14%) | 5 22 |
| 46 | R0 | 65/67 (97%) | 60 (92%) | 5 (8%) | 16 54 |
| 46 | Y0 | 65/67 (97%) | 61 (94%) | 4 (6%) | 23 64 |
| 47 | R1 | 82/83 (99%) | 67 (82%) | 15 (18%) | 2 11 |
| 47 | Y1 | 82/83 (99%) | 67 (82%) | 15 (18%) | 2 11 |
| 48 | R2 | 64/67 (96%) | 57 (89%) | 7 (11%) | 8 33 |
| 48 | Y2 | 64/67 (96%) | 57 (89%) | 7 (11%) | 8 33 |
| 49 | R3 | 51/52 (98%) | 40 (78%) | 11 (22%) | 1 7 |
| 49 | Y3 | 51/52 (98%) | 40 (78%) | 11 (22%) | 1 7 |
| 50 | R4 | 63/63 (100%) | 44 (70%) | 19 (30%) | 0 1 |
| 50 | Y4 | 63/63 (100%) | 44 (70%) | 19 (30%) | 0 1 |
| 51 | R5 | 51/52 (98%) | 39 (76%) | 12 (24%) | 1 4 |
| 51 | Y5 | 51/52 (98%) | 39 (76%) | 12 (24%) | 1 4 |
| 52 | R6 | 48/52 (92%) | 38 (79%) | 10 (21%) | 1 7 |
| 52 | Y6 | 48/52 (92%) | 38 (79%) | 10 (21%) | 1 7 |
| 53 | R7 | 42/42 (100%) | 39 (93%) | 3 (7%) | 18 57 |
| 53 | Y7 | 42/42 (100%) | 39 (93%) | 3 (7%) | 18 57 |
| 54 | R8 | 54/55 (98%) | 39 (72%) | 15 (28%) | 0 2 |
| 54 | Y8 | 54/55 (98%) | 39 (72%) | 15 (28%) | 0 2 |
| 55 | R9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 24 65 |
| 55 | Y9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 24 65 |
| All | All | 9702/10066 (96%) | 8287 (85%) | 1415 (15%) | 4 18 |

5 of 1415 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | R3 | 4 | LEU |
| 7 | XG | 78 | ARG |
| 45 | YZ | 112 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | R4 | 48 | ARG |
| 2 | XB | 36 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | R0 | 29 | GLN |
| 5 | XE | 72 | GLN |
| 43 | YX | 87 | GLN |
| 47 | R1 | 56 | GLN |
| 49 | R3 | 32 | GLN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | QA | 1499/1522 (98%) | 296 (19%) | 46 (3%) |
| 1 | XA | 1499/1522 (98%) | 294 (19%) | 52 (3%) |
| 22 | QV | 76/77 (98%) | 30 (39%) | 1 (1%) |
| 22 | XV | 76/77 (98%) | 30 (39%) | 1 (1%) |
| 23 | QX | 7/25 (28%) | 5 (71%) | 1 (14%) |
| 23 | XX | 7/25 (28%) | 5 (71%) | 0 |
| 24 | QY | 13/18 (72%) | 5 (38%) | 1 (7%) |
| 24 | XY | 13/18 (72%) | 5 (38%) | 1 (7%) |
| 25 | RA | 2879/2916 (98%) | 623 (21%) | 73 (2%) |
| 25 | YA | 2880/2916 (98%) | 626 (21%) | 70 (2%) |
| 26 | RB | 119/122 (97%) | 25 (21%) | 2 (1%) |
| 26 | YB | 119/122 (97%) | 30 (25%) | 1 (0%) |
| 56 | Z6 | 1/3 (33%) | 0 | 0 |
| 56 | Z8 | 1/3 (33%) | 0 | 0 |
| All | All | 9189/9366 (98%) | 1974 (21%) | 249 (2%) |

5 of 1974 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | QA | 6 | G |
| 1 | QA | 7 | G |
| 1 | QA | 8 | A |
| 1 | QA | 9 | G |
| 1 | QA | 32 | A |

5 of 249 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | RA | 2518 | A |
| 1 | XA | 412 | A |
| 25 | YA | 1992 | G |
| 25 | RA | 2689 | U |
| 1 | XA | 60 | A |

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 24 | 1MG | QY | 37 | 24 | 16,26,27 | 2.90 | 3 (18%) | 19,39,42 | 1.56 | 4 (21%) |
| 24 | 1MG | XY | 37 | 24 | 16,26,27 | 2.92 | 3 (18%) | 19,39,42 | 1.57 | 4 (21%) |
| 56 | PPU | Z6 | 76 | 25,56 | 30,40,41 | 2.59 | 6 (20%) | 37,57,60 | 3.25 | 11 (29%) |
| 56 | PPU | Z8 | 76 | 25,56 | 30,40,41 | 2.57 | 6 (20%) | 37,57,60 | 3.25 | 11 (29%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | 1MG | QY | 37 | 24 | - | 0/3/25/26 | 0/3/3/3 |
| 24 | 1MG | XY | 37 | 24 | - | 0/3/25/26 | 0/3/3/3 |
| 56 | PPU | Z6 | 76 | 25,56 | - | 0/21/43/44 | 0/4/4/4 |
| 56 | PPU | Z8 | 76 | 25,56 | - | 0/21/43/44 | 0/4/4/4 |

The worst 5 of 18 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 56 | Z6 | 76 | PPU | C9-N6 | -5.63 | 1.31 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 56 | Z8 | 76 | PPU | C9-N6 | -5.61 | 1.32 | 1.45 |
| 56 | Z6 | 76 | PPU | C10-N6 | -5.30 | 1.32 | 1.45 |
| 56 | Z8 | 76 | PPU | C10-N6 | -5.29 | 1.32 | 1.45 |
| 56 | Z6 | 76 | PPU | C5-N7 | -2.01 | 1.32 | 1.39 |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 56 | Z8 | 76 | PPU | C2'-C1'-N9 | -10.33 | 98.50 | 114.29 |
| 56 | Z6 | 76 | PPU | C2'-C1'-N9 | -10.32 | 98.52 | 114.29 |
| 56 | Z8 | 76 | PPU | N3-C2-N1 | -9.82 | 121.37 | 128.89 |
| 56 | Z6 | 76 | PPU | N3-C2-N1 | -9.76 | 121.42 | 128.89 |
| 56 | Z6 | 76 | PPU | C3'-N3'-C | -8.24 | 110.21 | 123.18 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | QY | 37 | 1MG | 1 | 0 |
| 24 | XY | 37 | 1MG | 1 | 0 |
| 56 | Z6 | 76 | PPU | 4 | 0 |
| 56 | Z8 | 76 | PPU | 6 | 0 |

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 687 ligands modelled in this entry, 685 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 58 | PAR | QA | 1667 | - | 45,45,45 | 1.31 | 7 (15%) | 59,67,67 | 1.41 | 7 (11%) |
| 58 | PAR | XA | 1673 | - | 45,45,45 | 1.35 | 6 (13%) | 59,67,67 | 1.34 | 5 (8%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 58 | PAR | QA | 1667 | - | - | 0/18/94/94 | 0/4/4/4 |
| 58 | PAR | XA | 1673 | - | - | 0/18/94/94 | 0/4/4/4 |

The worst 5 of 13 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 58 | QA | 1667 | PAR | C14-C24 | 2.03 | 1.56 | 1.52 |
| 58 | QA | 1667 | PAR | C11-C21 | 2.18 | 1.56 | 1.52 |
| 58 | QA | 1667 | PAR | C31-C21 | 2.19 | 1.56 | 1.53 |
| 58 | XA | 1673 | PAR | C14-C24 | 2.21 | 1.56 | 1.52 |
| 58 | QA | 1667 | PAR | O51-C11 | 2.30 | 1.47 | 1.41 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 58 | QA | 1667 | PAR | O11-C42-C32 | -2.97 | 101.73 | 108.92 |
| 58 | QA | 1667 | PAR | O54-C54-C44 | -2.07 | 105.80 | 109.68 |
| 58 | XA | 1673 | PAR | C11-O51-C51 | 2.59 | 118.76 | 113.75 |
| 58 | XA | 1673 | PAR | O54-C54-C64 | 2.68 | 111.33 | 106.10 |
| 58 | QA | 1667 | PAR | O54-C54-C64 | 2.79 | 111.55 | 106.10 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 58 | QA | 1667 | PAR | 1 | 0 |
| 58 | XA | 1673 | PAR | 1 | 0 |

## 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, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | QA | 1500/1522 (98%) | 0.21 | 53 (3%) 48 34 | 49, 89, 176, 309 | 0 |
| 1 | XA | 1500/1522 (98%) | 0.16 | 50 (3%) 50 37 | 41, 81, 178, 324 | 0 |
| 2 | QB | 237/256 (92%) | 0.59 | 21 (8%) 12 7 | 88, 147, 217, 264 | 0 |
| 2 | XB | 237/256 (92%) | 0.43 | 16 (6%) 20 12 | 70, 122, 194, 242 | 0 |
| 3 | QC | 205/239 (85%) | 0.68 | 19 (9%) 11 7 | 81, 126, 182, 248 | 0 |
| 3 | XC | 205/239 (85%) | 0.17 | 5 (2%) 62 50 | 56, 100, 159, 208 | 0 |
| 4 | QD | 208/209 (99%) | 0.29 | 8 (3%) 44 30 | 53, 96, 150, 208 | 0 |
| 4 | XD | 208/209 (99%) | 0.38 | 10 (4%) 34 23 | 45, 95, 147, 226 | 0 |
| 5 | QE | 151/162 (93%) | 0.51 | 11 (7%) 18 11 | 54, 107, 156, 244 | 0 |
| 5 | XE | 151/162 (93%) | 0.09 | 4 (2%) 59 47 | 47, 84, 135, 167 | 0 |
| 6 | QF | 101/101 (100%) | 0.25 | 1 (0%) 84 77 | 45, 90, 129, 174 | 0 |
| 6 | XF | 101/101 (100%) | 0.20 | 2 (1%) 68 56 | 48, 87, 125, 178 | 0 |
| 7 | QG | 155/156 (99%) | 0.43 | 14 (9%) 12 7 | 66, 115, 166, 229 | 0 |
| 7 | XG | 155/156 (99%) | 0.25 | 11 (7%) 19 12 | 68, 107, 155, 214 | 0 |
| 8 | QH | 138/138 (100%) | 0.31 | 7 (5%) 32 20 | 55, 103, 153, 176 | 0 |
| 8 | XH | 138/138 (100%) | 0.04 | 2 (1%) 78 67 | 53, 90, 130, 158 | 0 |
| 9 | QI | 127/128 (99%) | 0.91 | 16 (12%) 5 3 | 71, 131, 193, 226 | 0 |
| 9 | XI | 127/128 (99%) | 0.76 | 11 (8%) 13 8 | 58, 121, 176, 214 | 0 |
| 10 | QJ | 99/105 (94%) | 1.71 | 35 (35%) 0 1 | 81, 161, 235, 275 | 0 |
| 10 | XJ | 99/105 (94%) | 0.98 | 13 (13%) 5 3 | 59, 128, 180, 212 | 0 |
| 11 | QK | 119/129 (92%) | 0.67 | 12 (10%) 9 6 | 56, 95, 161, 209 | 0 |
| 11 | XK | 119/129 (92%) | 0.33 | 4 (3%) 49 35 | 47, 86, 151, 204 | 0 |
| 12 | QL | 125/132 (94%) | 0.48 | 6 (4%) 34 23 | 56, 93, 157, 241 | 0 |
| 12 | XL | 125/132 (94%) | 0.22 | 7 (5%) 28 17 | 33, 70, 130, 235 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | QM | 121/126 (96%) | 0.70 | 12 (9%) 9 6 | 59, 130, 190, 293 | 0 |
| 13 | XM | 121/126 (96%) | 0.38 | 8 (6%) 22 13 | 63, 114, 165, 262 | 0 |
| 14 | QN | 60/61 (98%) | 1.12 | 11 (18%) 2 1 | 72, 123, 164, 178 | 0 |
| 14 | XN | 60/61 (98%) | 0.51 | 3 (5%) 32 21 | 59, 92, 132, 161 | 0 |
| 15 | QO | 88/89 (98%) | 0.34 | 6 (6%) 20 12 | 56, 98, 153, 188 | 0 |
| 15 | XO | 88/89 (98%) | 0.44 | 7 (7%) 15 9 | 46, 84, 134, 150 | 0 |
| 16 | QP | 84/88 (95%) | 0.35 | 0 100 100 | 48, 87, 135, 191 | 0 |
| 16 | XP | 84/88 (95%) | 0.26 | 3 (3%) 46 33 | 59, 97, 142, 225 | 0 |
| 17 | QQ | 100/105 (95%) | 0.54 | 3 (3%) 54 41 | 60, 100, 144, 205 | 0 |
| 17 | XQ | 100/105 (95%) | 0.34 | 6 (6%) 25 15 | 60, 100, 147, 175 | 0 |
| 18 | QR | 70/88 (79%) | 0.36 | 2 (2%) 55 42 | 44, 94, 144, 177 | 0 |
| 18 | XR | 70/88 (79%) | 0.14 | 2 (2%) 55 42 | 50, 88, 136, 179 | 0 |
| 19 | QS | 84/93 (90%) | 0.94 | 14 (16%) 2 2 | 94, 142, 188, 229 | 0 |
| 19 | XS | 84/93 (90%) | 0.56 | 6 (7%) 19 12 | 74, 117, 173, 225 | 0 |
| 20 | QT | 99/106 (93%) | 0.52 | 6 (6%) 25 15 | 66, 105, 159, 206 | 0 |
| 20 | XT | 99/106 (93%) | 0.36 | 5 (5%) 32 20 | 60, 108, 168, 201 | 0 |
| 21 | QU | 25/27 (92%) | 2.45 | 11 (44%) 0 0 | 76, 114, 154, 186 | 0 |
| 21 | XU | 25/27 (92%) | 1.43 | 7 (28%) 1 1 | 59, 101, 140, 155 | 0 |
| 22 | QV | 77/77 (100%) | 0.58 | 7 (9%) 11 7 | 49, 107, 178, 226 | 0 |
| 22 | XV | 77/77 (100%) | 0.34 | 1 (1%) 79 69 | 43, 92, 154, 198 | 0 |
| 23 | QX | 8/25 (32%) | 0.98 | 0 100 100 | 66, 95, 136, 155 | 0 |
| 23 | XX | 8/25 (32%) | 0.77 | 1 (12%) 5 3 | 56, 74, 96, 136 | 0 |
| 24 | QY | 13/18 (72%) | 2.15 | 4 (30%) 1 1 | 103, 170, 239, 259 | 0 |
| 24 | XY | 13/18 (72%) | 2.05 | 6 (46%) 0 0 | 71, 145, 218, 228 | 0 |
| 25 | RA | 2882/2916 (98%) | 0.26 | 179 (6%) 24 15 | 37, 67, 225, 362 | 0 |
| 25 | YA | 2883/2916 (98%) | 0.11 | 134 (4%) 36 24 | 28, 58, 202, 336 | 0 |
| 26 | RB | 120/122 (98%) | 0.19 | 1 (0%) 87 80 | 70, 97, 127, 172 | 0 |
| 26 | YB | 120/122 (98%) | 0.07 | 2 (1%) 73 62 | 57, 84, 112, 160 | 0 |
| 27 | RD | 272/276 (98%) | 0.02 | 3 (1%) 82 73 | 30, 64, 103, 185 | 0 |
| 27 | YD | 272/276 (98%) | -0.16 | 2 (0%) 89 83 | 21, 55, 91, 213 | 0 |
| 28 | RE | 205/206 (99%) | 0.16 | 6 (2%) 55 42 | 37, 75, 150, 272 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | YE | 205/206 (99%) | 0.10 | 3 (1%) 76 65 | 33, 73, 141, 240 | 0 |
| 29 | RF | 202/210 (96%) | 0.01 | 2 (0%) 84 77 | 35, 81, 142, 186 | 0 |
| 29 | YF | 202/210 (96%) | -0.15 | 1 (0%) 91 87 | 19, 62, 127, 157 | 0 |
| 30 | RG | 181/182 (99%) | 1.82 | 73 (40%) 0 0 | 79, 152, 236, 277 | 0 |
| 30 | YG | 181/182 (99%) | 0.52 | 15 (8%) 14 8 | 59, 103, 159, 224 | 0 |
| 31 | RH | 170/180 (94%) | 1.47 | 49 (28%) 1 1 | 89, 159, 219, 257 | 0 |
| 31 | YH | 170/180 (94%) | 0.39 | 9 (5%) 30 19 | 50, 97, 137, 194 | 0 |
| 32 | RI | 146/148 (98%) | 0.73 | 19 (13%) 5 3 | 53, 122, 189, 282 | 0 |
| 32 | YI | 146/148 (98%) | 0.19 | 8 (5%) 29 18 | 48, 107, 166, 198 | 0 |
| 33 | RN | 138/140 (98%) | 0.32 | 7 (5%) 32 20 | 52, 90, 138, 201 | 0 |
| 33 | YN | 138/140 (98%) | -0.06 | 1 (0%) 89 83 | 45, 73, 129, 177 | 0 |
| 34 | RO | 122/122 (100%) | 0.02 | 0 100 100 | 39, 77, 111, 136 | 0 |
| 34 | YO | 122/122 (100%) | -0.14 | 0 100 100 | 36, 67, 96, 125 | 0 |
| 35 | RP | 150/150 (100%) | 0.47 | 12 (8%) 15 9 | 34, 88, 161, 221 | 0 |
| 35 | YP | 150/150 (100%) | 0.21 | 4 (2%) 58 45 | 24, 73, 137, 220 | 0 |
| 36 | RQ | 141/141 (100%) | 0.30 | 9 (6%) 23 14 | 45, 87, 138, 207 | 0 |
| 36 | YQ | 141/141 (100%) | 0.11 | 5 (3%) 48 34 | 35, 69, 135, 176 | 0 |
| 37 | RR | 118/118 (100%) | -0.08 | 1 (0%) 87 80 | 40, 70, 105, 146 | 0 |
| 37 | YR | 118/118 (100%) | -0.12 | 0 100 100 | 39, 69, 108, 143 | 0 |
| 38 | RS | 111/112 (99%) | 0.25 | 3 (2%) 58 45 | 61, 98, 149, 192 | 0 |
| 38 | YS | 111/112 (99%) | 0.10 | 3 (2%) 58 45 | 51, 87, 133, 188 | 0 |
| 39 | RT | 137/146 (93%) | 0.46 | 13 (9%) 10 7 | 46, 85, 188, 243 | 0 |
| 39 | YT | 137/146 (93%) | 0.19 | 8 (5%) 26 16 | 47, 77, 174, 265 | 0 |
| 40 | RU | 117/118 (99%) | 0.24 | 4 (3%) 49 35 | 36, 76, 134, 205 | 0 |
| 40 | YU | 117/118 (99%) | -0.10 | 2 (1%) 73 62 | 26, 59, 118, 220 | 0 |
| 41 | RV | 101/101 (100%) | 0.25 | 3 (2%) 54 41 | 42, 96, 169, 265 | 0 |
| 41 | YV | 101/101 (100%) | -0.03 | 2 (1%) 68 56 | 38, 85, 145, 208 | 0 |
| 42 | RW | 113/113 (100%) | 0.11 | 3 (2%) 58 45 | 39, 63, 114, 239 | 0 |
| 42 | YW | 113/113 (100%) | 0.06 | 1 (0%) 85 79 | 35, 60, 116, 221 | 0 |
| 43 | RX | 92/96 (95%) | 0.27 | 5 (5%) 29 19 | 49, 75, 117, 147 | 0 |
| 43 | YX | 92/96 (95%) | 0.02 | 0 100 100 | 38, 61, 99, 127 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | RY | 102/110 (92%) | 1.02 | 21 (20%) 1 1 | 63, 121, 197, 242 | 0 |
| 44 | YY | 102/110 (92%) | 0.30 | 6 (5%) 26 15 | 46, 89, 170, 226 | 0 |
| 45 | RZ | 183/206 (88%) | 0.69 | 23 (12%) 5 3 | 66, 122, 199, 239 | 0 |
| 45 | YZ | 183/206 (88%) | 0.56 | 17 (9%) 11 7 | 54, 112, 199, 258 | 0 |
| 46 | R0 | 82/85 (96%) | 0.17 | 1 (1%) 81 71 | 52, 75, 101, 157 | 0 |
| 46 | Y0 | 82/85 (96%) | -0.07 | 0 100 100 | 43, 71, 90, 104 | 0 |
| 47 | R1 | 97/98 (98%) | 0.64 | 11 (11%) 7 5 | 44, 76, 158, 289 | 0 |
| 47 | Y1 | 97/98 (98%) | 0.40 | 6 (6%) 24 15 | 36, 65, 174, 221 | 0 |
| 48 | R2 | 69/72 (95%) | 0.22 | 1 (1%) 78 67 | 53, 99, 158, 195 | 0 |
| 48 | Y2 | 69/72 (95%) | 0.18 | 3 (4%) 39 26 | 32, 74, 159, 183 | 0 |
| 49 | R3 | 59/60 (98%) | 0.55 | 7 (11%) 6 4 | 51, 87, 139, 197 | 0 |
| 49 | Y3 | 59/60 (98%) | 0.18 | 3 (5%) 32 20 | 49, 74, 125, 182 | 0 |
| 50 | R4 | 71/71 (100%) | 1.92 | 28 (39%) 0 0 | 126, 200, 274, 317 | 0 |
| 50 | Y4 | 71/71 (100%) | 1.14 | 18 (25%) 1 1 | 88, 160, 235, 285 | 0 |
| 51 | R5 | 59/60 (98%) | 1.03 | 12 (20%) 1 1 | 39, 79, 219, 237 | 0 |
| 51 | Y5 | 59/60 (98%) | 0.50 | 8 (13%) 4 3 | 32, 77, 222, 240 | 0 |
| 52 | R6 | 49/54 (90%) | 2.14 | 23 (46%) 0 0 | 93, 153, 224, 237 | 0 |
| 52 | Y6 | 49/54 (90%) | 2.10 | 24 (48%) 0 0 | 83, 146, 203, 230 | 0 |
| 53 | R7 | 49/49 (100%) | 0.15 | 4 (8%) 14 8 | 36, 52, 107, 191 | 0 |
| 53 | Y7 | 49/49 (100%) | 0.03 | 3 (6%) 25 15 | 29, 41, 104, 206 | 0 |
| 54 | R8 | 64/65 (98%) | 0.60 | 6 (9%) 11 7 | 48, 73, 141, 217 | 0 |
| 54 | Y8 | 64/65 (98%) | 0.40 | 2 (3%) 52 40 | 36, 66, 121, 208 | 0 |
| 55 | R9 | 37/37 (100%) | 3.40 | 28 (75%) 0 0 | 86, 127, 179, 254 | 0 |
| 55 | Y9 | 37/37 (100%) | 2.11 | 19 (51%) 0 0 | 72, 109, 161, 206 | 0 |
| 56 | Z6 | 2/3 (66%) | 0.61 | 0 100 100 | 57, 57, 57, 66 | 0 |
| 56 | Z8 | 2/3 (66%) | 0.14 | 0 100 100 | 47, 47, 47, 55 | 0 |
| All | All | 20871/21494 (97%) | 0.32 | 1335 (6%) 23 14 | 19, 84, 183, 362 | 0 |

The worst 5 of 1335 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 25 | RA | 1096 | A | 17.1 |
| 25 | RA | 2116 | G | 14.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 25 | YA | 2125 | G | 13.5 |
| 12 | QL | 129 | ALA | 13.0 |
| 7 | QG | 81 | GLY | 12.9 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 56 | PPU | Z6 | 76 | 37/38 | 0.94 | 0.26 | - | 57,57,57,57 | 0 |
| 56 | PPU | Z8 | 76 | 37/38 | 0.94 | 0.25 | - | 45,45,45,45 | 0 |
| 24 | 1MG | XY | 37 | 24/25 | 0.93 | 0.16 | - | 79,79,79,79 | 0 |
| 24 | 1MG | QY | 37 | 24/25 | 0.93 | 0.17 | - | 98,98,98,98 | 0 |

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3049 | 1/1 | 0.94 | 0.48 | 45.33 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3173 | 1/1 | 0.92 | 0.79 | 39.26 | 52,52,52,52 | 0 |
| 57 | MG | YA | 3259 | 1/1 | 0.99 | 0.51 | 37.84 | 28,28,28,28 | 0 |
| 57 | MG | YA | 3109 | 1/1 | 0.99 | 0.35 | 35.64 | 27,27,27,27 | 0 |
| 57 | MG | YA | 3255 | 1/1 | 0.98 | 0.55 | 34.12 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3098 | 1/1 | 0.98 | 0.43 | 33.81 | 25,25,25,25 | 0 |
| 57 | MG | RA | 3124 | 1/1 | 0.86 | 0.53 | 29.57 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | XA | 1621 | 1/1 | 0.94 | 0.56 | 28.29 | 48,48,48,48 | 0 |
| 57 | MG | YA | 3050 | 1/1 | 0.97 | 0.38 | 27.55 | 27,27,27,27 | 0 |
| 57 | MG | YA | 3009 | 1/1 | 0.98 | 0.55 | 25.93 | 28,28,28,28 | 0 |
| 57 | MG | XA | 1656 | 1/1 | 0.92 | 0.42 | 24.86 | 48,48,48,48 | 0 |
| 57 | MG | YA | 3237 | 1/1 | 0.96 | 0.35 | 24.83 | 59,59,59,59 | 0 |
| 57 | MG | YA | 3091 | 1/1 | 0.98 | 0.42 | 24.34 | 27,27,27,27 | 0 |
| 57 | MG | RA | 3077 | 1/1 | 0.97 | 0.43 | 22.91 | 42,42,42,42 | 0 |
| 57 | MG | YA | 3200 | 1/1 | 0.85 | 0.41 | 22.37 | 76,76,76,76 | 0 |
| 57 | MG | YA | 3161 | 1/1 | 0.94 | 0.33 | 22.14 | 36,36,36,36 | 0 |
| 57 | MG | XA | 1634 | 1/1 | 0.93 | 0.21 | 21.89 | 33,33,33,33 | 0 |
| 57 | MG | YA | 3182 | 1/1 | 0.88 | 0.42 | 21.39 | 64,64,64,64 | 0 |
| 57 | MG | YA | 3015 | 1/1 | 0.98 | 0.59 | 21.12 | 18,18,18,18 | 0 |
| 57 | MG | YA | 3145 | 1/1 | 0.83 | 0.39 | 19.45 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3095 | 1/1 | 0.90 | 0.47 | 18.64 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3069 | 1/1 | 0.98 | 0.47 | 18.26 | 42,42,42,42 | 0 |
| 57 | MG | YA | 3110 | 1/1 | 0.98 | 0.37 | 17.00 | 29,29,29,29 | 0 |
| 57 | MG | YA | 3265 | 1/1 | 0.97 | 0.52 | 16.83 | 39,39,39,39 | 0 |
| 57 | MG | QA | 1620 | 1/1 | 0.88 | 0.58 | 16.71 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3002 | 1/1 | 0.98 | 0.67 | 16.65 | 37,37,37,37 | 0 |
| 57 | MG | RA | 3015 | 1/1 | 0.99 | 0.39 | 16.36 | 22,22,22,22 | 0 |
| 57 | MG | RA | 3056 | 1/1 | 0.97 | 0.40 | 16.31 | 28,28,28,28 | 0 |
| 57 | MG | YA | 3026 | 1/1 | 0.99 | 0.43 | 16.02 | 12,12,12,12 | 0 |
| 57 | MG | YA | 3011 | 1/1 | 0.99 | 0.47 | 15.97 | 27,27,27,27 | 0 |
| 57 | MG | RA | 3170 | 1/1 | 0.90 | 0.38 | 15.60 | 46,46,46,46 | 0 |
| 57 | MG | XA | 1604 | 1/1 | 0.96 | 0.65 | 15.55 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3022 | 1/1 | 0.96 | 0.50 | 15.30 | 25,25,25,25 | 0 |
| 57 | MG | YA | 3101 | 1/1 | 0.89 | 0.39 | 15.10 | 32,32,32,32 | 0 |
| 57 | MG | YA | 3207 | 1/1 | 0.95 | 0.42 | 15.04 | 61,61,61,61 | 0 |
| 57 | MG | RA | 3079 | 1/1 | 0.95 | 0.52 | 14.96 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3037 | 1/1 | 0.94 | 0.36 | 14.94 | 26,26,26,26 | 0 |
| 57 | MG | QA | 1613 | 1/1 | 0.89 | 0.46 | 14.80 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3040 | 1/1 | 0.96 | 0.40 | 14.60 | 22,22,22,22 | 0 |
| 57 | MG | RA | 3081 | 1/1 | 0.98 | 0.58 | 14.42 | 46,46,46,46 | 0 |
| 57 | MG | XA | 1636 | 1/1 | 0.91 | 0.38 | 14.27 | 46,46,46,46 | 0 |
| 57 | MG | RA | 3087 | 1/1 | 0.94 | 0.41 | 14.05 | 35,35,35,35 | 0 |
| 57 | MG | RA | 3106 | 1/1 | 0.95 | 0.24 | 13.94 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3221 | 1/1 | 0.67 | 0.43 | 13.89 | 65,65,65,65 | 0 |
| 57 | MG | RA | 3020 | 1/1 | 0.99 | 0.48 | 13.87 | 20,20,20,20 | 0 |
| 57 | MG | YA | 3100 | 1/1 | 0.97 | 0.45 | 13.84 | 20,20,20,20 | 0 |
| 57 | MG | RA | 3161 | 1/1 | 0.81 | 0.27 | 13.33 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3034 | 1/1 | 0.96 | 0.52 | 12.94 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3131 | 1/1 | 0.95 | 0.53 | 12.77 | 46,46,46,46 | 0 |
| 57 | MG | RA | 3239 | 1/1 | 0.94 | 0.53 | 12.60 | 37,37,37,37 | 0 |
| 57 | MG | RA | 3008 | 1/1 | 0.90 | 0.41 | 12.56 | 46,46,46,46 | 0 |
| 57 | MG | QA | 1614 | 1/1 | 0.99 | 0.44 | 12.50 | 38,38,38,38 | 0 |
| 57 | MG | RA | 3107 | 1/1 | 0.96 | 0.36 | 12.22 | 45,45,45,45 | 0 |
| 57 | MG | RA | 3021 | 1/1 | 0.97 | 0.38 | 11.72 | 27,27,27,27 | 0 |
| 57 | MG | YA | 3092 | 1/1 | 0.98 | 0.34 | 11.69 | 44,44,44,44 | 0 |
| 57 | MG | YA | 3013 | 1/1 | 0.96 | 0.45 | 11.54 | 20,20,20,20 | 0 |
| 57 | MG | YA | 3081 | 1/1 | 0.98 | 0.43 | 11.51 | 28,28,28,28 | 0 |
| 57 | MG | YA | 3031 | 1/1 | 0.97 | 0.41 | 11.35 | 24,24,24,24 | 0 |
| 57 | MG | RA | 3130 | 1/1 | 0.96 | 0.35 | 11.03 | 43,43,43,43 | 0 |
| 57 | MG | YA | 3088 | 1/1 | 0.98 | 0.43 | 11.03 | 35,35,35,35 | 0 |
| 57 | MG | RA | 3062 | 1/1 | 0.98 | 0.50 | 10.97 | 18,18,18,18 | 0 |
| 57 | MG | Y7 | 101 | 1/1 | 0.89 | 0.43 | 10.94 | 48,48,48,48 | 0 |
| 57 | MG | XA | 1619 | 1/1 | 0.87 | 0.30 | 10.93 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3068 | 1/1 | 0.95 | 0.27 | 10.85 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3120 | 1/1 | 0.99 | 0.39 | 10.75 | 52,52,52,52 | 0 |
| 57 | MG | YA | 3221 | 1/1 | 0.87 | 0.54 | 10.72 | 65,65,65,65 | 0 |
| 57 | MG | XA | 1615 | 1/1 | 0.96 | 0.39 | 10.35 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3052 | 1/1 | 0.98 | 0.32 | 10.22 | 18,18,18,18 | 0 |
| 57 | MG | QA | 1618 | 1/1 | 0.88 | 0.46 | 10.17 | 45,45,45,45 | 0 |
| 57 | MG | RA | 3004 | 1/1 | 0.92 | 0.42 | 10.11 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3024 | 1/1 | 0.93 | 0.34 | 10.08 | 21,21,21,21 | 0 |
| 57 | MG | RA | 3059 | 1/1 | 0.99 | 0.32 | 10.03 | 19,19,19,19 | 0 |
| 57 | MG | YA | 3034 | 1/1 | 0.94 | 0.41 | 9.98 | 19,19,19,19 | 0 |
| 57 | MG | YA | 3203 | 1/1 | 0.91 | 0.21 | 9.88 | 28,28,28,28 | 0 |
| 57 | MG | QA | 1647 | 1/1 | 0.94 | 0.65 | 9.72 | 50,50,50,50 | 0 |
| 57 | MG | RA | 3058 | 1/1 | 0.95 | 0.32 | 9.64 | 19,19,19,19 | 0 |
| 57 | MG | RA | 3197 | 1/1 | 0.96 | 0.38 | 9.51 | 37,37,37,37 | 0 |
| 57 | MG | RA | 3141 | 1/1 | 0.80 | 0.34 | 9.41 | 61,61,61,61 | 0 |
| 57 | MG | RA | 3085 | 1/1 | 0.99 | 0.40 | 9.08 | 32,32,32,32 | 0 |
| 57 | MG | YA | 3138 | 1/1 | 0.88 | 0.24 | 8.96 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3120 | 1/1 | 0.98 | 0.54 | 8.91 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3006 | 1/1 | 0.96 | 0.53 | 8.87 | 30,30,30,30 | 0 |
| 57 | MG | QA | 1660 | 1/1 | 0.96 | 0.36 | 8.74 | 59,59,59,59 | 0 |
| 57 | MG | YA | 3105 | 1/1 | 0.99 | 0.34 | 8.67 | 24,24,24,24 | 0 |
| 57 | MG | RA | 3123 | 1/1 | 0.95 | 0.35 | 8.66 | 53,53,53,53 | 0 |
| 57 | MG | RA | 3174 | 1/1 | 0.80 | 0.27 | 8.57 | 39,39,39,39 | 0 |
| 57 | MG | XA | 1610 | 1/1 | 0.96 | 0.31 | 8.53 | 32,32,32,32 | 0 |
| 57 | MG | XA | 1628 | 1/1 | 0.86 | 0.25 | 8.20 | 29,29,29,29 | 0 |
| 57 | MG | RA | 3121 | 1/1 | 0.95 | 0.37 | 8.19 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3220 | 1/1 | 0.73 | 0.26 | 8.17 | 72,72,72,72 | 0 |
| 57 | MG | RA | 3063 | 1/1 | 0.94 | 0.51 | 8.10 | 31,31,31,31 | 0 |
| 57 | MG | YA | 3083 | 1/1 | 0.94 | 0.22 | 8.10 | 24,24,24,24 | 0 |
| 57 | MG | YA | 3141 | 1/1 | 0.95 | 0.43 | 7.91 | 41,41,41,41 | 0 |
| 57 | MG | YA | 3117 | 1/1 | 0.90 | 0.44 | 7.87 | 73,73,73,73 | 0 |
| 57 | MG | XA | 1637 | 1/1 | 0.98 | 0.49 | 7.86 | 53,53,53,53 | 0 |
| 57 | MG | YA | 3072 | 1/1 | 0.59 | 0.40 | 7.67 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3149 | 1/1 | 0.83 | 0.25 | 7.59 | 53,53,53,53 | 0 |
| 57 | MG | YA | 3262 | 1/1 | 0.95 | 0.39 | 7.43 | 35,35,35,35 | 0 |
| 57 | MG | RA | 3227 | 1/1 | 0.70 | 0.31 | 7.22 | 55,55,55,55 | 0 |
| 57 | MG | YA | 3126 | 1/1 | 0.83 | 0.31 | 7.13 | 38,38,38,38 | 0 |
| 57 | MG | XA | 1659 | 1/1 | 0.96 | 0.44 | 7.03 | 71,71,71,71 | 0 |
| 57 | MG | RA | 3050 | 1/1 | 0.98 | 0.34 | 6.84 | 25,25,25,25 | 0 |
| 57 | MG | YA | 3016 | 1/1 | 0.85 | 0.24 | 6.75 | 29,29,29,29 | 0 |
| 57 | MG | YA | 3210 | 1/1 | 0.59 | 0.26 | 6.71 | 60,60,60,60 | 0 |
| 57 | MG | YA | 3211 | 1/1 | 0.89 | 0.24 | 6.59 | 32,32,32,32 | 0 |
| 57 | MG | YA | 3059 | 1/1 | 0.98 | 0.32 | 6.52 | 13,13,13,13 | 0 |
| 57 | MG | YA | 3096 | 1/1 | 0.89 | 0.40 | 6.50 | 33,33,33,33 | 0 |
| 57 | MG | YA | 3047 | 1/1 | 0.97 | 0.34 | 6.47 | 23,23,23,23 | 0 |
| 57 | MG | YA | 3032 | 1/1 | 0.96 | 0.38 | 6.45 | 22,22,22,22 | 0 |
| 57 | MG | YA | 3102 | 1/1 | 0.96 | 0.34 | 6.41 | 26,26,26,26 | 0 |
| 57 | MG | RA | 3064 | 1/1 | 0.99 | 0.26 | 6.31 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3240 | 1/1 | 0.96 | 0.50 | 6.29 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3023 | 1/1 | 0.97 | 0.31 | 6.28 | 21,21,21,21 | 0 |
| 57 | MG | QA | 1650 | 1/1 | 0.92 | 0.34 | 6.27 | 72,72,72,72 | 0 |
| 57 | MG | RA | 3097 | 1/1 | 0.97 | 0.28 | 6.19 | 26,26,26,26 | 0 |
| 57 | MG | YA | 3044 | 1/1 | 0.96 | 0.24 | 6.18 | 15,15,15,15 | 0 |
| 57 | MG | XA | 1618 | 1/1 | 0.92 | 0.46 | 6.07 | 41,41,41,41 | 0 |
| 57 | MG | RA | 3222 | 1/1 | 0.65 | 0.32 | 5.97 | 67,67,67,67 | 0 |
| 57 | MG | YA | 3008 | 1/1 | 0.96 | 0.32 | 5.90 | 20,20,20,20 | 0 |
| 57 | MG | YA | 3002 | 1/1 | 0.97 | 0.32 | 5.90 | 16,16,16,16 | 0 |
| 57 | MG | YA | 3049 | 1/1 | 0.92 | 0.41 | 5.88 | 30,30,30,30 | 0 |
| 57 | MG | RA | 3119 | 1/1 | 0.94 | 0.41 | 5.85 | 66,66,66,66 | 0 |
| 57 | MG | RP | 201 | 1/1 | 0.92 | 0.46 | 5.81 | 41,41,41,41 | 0 |
| 57 | MG | RA | 3038 | 1/1 | 0.96 | 0.27 | 5.79 | 26,26,26,26 | 0 |
| 57 | MG | YA | 3106 | 1/1 | 0.71 | 0.26 | 5.76 | 28,28,28,28 | 0 |
| 57 | MG | RA | 3033 | 1/1 | 0.95 | 0.39 | 5.54 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3004 | 1/1 | 0.95 | 0.28 | 5.45 | 11,11,11,11 | 0 |
| 57 | MG | RA | 3088 | 1/1 | 0.99 | 0.35 | 5.43 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3245 | 1/1 | 0.93 | 0.34 | 5.42 | 60,60,60,60 | 0 |
| 57 | MG | RA | 3005 | 1/1 | 0.92 | 0.46 | 5.38 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | YA | 3178 | 1/1 | 0.98 | 0.30 | 5.30 | 44,44,44,44 | 0 |
| 57 | MG | YA | 3230 | 1/1 | 0.77 | 0.30 | 5.28 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3014 | 1/1 | 0.94 | 0.39 | 5.25 | 22,22,22,22 | 0 |
| 57 | MG | YA | 3143 | 1/1 | 0.96 | 0.24 | 5.22 | 35,35,35,35 | 0 |
| 57 | MG | XA | 1635 | 1/1 | 0.93 | 0.43 | 5.21 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3019 | 1/1 | 0.96 | 0.31 | 5.11 | 26,26,26,26 | 0 |
| 57 | MG | RA | 3094 | 1/1 | 0.97 | 0.46 | 5.11 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3214 | 1/1 | 0.86 | 0.28 | 5.04 | 47,47,47,47 | 0 |
| 57 | MG | QA | 1615 | 1/1 | 0.98 | 0.29 | 4.95 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3042 | 1/1 | 0.97 | 0.32 | 4.88 | 19,19,19,19 | 0 |
| 57 | MG | RA | 3012 | 1/1 | 0.94 | 0.35 | 4.70 | 28,28,28,28 | 0 |
| 57 | MG | QA | 1658 | 1/1 | 0.59 | 0.25 | 4.65 | 58,58,58,58 | 0 |
| 57 | MG | RA | 3031 | 1/1 | 0.99 | 0.34 | 4.56 | 35,35,35,35 | 0 |
| 57 | MG | RA | 3086 | 1/1 | 0.97 | 0.33 | 4.54 | 45,45,45,45 | 0 |
| 57 | MG | RA | 3105 | 1/1 | 0.95 | 0.27 | 4.54 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3186 | 1/1 | 0.89 | 0.24 | 4.51 | 43,43,43,43 | 0 |
| 57 | MG | RA | 3191 | 1/1 | 0.92 | 0.39 | 4.51 | 51,51,51,51 | 0 |
| 57 | MG | YA | 3060 | 1/1 | 0.96 | 0.27 | 4.48 | 25,25,25,25 | 0 |
| 57 | MG | YA | 3033 | 1/1 | 0.99 | 0.43 | 4.45 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3074 | 1/1 | 0.98 | 0.34 | 4.36 | 35,35,35,35 | 0 |
| 57 | MG | XA | 1651 | 1/1 | 0.76 | 0.23 | 4.30 | 55,55,55,55 | 0 |
| 57 | MG | RA | 3065 | 1/1 | 0.97 | 0.34 | 4.29 | 36,36,36,36 | 0 |
| 57 | MG | RA | 3153 | 1/1 | 0.93 | 0.27 | 4.23 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3041 | 1/1 | 0.95 | 0.30 | 4.20 | 17,17,17,17 | 0 |
| 57 | MG | QA | 1604 | 1/1 | 0.94 | 0.36 | 4.09 | 36,36,36,36 | 0 |
| 57 | MG | XA | 1626 | 1/1 | 0.95 | 0.29 | 4.09 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3042 | 1/1 | 0.98 | 0.26 | 4.06 | 26,26,26,26 | 0 |
| 57 | MG | YE | 302 | 1/1 | 0.95 | 0.31 | 4.00 | 35,35,35,35 | 0 |
| 57 | MG | YA | 3017 | 1/1 | 0.96 | 0.22 | 3.95 | 25,25,25,25 | 0 |
| 57 | MG | XA | 1638 | 1/1 | 0.80 | 0.18 | 3.84 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3115 | 1/1 | 0.97 | 0.34 | 3.70 | 31,31,31,31 | 0 |
| 57 | MG | YA | 3185 | 1/1 | 0.94 | 0.23 | 3.67 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3143 | 1/1 | 0.96 | 0.36 | 3.60 | 37,37,37,37 | 0 |
| 57 | MG | XA | 1603 | 1/1 | 0.95 | 0.24 | 3.54 | 32,32,32,32 | 0 |
| 57 | MG | QV | 101 | 1/1 | 0.97 | 0.24 | 3.39 | 36,36,36,36 | 0 |
| 57 | MG | YA | 3048 | 1/1 | 0.97 | 0.28 | 3.36 | 26,26,26,26 | 0 |
| 57 | MG | YA | 3006 | 1/1 | 0.98 | 0.43 | 3.18 | 11,11,11,11 | 0 |
| 57 | MG | YA | 3256 | 1/1 | 0.88 | 0.32 | 3.16 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3175 | 1/1 | 0.81 | 0.28 | 2.95 | 58,58,58,58 | 0 |
| 57 | MG | RA | 3026 | 1/1 | 0.94 | 0.38 | 2.91 | 18,18,18,18 | 0 |
| 57 | MG | YA | 3266 | 1/1 | 0.96 | 0.22 | 2.76 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | QA | 1611 | 1/1 | 0.94 | 0.26 | 2.73 | 27,27,27,27 | 0 |
| 57 | MG | YA | 3217 | 1/1 | 0.84 | 0.24 | 2.58 | 70,70,70,70 | 0 |
| 57 | MG | YA | 3080 | 1/1 | 0.93 | 0.25 | 2.54 | 33,33,33,33 | 0 |
| 57 | MG | YA | 3118 | 1/1 | 0.89 | 0.28 | 2.49 | 27,27,27,27 | 0 |
| 57 | MG | RA | 3212 | 1/1 | 0.81 | 0.22 | 2.48 | 64,64,64,64 | 0 |
| 57 | MG | QA | 1655 | 1/1 | 0.77 | 0.23 | 2.46 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3188 | 1/1 | 0.91 | 0.32 | 2.43 | 41,41,41,41 | 0 |
| 57 | MG | RA | 3136 | 1/1 | 0.92 | 0.30 | 2.37 | 33,33,33,33 | 0 |
| 58 | PAR | QA | 1667 | 42/42 | 0.90 | 0.25 | 2.29 | 75,75,75,75 | 0 |
| 57 | MG | RA | 3199 | 1/1 | 0.69 | 0.20 | 2.27 | 58,58,58,58 | 0 |
| 57 | MG | RA | 3035 | 1/1 | 0.92 | 0.28 | 2.15 | 24,24,24,24 | 0 |
| 57 | MG | XA | 1620 | 1/1 | 0.94 | 0.26 | 2.14 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3036 | 1/1 | 0.98 | 0.27 | 2.13 | 23,23,23,23 | 0 |
| 57 | MG | RA | 3210 | 1/1 | 0.72 | 0.40 | 2.12 | 76,76,76,76 | 0 |
| 57 | MG | YA | 3169 | 1/1 | 0.93 | 0.23 | 2.09 | 43,43,43,43 | 0 |
| 57 | MG | YA | 3177 | 1/1 | 0.94 | 0.22 | 2.09 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3205 | 1/1 | 0.95 | 0.29 | 2.07 | 38,38,38,38 | 0 |
| 57 | MG | XV | 101 | 1/1 | 0.97 | 0.20 | 2.06 | 31,31,31,31 | 0 |
| 57 | MG | QA | 1610 | 1/1 | 0.97 | 0.26 | 1.98 | 33,33,33,33 | 0 |
| 57 | MG | YA | 3114 | 1/1 | 0.94 | 0.19 | 1.92 | 39,39,39,39 | 0 |
| 57 | MG | XA | 1611 | 1/1 | 0.98 | 0.35 | 1.89 | 28,28,28,28 | 0 |
| 57 | MG | YA | 3005 | 1/1 | 0.93 | 0.21 | 1.86 | 20,20,20,20 | 0 |
| 57 | MG | YA | 3187 | 1/1 | 0.85 | 0.20 | 1.84 | 36,36,36,36 | 0 |
| 57 | MG | RA | 3072 | 1/1 | 0.95 | 0.23 | 1.78 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3224 | 1/1 | 0.80 | 0.20 | 1.75 | 59,59,59,59 | 0 |
| 57 | MG | RA | 3154 | 1/1 | 0.83 | 0.22 | 1.60 | 31,31,31,31 | 0 |
| 57 | MG | RA | 3192 | 1/1 | 0.45 | 0.28 | 1.59 | 81,81,81,81 | 0 |
| 57 | MG | RA | 3017 | 1/1 | 0.96 | 0.20 | 1.53 | 29,29,29,29 | 0 |
| 57 | MG | YA | 3027 | 1/1 | 0.99 | 0.19 | 1.52 | 21,21,21,21 | 0 |
| 57 | MG | YA | 3057 | 1/1 | 0.92 | 0.21 | 1.47 | 10,10,10,10 | 0 |
| 57 | MG | RA | 3024 | 1/1 | 0.98 | 0.18 | 1.46 | 25,25,25,25 | 0 |
| 57 | MG | RA | 3150 | 1/1 | 0.86 | 0.21 | 1.42 | 47,47,47,47 | 0 |
| 57 | MG | RE | 302 | 1/1 | 0.85 | 0.28 | 1.39 | 43,43,43,43 | 0 |
| 57 | MG | QA | 1617 | 1/1 | 0.93 | 0.26 | 1.25 | 40,40,40,40 | 0 |
| 58 | PAR | XA | 1673 | 42/42 | 0.94 | 0.22 | 1.24 | 64,64,64,64 | 0 |
| 57 | MG | YA | 3116 | 1/1 | 0.95 | 0.21 | 1.17 | 42,42,42,42 | 0 |
| 57 | MG | XA | 1665 | 1/1 | 0.88 | 0.18 | 1.08 | 53,53,53,53 | 0 |
| 57 | MG | RU | 201 | 1/1 | 0.95 | 0.23 | 0.89 | 90,90,90,90 | 0 |
| 57 | MG | XA | 1607 | 1/1 | 0.92 | 0.23 | 0.84 | 49,49,49,49 | 0 |
| 57 | MG | RA | 3184 | 1/1 | 0.89 | 0.17 | 0.79 | 41,41,41,41 | 0 |
| 57 | MG | XA | 1671 | 1/1 | 0.94 | 0.19 | 0.79 | 52,52,52,52 | 0 |
| 57 | MG | QA | 1644 | 1/1 | 0.87 | 0.36 | 0.77 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | YA | 3139 | 1/1 | 0.96 | 0.19 | 0.74 | 35,35,35,35 | 0 |
| 57 | MG | QA | 1636 | 1/1 | 0.93 | 0.20 | 0.74 | 46,46,46,46 | 0 |
| 57 | MG | YA | 3154 | 1/1 | 0.87 | 0.26 | 0.65 | 36,36,36,36 | 0 |
| 57 | MG | RA | 3100 | 1/1 | 0.87 | 0.20 | 0.62 | 26,26,26,26 | 0 |
| 57 | MG | YA | 3038 | 1/1 | 0.98 | 0.16 | 0.61 | 17,17,17,17 | 0 |
| 57 | MG | RA | 3179 | 1/1 | 0.93 | 0.17 | 0.60 | 32,32,32,32 | 0 |
| 57 | MG | QA | 1616 | 1/1 | 0.84 | 0.18 | 0.54 | 66,66,66,66 | 0 |
| 57 | MG | QA | 1606 | 1/1 | 0.94 | 0.20 | 0.53 | 35,35,35,35 | 0 |
| 57 | MG | YA | 3155 | 1/1 | 0.91 | 0.17 | 0.52 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3215 | 1/1 | 0.77 | 0.21 | 0.51 | 50,50,50,50 | 0 |
| 57 | MG | RA | 3203 | 1/1 | 0.72 | 0.21 | 0.46 | 73,73,73,73 | 0 |
| 57 | MG | XA | 1614 | 1/1 | 0.93 | 0.22 | 0.45 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3025 | 1/1 | 0.98 | 0.20 | 0.43 | 13,13,13,13 | 0 |
| 57 | MG | RA | 3135 | 1/1 | 0.95 | 0.18 | 0.43 | 38,38,38,38 | 0 |
| 57 | MG | RA | 3158 | 1/1 | 0.87 | 0.16 | 0.33 | 41,41,41,41 | 0 |
| 57 | MG | RA | 3075 | 1/1 | 0.98 | 0.17 | 0.31 | 21,21,21,21 | 0 |
| 57 | MG | RA | 3115 | 1/1 | 0.87 | 0.17 | 0.27 | 25,25,25,25 | 0 |
| 57 | MG | YA | 3073 | 1/1 | 0.97 | 0.20 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | YA | 3172 | 1/1 | 0.74 | 0.15 | 0.17 | 65,65,65,65 | 0 |
| 57 | MG | YA | 3130 | 1/1 | 0.97 | 0.19 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3014 | 1/1 | 0.95 | 0.21 | 0.14 | 25,25,25,25 | 0 |
| 57 | MG | RD | 301 | 1/1 | 0.81 | 0.25 | 0.03 | 64,64,64,64 | 0 |
| 57 | MG | XA | 1612 | 1/1 | 0.90 | 0.17 | -0.00 | 31,31,31,31 | 0 |
| 57 | MG | YA | 3180 | 1/1 | 0.90 | 0.17 | -0.02 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3080 | 1/1 | 0.96 | 0.20 | -0.03 | 36,36,36,36 | 0 |
| 57 | MG | XA | 1633 | 1/1 | 0.91 | 0.20 | -0.04 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3028 | 1/1 | 0.97 | 0.17 | -0.05 | 17,17,17,17 | 0 |
| 57 | MG | XA | 1655 | 1/1 | 0.92 | 0.23 | -0.10 | 44,44,44,44 | 0 |
| 57 | MG | YA | 3068 | 1/1 | 0.98 | 0.17 | -0.16 | 35,35,35,35 | 0 |
| 57 | MG | RP | 202 | 1/1 | 0.93 | 0.19 | -0.21 | 157,157,157,157 | 0 |
| 59 | ZN | XN | 101 | 1/1 | 0.80 | 0.23 | -0.32 | 97,97,97,97 | 0 |
| 57 | MG | YX | 101 | 1/1 | 0.89 | 0.16 | -0.33 | 109,109,109,109 | 0 |
| 57 | MG | RA | 3156 | 1/1 | 0.96 | 0.18 | -0.41 | 47,47,47,47 | 0 |
| 57 | MG | XA | 1646 | 1/1 | 0.70 | 0.18 | -0.41 | 55,55,55,55 | 0 |
| 57 | MG | QA | 1640 | 1/1 | 0.95 | 0.14 | -0.44 | 44,44,44,44 | 0 |
| 57 | MG | YA | 3199 | 1/1 | 0.96 | 0.18 | -0.45 | 45,45,45,45 | 0 |
| 59 | ZN | QD | 301 | 1/1 | 0.96 | 0.30 | -0.51 | 54,54,54,54 | 0 |
| 57 | MG | RA | 3054 | 1/1 | 0.85 | 0.17 | -0.54 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3240 | 1/1 | 0.95 | 0.17 | -0.55 | 60,60,60,60 | 0 |
| 57 | MG | YA | 3179 | 1/1 | 0.70 | 0.14 | -0.56 | 44,44,44,44 | 0 |
| 57 | MG | QA | 1666 | 1/1 | 0.87 | 0.22 | -0.60 | 52,52,52,52 | 0 |
| 57 | MG | YD | 301 | 1/1 | 0.98 | 0.18 | -0.62 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3208 | 1/1 | 0.92 | 0.14 | -0.71 | 31,31,31,31 | 0 |
| 57 | MG | RF | 301 | 1/1 | 0.93 | 0.23 | -0.79 | 50,50,50,50 | 0 |
| 57 | MG | RA | 3185 | 1/1 | 0.93 | 0.17 | -0.81 | 44,44,44,44 | 0 |
| 59 | ZN | XD | 301 | 1/1 | 0.86 | 0.30 | -0.90 | 52,52,52,52 | 0 |
| 57 | MG | XA | 1608 | 1/1 | 0.89 | 0.14 | -0.92 | 57,57,57,57 | 0 |
| 57 | MG | RA | 3102 | 1/1 | 0.89 | 0.16 | -0.94 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3127 | 1/1 | 0.96 | 0.16 | -0.96 | 34,34,34,34 | 0 |
| 57 | MG | QA | 1609 | 1/1 | 0.86 | 0.19 | -1.03 | 62,62,62,62 | 0 |
| 57 | MG | QA | 1621 | 1/1 | 0.98 | 0.10 | -1.10 | 36,36,36,36 | 0 |
| 59 | ZN | Y9 | 101 | 1/1 | 0.88 | 0.25 | -1.15 | 166,166,166,166 | 0 |
| 57 | MG | YA | 3183 | 1/1 | 0.95 | 0.14 | -1.25 | 45,45,45,45 | 0 |
| 57 | MG | QA | 1631 | 1/1 | 0.80 | 0.17 | -1.27 | 53,53,53,53 | 0 |
| 57 | MG | YA | 3226 | 1/1 | 0.94 | 0.13 | -1.40 | 41,41,41,41 | 0 |
| 59 | ZN | QN | 100 | 1/1 | 0.83 | 0.13 | -1.58 | 100,100,100,100 | 0 |
| 57 | MG | XA | 1666 | 1/1 | 0.88 | 0.17 | -1.70 | 54,54,54,54 | 0 |
| 57 | MG | XA | 1661 | 1/1 | 0.95 | 0.11 | -1.75 | 67,67,67,67 | 0 |
| 57 | MG | RA | 3164 | 1/1 | 0.89 | 0.10 | -1.77 | 32,32,32,32 | 0 |
| 57 | MG | QM | 201 | 1/1 | 0.93 | 0.10 | -1.85 | 81,81,81,81 | 0 |
| 57 | MG | XA | 1660 | 1/1 | 0.97 | 0.14 | -1.86 | 26,26,26,26 | 0 |
| 57 | MG | YA | 3066 | 1/1 | 0.94 | 0.13 | -1.88 | 23,23,23,23 | 0 |
| 57 | MG | YA | 3148 | 1/1 | 0.94 | 0.13 | -1.88 | 33,33,33,33 | 0 |
| 57 | MG | YA | 3202 | 1/1 | 0.94 | 0.13 | -1.89 | 55,55,55,55 | 0 |
| 57 | MG | QA | 1646 | 1/1 | 0.93 | 0.10 | -1.91 | 52,52,52,52 | 0 |
| 57 | MG | XA | 1649 | 1/1 | 0.81 | 0.15 | -1.94 | 61,61,61,61 | 0 |
| 57 | MG | YA | 3220 | 1/1 | 0.94 | 0.12 | -1.98 | 38,38,38,38 | 0 |
| 57 | MG | RA | 3132 | 1/1 | 0.93 | 0.11 | -1.99 | 40,40,40,40 | 0 |
| 59 | ZN | R9 | 101 | 1/1 | 0.81 | 0.21 | -2.16 | 179,179,179,179 | 0 |
| 57 | MG | YA | 3062 | 1/1 | 0.94 | 0.15 | -2.23 | 30,30,30,30 | 0 |
| 57 | MG | RA | 3074 | 1/1 | 0.82 | 0.10 | -2.27 | 51,51,51,51 | 0 |
| 57 | MG | QA | 1630 | 1/1 | 0.95 | 0.15 | -2.27 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3186 | 1/1 | 0.93 | 0.09 | -2.33 | 27,27,27,27 | 0 |
| 57 | MG | RA | 3099 | 1/1 | 0.94 | 0.12 | -2.54 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3208 | 1/1 | 0.82 | 0.16 | -2.58 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3236 | 1/1 | 0.89 | 0.11 | -2.65 | 43,43,43,43 | 0 |
| 57 | MG | YA | 3188 | 1/1 | 0.89 | 0.12 | -2.73 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3159 | 1/1 | 0.97 | 0.12 | -2.87 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3136 | 1/1 | 0.95 | 0.07 | -3.00 | 30,30,30,30 | 0 |
| 57 | MG | XA | 1625 | 1/1 | 0.86 | 0.12 | -3.10 | 32,32,32,32 | 0 |
| 57 | MG | YA | 3192 | 1/1 | 0.95 | 0.09 | -3.30 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3133 | 1/1 | 0.97 | 0.10 | -3.47 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3075 | 1/1 | 0.89 | 0.11 | -3.48 | 23,23,23,23 | 0 |
| 57 | MG | YA | 3219 | 1/1 | 0.94 | 0.10 | -4.06 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | YA | 3071 | 1/1 | 0.93 | 0.10 | -4.12 | 17,17,17,17 | 0 |
| 57 | MG | YA | 3213 | 1/1 | 0.86 | 0.13 | -4.24 | 35,35,35,35 | 0 |
| 57 | MG | QA | 1632 | 1/1 | 0.89 | 0.10 | -4.56 | 58,58,58,58 | 0 |
| 57 | MG | YA | 3170 | 1/1 | 0.96 | 0.07 | -4.81 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3113 | 1/1 | 0.99 | 0.07 | -4.98 | 35,35,35,35 | 0 |
| 57 | MG | RB | 201 | 1/1 | 0.93 | 0.11 | -5.32 | 76,76,76,76 | 0 |
| 57 | MG | YA | 3242 | 1/1 | 0.99 | 0.09 | -5.56 | 55,55,55,55 | 0 |
| 57 | MG | QA | 1607 | 1/1 | 0.94 | 0.11 | -6.00 | 61,61,61,61 | 0 |
| 57 | MG | XA | 1622 | 1/1 | 0.97 | 0.12 | -7.09 | 37,37,37,37 | 0 |
| 57 | MG | YB | 203 | 1/1 | 0.95 | 0.08 | -7.10 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3146 | 1/1 | 0.97 | 0.10 | -9.19 | 31,31,31,31 | 0 |
| 57 | MG | YA | 3167 | 1/1 | 0.52 | 0.36 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3204 | 1/1 | 0.92 | 0.37 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3155 | 1/1 | 0.95 | 0.39 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3183 | 1/1 | 0.85 | 0.16 | - | 49,49,49,49 | 0 |
| 57 | MG | XA | 1602 | 1/1 | 0.99 | 0.28 | - | 26,26,26,26 | 0 |
| 57 | MG | YA | 3251 | 1/1 | 0.92 | 0.38 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3007 | 1/1 | 0.96 | 0.19 | - | 21,21,21,21 | 0 |
| 57 | MG | YA | 3229 | 1/1 | 0.93 | 0.35 | - | 33,33,33,33 | 0 |
| 57 | MG | XA | 1647 | 1/1 | 0.85 | 0.24 | - | 58,58,58,58 | 0 |
| 57 | MG | YA | 3053 | 1/1 | 0.93 | 0.30 | - | 27,27,27,27 | 0 |
| 57 | MG | RA | 3116 | 1/1 | 0.81 | 0.18 | - | 77,77,77,77 | 0 |
| 57 | MG | YA | 3128 | 1/1 | 0.59 | 0.55 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3003 | 1/1 | 0.99 | 0.27 | - | 18,18,18,18 | 0 |
| 57 | MG | QA | 1648 | 1/1 | 0.97 | 0.12 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3201 | 1/1 | 0.95 | 0.25 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3144 | 1/1 | 0.95 | 0.13 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3053 | 1/1 | 0.96 | 0.13 | - | 19,19,19,19 | 0 |
| 57 | MG | YA | 3152 | 1/1 | 0.89 | 0.46 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3238 | 1/1 | 0.93 | 0.43 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3064 | 1/1 | 0.86 | 0.27 | - | 25,25,25,25 | 0 |
| 57 | MG | RA | 3039 | 1/1 | 0.95 | 0.26 | - | 30,30,30,30 | 0 |
| 57 | MG | RA | 3232 | 1/1 | 0.95 | 0.48 | - | 33,33,33,33 | 0 |
| 57 | MG | RA | 3030 | 1/1 | 0.98 | 0.31 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3187 | 1/1 | 0.93 | 0.21 | - | 63,63,63,63 | 0 |
| 57 | MG | R5 | 101 | 1/1 | 0.94 | 0.21 | - | 38,38,38,38 | 0 |
| 57 | MG | QA | 1612 | 1/1 | 0.98 | 0.33 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3145 | 1/1 | 0.96 | 0.20 | - | 53,53,53,53 | 0 |
| 57 | MG | QA | 1627 | 1/1 | 0.95 | 0.14 | - | 38,38,38,38 | 0 |
| 57 | MG | RA | 3045 | 1/1 | 0.94 | 0.12 | - | 28,28,28,28 | 0 |
| 57 | MG | QA | 1651 | 1/1 | 0.89 | 0.32 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3181 | 1/1 | 0.92 | 0.17 | - | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | YA | 3261 | 1/1 | 0.94 | 0.33 | - | 29,29,29,29 | 0 |
| 57 | MG | YA | 3036 | 1/1 | 0.95 | 0.21 | - | 19,19,19,19 | 0 |
| 57 | MG | YA | 3190 | 1/1 | 0.95 | 0.54 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3043 | 1/1 | 0.91 | 0.28 | - | 43,43,43,43 | 0 |
| 57 | MG | XA | 1653 | 1/1 | 0.93 | 0.21 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3164 | 1/1 | 0.96 | 0.22 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3198 | 1/1 | 0.60 | 0.18 | - | 56,56,56,56 | 0 |
| 57 | MG | XA | 1645 | 1/1 | 0.95 | 0.36 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3216 | 1/1 | 0.97 | 0.26 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3253 | 1/1 | 0.82 | 0.85 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3238 | 1/1 | 0.97 | 0.19 | - | 34,34,34,34 | 0 |
| 57 | MG | YA | 3132 | 1/1 | 0.95 | 0.16 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3200 | 1/1 | 0.93 | 0.42 | - | 43,43,43,43 | 0 |
| 57 | MG | XA | 1664 | 1/1 | 0.82 | 0.37 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3229 | 1/1 | 0.71 | 0.36 | - | 80,80,80,80 | 0 |
| 57 | MG | RA | 3142 | 1/1 | 0.91 | 0.20 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3086 | 1/1 | 0.83 | 0.23 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3082 | 1/1 | 0.97 | 0.40 | - | 23,23,23,23 | 0 |
| 57 | MG | RA | 3211 | 1/1 | 0.91 | 0.23 | - | 50,50,50,50 | 0 |
| 57 | MG | QA | 1649 | 1/1 | 0.99 | 0.22 | - | 49,49,49,49 | 0 |
| 57 | MG | RA | 3126 | 1/1 | 0.95 | 0.24 | - | 53,53,53,53 | 0 |
| 57 | MG | XA | 1624 | 1/1 | 0.93 | 0.45 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3089 | 1/1 | 0.93 | 0.53 | - | 35,35,35,35 | 0 |
| 57 | MG | RA | 3209 | 1/1 | 0.82 | 0.20 | - | 67,67,67,67 | 0 |
| 57 | MG | RA | 3078 | 1/1 | 0.97 | 0.40 | - | 46,46,46,46 | 0 |
| 57 | MG | XA | 1654 | 1/1 | 0.91 | 0.31 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3213 | 1/1 | 0.86 | 0.19 | - | 40,40,40,40 | 0 |
| 57 | MG | XA | 1669 | 1/1 | 0.91 | 0.12 | - | 75,75,75,75 | 0 |
| 57 | MG | YA | 3129 | 1/1 | 0.93 | 0.37 | - | 35,35,35,35 | 0 |
| 57 | MG | YA | 3131 | 1/1 | 0.60 | 0.20 | - | 25,25,25,25 | 0 |
| 57 | MG | QA | 1638 | 1/1 | 0.84 | 0.28 | - | 47,47,47,47 | 0 |
| 57 | MG | QA | 1643 | 1/1 | 0.97 | 0.28 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3061 | 1/1 | 0.93 | 0.38 | - | 19,19,19,19 | 0 |
| 57 | MG | YA | 3122 | 1/1 | 0.98 | 0.32 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3250 | 1/1 | 0.95 | 0.57 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3223 | 1/1 | 0.76 | 0.38 | - | 67,67,67,67 | 0 |
| 57 | MG | YA | 3137 | 1/1 | 0.96 | 0.20 | - | 30,30,30,30 | 0 |
| 57 | MG | RA | 3134 | 1/1 | 0.63 | 0.30 | - | 36,36,36,36 | 0 |
| 57 | MG | RA | 3093 | 1/1 | 0.99 | 0.38 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3076 | 1/1 | 0.98 | 0.34 | - | 37,37,37,37 | 0 |
| 57 | MG | RA | 3166 | 1/1 | 0.61 | 0.15 | - | 44,44,44,44 | 0 |
| 57 | MG | QA | 1656 | 1/1 | 0.87 | 0.29 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | YA | 3158 | 1/1 | 0.92 | 0.22 | - | 40,40,40,40 | 0 |
| 57 | MG | YA | 3051 | 1/1 | 0.98 | 0.31 | - | 20,20,20,20 | 0 |
| 57 | MG | XM | 201 | 1/1 | 0.82 | 0.14 | - | 79,79,79,79 | 0 |
| 57 | MG | RA | 3178 | 1/1 | 0.66 | 0.40 | - | 48,48,48,48 | 0 |
| 57 | MG | XA | 1623 | 1/1 | 0.94 | 0.12 | - | 34,34,34,34 | 0 |
| 57 | MG | RA | 3118 | 1/1 | 0.79 | 0.26 | - | 40,40,40,40 | 0 |
| 57 | MG | YA | 3193 | 1/1 | 0.92 | 0.43 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3231 | 1/1 | 0.93 | 0.55 | - | 27,27,27,27 | 0 |
| 57 | MG | RA | 3003 | 1/1 | 0.96 | 0.44 | - | 28,28,28,28 | 0 |
| 57 | MG | YA | 3227 | 1/1 | 0.94 | 0.39 | - | 27,27,27,27 | 0 |
| 57 | MG | RA | 3083 | 1/1 | 0.57 | 0.41 | - | 40,40,40,40 | 0 |
| 57 | MG | XA | 1662 | 1/1 | 0.63 | 0.60 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3169 | 1/1 | 0.93 | 0.22 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3093 | 1/1 | 0.98 | 0.21 | - | 37,37,37,37 | 0 |
| 57 | MG | YA | 3108 | 1/1 | 0.95 | 0.42 | - | 34,34,34,34 | 0 |
| 57 | MG | QA | 1654 | 1/1 | 0.98 | 0.10 | - | 77,77,77,77 | 0 |
| 57 | MG | YA | 3030 | 1/1 | 0.98 | 0.48 | - | 30,30,30,30 | 0 |
| 57 | MG | RA | 3111 | 1/1 | 0.92 | 0.28 | - | 45,45,45,45 | 0 |
| 57 | MG | QA | 1602 | 1/1 | 0.97 | 0.39 | - | 37,37,37,37 | 0 |
| 57 | MG | RB | 202 | 1/1 | 0.94 | 0.08 | - | 63,63,63,63 | 0 |
| 57 | MG | YA | 3151 | 1/1 | 0.96 | 0.07 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3054 | 1/1 | 0.95 | 0.29 | - | 26,26,26,26 | 0 |
| 57 | MG | YA | 3084 | 1/1 | 0.95 | 0.41 | - | 25,25,25,25 | 0 |
| 57 | MG | YA | 3225 | 1/1 | 0.84 | 0.17 | - | 36,36,36,36 | 0 |
| 57 | MG | QH | 201 | 1/1 | 0.87 | 0.15 | - | 81,81,81,81 | 0 |
| 57 | MG | RA | 3091 | 1/1 | 0.96 | 0.36 | - | 28,28,28,28 | 0 |
| 57 | MG | YA | 3021 | 1/1 | 0.93 | 0.37 | - | 22,22,22,22 | 0 |
| 57 | MG | YA | 3269 | 1/1 | 0.95 | 0.59 | - | 52,52,52,52 | 0 |
| 57 | MG | RA | 3241 | 1/1 | 0.94 | 0.20 | - | 34,34,34,34 | 0 |
| 57 | MG | YA | 3001 | 1/1 | 0.96 | 0.46 | - | 21,21,21,21 | 0 |
| 57 | MG | YA | 3085 | 1/1 | 0.79 | 0.27 | - | 35,35,35,35 | 0 |
| 57 | MG | YA | 3252 | 1/1 | 0.94 | 0.50 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3138 | 1/1 | 0.76 | 0.27 | - | 59,59,59,59 | 0 |
| 57 | MG | YA | 3099 | 1/1 | 0.99 | 0.24 | - | 28,28,28,28 | 0 |
| 57 | MG | YA | 3189 | 1/1 | 0.90 | 0.12 | - | 57,57,57,57 | 0 |
| 57 | MG | YB | 202 | 1/1 | 0.93 | 0.35 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3159 | 1/1 | 0.94 | 0.16 | - | 25,25,25,25 | 0 |
| 57 | MG | YA | 3134 | 1/1 | 0.86 | 0.53 | - | 28,28,28,28 | 0 |
| 57 | MG | RA | 3011 | 1/1 | 0.97 | 0.23 | - | 31,31,31,31 | 0 |
| 57 | MG | YA | 3067 | 1/1 | 0.96 | 0.48 | - | 33,33,33,33 | 0 |
| 57 | MG | YA | 3232 | 1/1 | 0.91 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | RA | 3016 | 1/1 | 0.99 | 0.33 | - | 16,16,16,16 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | QA | 1639 | 1/1 | 0.95 | 0.34 | - | 35,35,35,35 | 0 |
| 57 | MG | YA | 3231 | 1/1 | 0.69 | 0.19 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3202 | 1/1 | 0.93 | 0.46 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3123 | 1/1 | 0.96 | 0.20 | - | 22,22,22,22 | 0 |
| 57 | MG | XA | 1640 | 1/1 | 0.91 | 0.55 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3122 | 1/1 | 0.93 | 0.22 | - | 61,61,61,61 | 0 |
| 57 | MG | YA | 3087 | 1/1 | 0.96 | 0.33 | - | 27,27,27,27 | 0 |
| 57 | MG | YA | 3153 | 1/1 | 0.83 | 0.75 | - | 67,67,67,67 | 0 |
| 57 | MG | XA | 1605 | 1/1 | 0.94 | 0.38 | - | 37,37,37,37 | 0 |
| 57 | MG | Y5 | 101 | 1/1 | 0.94 | 0.19 | - | 35,35,35,35 | 0 |
| 57 | MG | RA | 3162 | 1/1 | 0.94 | 0.27 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3129 | 1/1 | 0.88 | 0.17 | - | 71,71,71,71 | 0 |
| 57 | MG | XA | 1648 | 1/1 | 0.94 | 0.37 | - | 40,40,40,40 | 0 |
| 57 | MG | QA | 1641 | 1/1 | 0.96 | 0.38 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3193 | 1/1 | 0.67 | 0.42 | - | 73,73,73,73 | 0 |
| 57 | MG | YA | 3233 | 1/1 | 0.91 | 0.38 | - | 55,55,55,55 | 0 |
| 57 | MG | RA | 3176 | 1/1 | 0.79 | 0.23 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3165 | 1/1 | 0.94 | 0.21 | - | 61,61,61,61 | 0 |
| 57 | MG | YA | 3156 | 1/1 | 0.79 | 0.30 | - | 50,50,50,50 | 0 |
| 57 | MG | RE | 301 | 1/1 | 0.92 | 0.17 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3189 | 1/1 | 0.93 | 0.14 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3056 | 1/1 | 0.99 | 0.22 | - | 20,20,20,20 | 0 |
| 57 | MG | YE | 301 | 1/1 | 0.93 | 0.20 | - | 21,21,21,21 | 0 |
| 57 | MG | QA | 1601 | 1/1 | 0.95 | 0.26 | - | 44,44,44,44 | 0 |
| 57 | MG | YA | 3162 | 1/1 | 0.37 | 0.27 | - | 71,71,71,71 | 0 |
| 57 | MG | YA | 3247 | 1/1 | 0.82 | 0.77 | - | 64,64,64,64 | 0 |
| 57 | MG | RA | 3218 | 1/1 | 0.80 | 0.34 | - | 66,66,66,66 | 0 |
| 57 | MG | XA | 1630 | 1/1 | 0.85 | 0.32 | - | 38,38,38,38 | 0 |
| 57 | MG | YA | 3035 | 1/1 | 0.99 | 0.33 | - | 18,18,18,18 | 0 |
| 57 | MG | YA | 3171 | 1/1 | 0.96 | 0.20 | - | 49,49,49,49 | 0 |
| 57 | MG | QA | 1664 | 1/1 | 0.96 | 0.07 | - | 118,118,118,118 | 0 |
| 57 | MG | RA | 3041 | 1/1 | 0.99 | 0.28 | - | 23,23,23,23 | 0 |
| 57 | MG | RA | 3110 | 1/1 | 0.94 | 0.30 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3108 | 1/1 | 0.95 | 0.12 | - | 29,29,29,29 | 0 |
| 57 | MG | XA | 1650 | 1/1 | 0.90 | 0.27 | - | 39,39,39,39 | 0 |
| 57 | MG | YB | 201 | 1/1 | 0.69 | 0.36 | - | 71,71,71,71 | 0 |
| 57 | MG | YA | 3098 | 1/1 | 0.98 | 0.25 | - | 34,34,34,34 | 0 |
| 57 | MG | XA | 1657 | 1/1 | 0.76 | 0.55 | - | 56,56,56,56 | 0 |
| 57 | MG | YA | 3078 | 1/1 | 0.97 | 0.20 | - | 27,27,27,27 | 0 |
| 57 | MG | RA | 3223 | 1/1 | 0.72 | 0.28 | - | 98,98,98,98 | 0 |
| 57 | MG | RA | 3230 | 1/1 | 0.98 | 0.31 | - | 22,22,22,22 | 0 |
| 57 | MG | RR | 201 | 1/1 | 0.89 | 0.33 | - | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | XA | 1632 | 1/1 | 0.96 | 0.42 | - | 40,40,40,40 | 0 |
| 57 | MG | RA | 3137 | 1/1 | 0.84 | 0.28 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3167 | 1/1 | 0.79 | 0.20 | - | 51,51,51,51 | 0 |
| 57 | MG | RA | 3109 | 1/1 | 0.92 | 0.30 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3039 | 1/1 | 0.91 | 0.32 | - | 43,43,43,43 | 0 |
| 57 | MG | XA | 1606 | 1/1 | 0.93 | 0.34 | - | 35,35,35,35 | 0 |
| 57 | MG | RA | 3027 | 1/1 | 0.97 | 0.24 | - | 27,27,27,27 | 0 |
| 57 | MG | RA | 3190 | 1/1 | 0.94 | 0.31 | - | 48,48,48,48 | 0 |
| 57 | MG | RA | 3096 | 1/1 | 0.97 | 0.31 | - | 25,25,25,25 | 0 |
| 57 | MG | QA | 1637 | 1/1 | 0.88 | 0.29 | - | 72,72,72,72 | 0 |
| 57 | MG | YA | 3070 | 1/1 | 0.96 | 0.26 | - | 33,33,33,33 | 0 |
| 57 | MG | RA | 3140 | 1/1 | 0.87 | 0.75 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3012 | 1/1 | 0.99 | 0.45 | - | 8,8,8,8 | 0 |
| 57 | MG | XA | 1613 | 1/1 | 0.97 | 0.08 | - | 36,36,36,36 | 0 |
| 57 | MG | RA | 3023 | 1/1 | 0.95 | 0.19 | - | 26,26,26,26 | 0 |
| 57 | MG | YA | 3234 | 1/1 | 0.95 | 0.20 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3222 | 1/1 | 0.98 | 0.28 | - | 56,56,56,56 | 0 |
| 57 | MG | RA | 3157 | 1/1 | 0.80 | 0.44 | - | 69,69,69,69 | 0 |
| 57 | MG | XA | 1663 | 1/1 | 0.92 | 0.34 | - | 55,55,55,55 | 0 |
| 57 | MG | RA | 3092 | 1/1 | 0.96 | 0.41 | - | 27,27,27,27 | 0 |
| 57 | MG | YA | 3244 | 1/1 | 0.94 | 0.20 | - | 71,71,71,71 | 0 |
| 57 | MG | YA | 3077 | 1/1 | 0.95 | 0.47 | - | 26,26,26,26 | 0 |
| 57 | MG | RA | 3057 | 1/1 | 0.92 | 0.42 | - | 44,44,44,44 | 0 |
| 57 | MG | YA | 3018 | 1/1 | 0.95 | 0.43 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3165 | 1/1 | 0.92 | 0.32 | - | 46,46,46,46 | 0 |
| 57 | MG | RA | 3194 | 1/1 | 0.76 | 0.42 | - | 40,40,40,40 | 0 |
| 57 | MG | YA | 3212 | 1/1 | 0.97 | 0.24 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3055 | 1/1 | 0.98 | 0.54 | - | 27,27,27,27 | 0 |
| 57 | MG | YA | 3174 | 1/1 | 0.85 | 0.12 | - | 64,64,64,64 | 0 |
| 57 | MG | RA | 3028 | 1/1 | 0.98 | 0.35 | - | 28,28,28,28 | 0 |
| 57 | MG | RA | 3139 | 1/1 | 0.97 | 0.29 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3198 | 1/1 | 0.90 | 0.20 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3090 | 1/1 | 0.98 | 0.28 | - | 11,11,11,11 | 0 |
| 57 | MG | RA | 3073 | 1/1 | 0.91 | 0.27 | - | 35,35,35,35 | 0 |
| 57 | MG | QA | 1661 | 1/1 | 0.93 | 0.32 | - | 56,56,56,56 | 0 |
| 57 | MG | QA | 1626 | 1/1 | 0.84 | 0.17 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3260 | 1/1 | 0.99 | 0.33 | - | 26,26,26,26 | 0 |
| 57 | MG | YA | 3107 | 1/1 | 0.97 | 0.15 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3163 | 1/1 | 0.94 | 0.10 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3151 | 1/1 | 0.95 | 0.28 | - | 54,54,54,54 | 0 |
| 57 | MG | XA | 1629 | 1/1 | 0.48 | 0.17 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3037 | 1/1 | 0.98 | 0.25 | - | 16,16,16,16 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3160 | 1/1 | 0.88 | 0.22 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3176 | 1/1 | 0.88 | 0.16 | - | 47,47,47,47 | 0 |
| 57 | MG | QA | 1623 | 1/1 | 0.95 | 0.29 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3246 | 1/1 | 0.81 | 0.31 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3084 | 1/1 | 0.94 | 0.19 | - | 45,45,45,45 | 0 |
| 57 | MG | QA | 1652 | 1/1 | 0.95 | 0.36 | - | 38,38,38,38 | 0 |
| 57 | MG | QA | 1624 | 1/1 | 0.97 | 0.33 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3217 | 1/1 | 0.81 | 0.13 | - | 74,74,74,74 | 0 |
| 57 | MG | RA | 3013 | 1/1 | 0.96 | 0.28 | - | 14,14,14,14 | 0 |
| 57 | MG | QV | 102 | 1/1 | 0.90 | 0.27 | - | 30,30,30,30 | 0 |
| 57 | MG | QA | 1653 | 1/1 | 0.89 | 0.18 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3076 | 1/1 | 0.94 | 0.21 | - | 29,29,29,29 | 0 |
| 57 | MG | XA | 1616 | 1/1 | 0.98 | 0.30 | - | 25,25,25,25 | 0 |
| 57 | MG | RA | 3236 | 1/1 | 0.92 | 0.36 | - | 44,44,44,44 | 0 |
| 57 | MG | QA | 1635 | 1/1 | 0.96 | 0.20 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3181 | 1/1 | 0.76 | 0.21 | - | 54,54,54,54 | 0 |
| 57 | MG | QA | 1629 | 1/1 | 0.76 | 0.57 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3147 | 1/1 | 0.90 | 0.32 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3124 | 1/1 | 0.93 | 0.27 | - | 35,35,35,35 | 0 |
| 57 | MG | YA | 3241 | 1/1 | 0.88 | 0.34 | - | 56,56,56,56 | 0 |
| 57 | MG | YA | 3127 | 1/1 | 0.88 | 0.32 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3191 | 1/1 | 0.91 | 0.20 | - | 34,34,34,34 | 0 |
| 57 | MG | YA | 3204 | 1/1 | 0.90 | 0.28 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3082 | 1/1 | 0.99 | 0.57 | - | 39,39,39,39 | 0 |
| 57 | MG | YA | 3157 | 1/1 | 0.90 | 0.35 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3160 | 1/1 | 0.92 | 0.18 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3066 | 1/1 | 0.98 | 0.35 | - | 28,28,28,28 | 0 |
| 57 | MG | RA | 3009 | 1/1 | 0.87 | 0.22 | - | 77,77,77,77 | 0 |
| 57 | MG | XA | 1627 | 1/1 | 0.96 | 0.26 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3029 | 1/1 | 0.95 | 0.32 | - | 20,20,20,20 | 0 |
| 57 | MG | YA | 3201 | 1/1 | 0.91 | 0.88 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3150 | 1/1 | 0.96 | 0.22 | - | 52,52,52,52 | 0 |
| 57 | MG | RA | 3125 | 1/1 | 0.83 | 0.27 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3065 | 1/1 | 0.91 | 0.42 | - | 52,52,52,52 | 0 |
| 57 | MG | XA | 1601 | 1/1 | 0.96 | 0.50 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3171 | 1/1 | 0.88 | 0.24 | - | 56,56,56,56 | 0 |
| 57 | MG | YA | 3218 | 1/1 | 0.92 | 0.37 | - | 63,63,63,63 | 0 |
| 57 | MG | YA | 3146 | 1/1 | 0.88 | 0.45 | - | 48,48,48,48 | 0 |
| 57 | MG | QA | 1622 | 1/1 | 0.98 | 0.17 | - | 46,46,46,46 | 0 |
| 57 | MG | QA | 1663 | 1/1 | 0.88 | 0.11 | - | 95,95,95,95 | 0 |
| 57 | MG | YA | 3095 | 1/1 | 0.96 | 0.40 | - | 24,24,24,24 | 0 |
| 57 | MG | YA | 3194 | 1/1 | 0.89 | 0.17 | - | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | XA | 1670 | 1/1 | 0.74 | 0.13 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3235 | 1/1 | 0.88 | 0.36 | - | 69,69,69,69 | 0 |
| 57 | MG | RA | 3104 | 1/1 | 0.97 | 0.34 | - | 29,29,29,29 | 0 |
| 57 | MG | YA | 3264 | 1/1 | 0.87 | 0.47 | - | 52,52,52,52 | 0 |
| 57 | MG | XA | 1667 | 1/1 | 0.85 | 0.29 | - | 50,50,50,50 | 0 |
| 57 | MG | RA | 3103 | 1/1 | 0.96 | 0.25 | - | 28,28,28,28 | 0 |
| 57 | MG | XX | 101 | 1/1 | 0.91 | 0.20 | - | 79,79,79,79 | 0 |
| 57 | MG | RA | 3180 | 1/1 | 0.88 | 0.17 | - | 34,34,34,34 | 0 |
| 57 | MG | QA | 1628 | 1/1 | 0.95 | 0.14 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3219 | 1/1 | 0.93 | 0.18 | - | 49,49,49,49 | 0 |
| 57 | MG | XA | 1643 | 1/1 | 0.94 | 0.31 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3032 | 1/1 | 0.99 | 0.40 | - | 21,21,21,21 | 0 |
| 57 | MG | YA | 3055 | 1/1 | 0.98 | 0.24 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3135 | 1/1 | 0.85 | 0.13 | - | 45,45,45,45 | 0 |
| 57 | MG | QA | 1603 | 1/1 | 0.95 | 0.67 | - | 36,36,36,36 | 0 |
| 57 | MG | YA | 3097 | 1/1 | 0.96 | 0.33 | - | 36,36,36,36 | 0 |
| 57 | MG | RA | 3044 | 1/1 | 0.92 | 0.44 | - | 43,43,43,43 | 0 |
| 57 | MG | RA | 3007 | 1/1 | 0.86 | 0.24 | - | 34,34,34,34 | 0 |
| 57 | MG | YA | 3063 | 1/1 | 0.94 | 0.29 | - | 23,23,23,23 | 0 |
| 57 | MG | RA | 3177 | 1/1 | 0.81 | 0.22 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3237 | 1/1 | 0.97 | 0.33 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3168 | 1/1 | 0.92 | 0.55 | - | 57,57,57,57 | 0 |
| 57 | MG | XA | 1641 | 1/1 | 0.83 | 0.30 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3029 | 1/1 | 0.97 | 0.29 | - | 32,32,32,32 | 0 |
| 57 | MG | YA | 3197 | 1/1 | 0.93 | 0.47 | - | 47,47,47,47 | 0 |
| 57 | MG | QA | 1662 | 1/1 | 0.52 | 0.33 | - | 119,119,119,119 | 0 |
| 57 | MG | RA | 3070 | 1/1 | 0.93 | 0.43 | - | 32,32,32,32 | 0 |
| 57 | MG | YA | 3043 | 1/1 | 0.96 | 0.43 | - | 17,17,17,17 | 0 |
| 57 | MG | YA | 3040 | 1/1 | 0.96 | 0.29 | - | 19,19,19,19 | 0 |
| 57 | MG | RA | 3235 | 1/1 | 0.88 | 0.57 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3207 | 1/1 | 0.99 | 0.08 | - | 93,93,93,93 | 0 |
| 57 | MG | QF | 201 | 1/1 | 0.94 | 0.41 | - | 68,68,68,68 | 0 |
| 57 | MG | YA | 3104 | 1/1 | 0.98 | 0.16 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3112 | 1/1 | 0.98 | 0.21 | - | 44,44,44,44 | 0 |
| 57 | MG | XA | 1631 | 1/1 | 0.78 | 0.18 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3209 | 1/1 | 0.74 | 0.32 | - | 71,71,71,71 | 0 |
| 57 | MG | RA | 3225 | 1/1 | 0.98 | 0.14 | - | 59,59,59,59 | 0 |
| 57 | MG | XA | 1652 | 1/1 | 0.97 | 0.18 | - | 105,105,105,105 | 0 |
| 57 | MG | RA | 3010 | 1/1 | 0.91 | 0.58 | - | 56,56,56,56 | 0 |
| 57 | MG | RA | 3152 | 1/1 | 0.94 | 0.13 | - | 56,56,56,56 | 0 |
| 57 | MG | QA | 1634 | 1/1 | 0.96 | 0.48 | - | 39,39,39,39 | 0 |
| 57 | MG | YA | 3052 | 1/1 | 0.92 | 0.61 | - | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | QA | 1659 | 1/1 | 0.93 | 0.29 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3228 | 1/1 | 0.64 | 0.29 | - | 36,36,36,36 | 0 |
| 57 | MG | YA | 3206 | 1/1 | 0.58 | 0.30 | - | 56,56,56,56 | 0 |
| 57 | MG | YA | 3224 | 1/1 | 0.91 | 0.20 | - | 51,51,51,51 | 0 |
| 57 | MG | XA | 1609 | 1/1 | 0.97 | 0.40 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3069 | 1/1 | 0.93 | 0.45 | - | 40,40,40,40 | 0 |
| 57 | MG | YA | 3079 | 1/1 | 0.99 | 0.42 | - | 25,25,25,25 | 0 |
| 57 | MG | YA | 3058 | 1/1 | 0.98 | 0.52 | - | 24,24,24,24 | 0 |
| 57 | MG | YA | 3205 | 1/1 | 0.92 | 0.08 | - | 48,48,48,48 | 0 |
| 57 | MG | QA | 1625 | 1/1 | 0.87 | 0.33 | - | 53,53,53,53 | 0 |
| 57 | MG | R8 | 101 | 1/1 | 0.92 | 0.28 | - | 33,33,33,33 | 0 |
| 57 | MG | RA | 3206 | 1/1 | 0.88 | 0.24 | - | 76,76,76,76 | 0 |
| 57 | MG | RA | 3196 | 1/1 | 0.91 | 0.09 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3101 | 1/1 | 0.95 | 0.33 | - | 38,38,38,38 | 0 |
| 57 | MG | YA | 3149 | 1/1 | 0.89 | 0.20 | - | 40,40,40,40 | 0 |
| 57 | MG | RA | 3018 | 1/1 | 0.98 | 0.27 | - | 23,23,23,23 | 0 |
| 57 | MG | XT | 201 | 1/1 | 0.49 | 0.34 | - | 77,77,77,77 | 0 |
| 57 | MG | XA | 1639 | 1/1 | 0.94 | 0.15 | - | 49,49,49,49 | 0 |
| 57 | MG | RA | 3025 | 1/1 | 0.87 | 0.20 | - | 18,18,18,18 | 0 |
| 57 | MG | RA | 3133 | 1/1 | 0.90 | 0.31 | - | 73,73,73,73 | 0 |
| 57 | MG | XA | 1644 | 1/1 | 0.96 | 0.16 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3061 | 1/1 | 0.94 | 0.16 | - | 68,68,68,68 | 0 |
| 57 | MG | YA | 3045 | 1/1 | 0.76 | 0.31 | - | 20,20,20,20 | 0 |
| 57 | MG | RA | 3168 | 1/1 | 0.97 | 0.43 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3142 | 1/1 | 0.95 | 0.35 | - | 54,54,54,54 | 0 |
| 57 | MG | QA | 1605 | 1/1 | 0.93 | 0.57 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3117 | 1/1 | 0.94 | 0.16 | - | 35,35,35,35 | 0 |
| 57 | MG | RA | 3172 | 1/1 | 0.78 | 0.22 | - | 51,51,51,51 | 0 |
| 57 | MG | RA | 3046 | 1/1 | 0.94 | 0.43 | - | 26,26,26,26 | 0 |
| 57 | MG | YA | 3248 | 1/1 | 0.91 | 0.52 | - | 38,38,38,38 | 0 |
| 57 | MG | XA | 1658 | 1/1 | 0.94 | 0.40 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3254 | 1/1 | 0.95 | 0.47 | - | 32,32,32,32 | 0 |
| 57 | MG | YA | 3103 | 1/1 | 0.95 | 0.30 | - | 32,32,32,32 | 0 |
| 57 | MG | YA | 3125 | 1/1 | 0.93 | 0.31 | - | 33,33,33,33 | 0 |
| 57 | MG | QA | 1645 | 1/1 | 0.97 | 0.15 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3112 | 1/1 | 0.97 | 0.16 | - | 36,36,36,36 | 0 |
| 57 | MG | RA | 3226 | 1/1 | 0.88 | 0.22 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3113 | 1/1 | 0.86 | 0.21 | - | 27,27,27,27 | 0 |
| 57 | MG | YA | 3166 | 1/1 | 0.77 | 0.26 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3001 | 1/1 | 0.94 | 0.49 | - | 42,42,42,42 | 0 |
| 57 | MG | YA | 3022 | 1/1 | 0.99 | 0.28 | - | 34,34,34,34 | 0 |
| 57 | MG | R0 | 101 | 1/1 | 0.95 | 0.27 | - | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | YA | 3010 | 1/1 | 0.99 | 0.27 | - | 17,17,17,17 | 0 |
| 57 | MG | QA | 1633 | 1/1 | 0.80 | 0.39 | - | 73,73,73,73 | 0 |
| 57 | MG | YA | 3257 | 1/1 | 0.99 | 0.25 | - | 12,12,12,12 | 0 |
| 57 | MG | RA | 3071 | 1/1 | 0.96 | 0.31 | - | 51,51,51,51 | 0 |
| 57 | MG | RA | 3182 | 1/1 | 0.94 | 0.19 | - | 33,33,33,33 | 0 |
| 57 | MG | YA | 3119 | 1/1 | 0.97 | 0.41 | - | 36,36,36,36 | 0 |
| 57 | MG | XA | 1668 | 1/1 | 0.89 | 0.65 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3114 | 1/1 | 0.97 | 0.33 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3228 | 1/1 | 0.80 | 0.23 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3215 | 1/1 | 0.94 | 0.41 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3175 | 1/1 | 0.92 | 0.11 | - | 49,49,49,49 | 0 |
| 57 | MG | RA | 3233 | 1/1 | 0.95 | 0.28 | - | 57,57,57,57 | 0 |
| 57 | MG | QA | 1657 | 1/1 | 0.93 | 0.32 | - | 55,55,55,55 | 0 |
| 57 | MG | RA | 3216 | 1/1 | 0.75 | 0.27 | - | 47,47,47,47 | 0 |
| 57 | MG | QA | 1642 | 1/1 | 0.97 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | YA | 3268 | 1/1 | 0.69 | 0.65 | - | 72,72,72,72 | 0 |
| 57 | MG | QA | 1608 | 1/1 | 0.97 | 0.08 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3144 | 1/1 | 0.94 | 0.40 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3051 | 1/1 | 0.91 | 0.35 | - | 26,26,26,26 | 0 |
| 57 | MG | RA | 3060 | 1/1 | 0.98 | 0.18 | - | 31,31,31,31 | 0 |
| 57 | MG | YA | 3121 | 1/1 | 0.36 | 0.43 | - | 76,76,76,76 | 0 |
| 57 | MG | RA | 3147 | 1/1 | 0.91 | 0.25 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3267 | 1/1 | 0.96 | 0.34 | - | 40,40,40,40 | 0 |
| 57 | MG | RA | 3090 | 1/1 | 0.55 | 0.56 | - | 71,71,71,71 | 0 |
| 57 | MG | YA | 3239 | 1/1 | 0.78 | 0.48 | - | 74,74,74,74 | 0 |
| 57 | MG | YA | 3263 | 1/1 | 0.97 | 0.38 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3173 | 1/1 | 0.86 | 0.09 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3243 | 1/1 | 0.74 | 0.22 | - | 46,46,46,46 | 0 |
| 57 | MG | XA | 1617 | 1/1 | 0.96 | 0.20 | - | 36,36,36,36 | 0 |
| 57 | MG | RA | 3234 | 1/1 | 0.87 | 0.49 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3048 | 1/1 | 0.91 | 0.25 | - | 30,30,30,30 | 0 |
| 57 | MG | XA | 1642 | 1/1 | 0.93 | 0.37 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3196 | 1/1 | 0.95 | 0.28 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3140 | 1/1 | 0.61 | 0.30 | - | 81,81,81,81 | 0 |
| 57 | MG | YA | 3184 | 1/1 | 0.92 | 0.31 | - | 67,67,67,67 | 0 |
| 57 | MG | RA | 3163 | 1/1 | 0.84 | 0.59 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3148 | 1/1 | 0.97 | 0.27 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3111 | 1/1 | 0.99 | 0.17 | - | 28,28,28,28 | 0 |
| 57 | MG | RA | 3195 | 1/1 | 0.92 | 0.20 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3249 | 1/1 | 0.88 | 0.34 | - | 74,74,74,74 | 0 |
| 57 | MG | QA | 1665 | 1/1 | 0.81 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3046 | 1/1 | 0.97 | 0.33 | - | 27,27,27,27 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 57 | MG | RA | 3128 | 1/1 | 0.97 | 0.12 | - | 39,39,39,39 | 0 |
| 57 | MG | YA | 3019 | 1/1 | 0.95 | 0.34 | - | 21,21,21,21 | 0 |
| 57 | MG | RA | 3067 | 1/1 | 0.93 | 0.29 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3047 | 1/1 | 0.97 | 0.41 | - | 19,19,19,19 | 0 |
| 57 | MG | YA | 3020 | 1/1 | 0.96 | 0.54 | - | 18,18,18,18 | 0 |
| 57 | MG | YA | 3258 | 1/1 | 0.97 | 0.26 | - | 28,28,28,28 | 0 |
| 57 | MG | XA | 1672 | 1/1 | 0.92 | 0.30 | - | 44,44,44,44 | 0 |
| 57 | MG | QA | 1619 | 1/1 | 0.92 | 0.40 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3089 | 1/1 | 0.95 | 0.46 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3094 | 1/1 | 0.97 | 0.31 | - | 27,27,27,27 | 0 |
| 57 | MG | YA | 3214 | 1/1 | 0.95 | 0.16 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3195 | 1/1 | 0.92 | 0.22 | - | 32,32,32,32 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.