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

Sep 14, 2023 – 07:25 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 4V9N |
| Title | : | Crystal structure of the 70S ribosome bound with the Q253P mutant of release factor RF2. |
| Authors | : | Santos, N.; Zhu, J.; Donohue, J.P.; Korostelev, A.A.; Noller, H.F. |
| Deposited on | : | 2013-04-26 |
| Resolution | : | 3.40 Å(reported) |

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

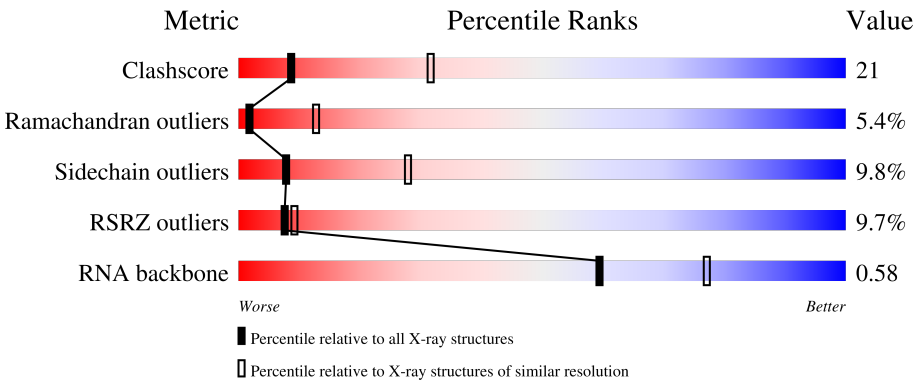
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

# 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 3.40 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 1055 (3.48-3.32) |
| Ramachandran outliers | 138981 | 1038 (3.48-3.32) |
| Sidechain outliers | 138945 | 1038 (3.48-3.32) |
| RSRZ outliers | 127900 | 2173 (3.50-3.30) |
| RNA backbone | 3102 | 1006 (3.84-2.96) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AA | 1504 | 2%, 44%, 46%, 10% |
| 1 | CA | 1504 | 3%, 44%, 46%, 10% |
| 2 | AV | 10 | 10%, 50%, 50% |
| 2 | CV | 10 | 30%, 40%, 60% |
| 3 | AW | 77 | ., 60%, 35%, 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | CW | 77 | %, 58%, 36%, 5% |
| 4 | AY | 362 | 35%, 48%, 43%, 8% |
| 4 | CY | 362 | 36%, 49%, 43%, 7% |
| 5 | AB | 234 | 23%, 46%, 47%, 7% |
| 5 | CB | 234 | 27%, 46%, 47%, 8% |
| 6 | AC | 206 | 12%, 44%, 46%, 10% |
| 6 | CC | 206 | 11%, 43%, 46%, 11% |
| 7 | AD | 208 | 2%, 46%, 42%, 11% |
| 7 | CD | 208 | 9%, 41%, 50%, 8% |
| 8 | AE | 151 | 9%, 45%, 50%, 5% |
| 8 | CE | 151 | 10%, 46%, 47%, 7% |
| 9 | AF | 101 | 17%, 55%, 41% |
| 9 | CF | 101 | 10%, 57%, 39% |
| 10 | AG | 155 | 11%, 56%, 43% |
| 10 | CG | 155 | 12%, 61%, 38% |
| 11 | AH | 138 | 5%, 46%, 49% |
| 11 | CH | 138 | 7%, 44%, 51% |
| 12 | AI | 127 | 32%, 41%, 52%, 7% |
| 12 | CI | 127 | 31%, 39%, 54%, 7% |
| 13 | AJ | 98 | 35%, 35%, 54%, 10% |
| 13 | CJ | 98 | 38%, 37%, 52%, 10% |
| 14 | AK | 114 | 17%, 55%, 39%, 5% |
| 14 | CK | 114 | 6%, 53%, 43% |
| 15 | AL | 122 | 2%, 48%, 46%, 7% |
| 15 | CL | 122 | 2%, 49%, 43%, 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 16 | AM | 117 | 13% 53% 41% 6% |
| 16 | CM | 117 | 17% 53% 41% 6% |
| 17 | AN | 60 | 17% 45% 47% 7% |
| 17 | CN | 60 | 18% 40% 53% 7% |
| 18 | AO | 88 | 2% 56% 34% 10% |
| 18 | CO | 88 | % 53% 35% 11% |
| 19 | AP | 83 | 5% 41% 51% 8% |
| 19 | CP | 83 | 31% 42% 51% 7% |
| 20 | AQ | 99 | 4% 48% 45% 6% |
| 20 | CQ | 99 | 6% 47% 46% 6% |
| 21 | AR | 70 | 40% 50% 49% |
| 21 | CR | 70 | 14% 46% 51% |
| 22 | AS | 78 | 32% 36% 46% 17% |
| 22 | CS | 78 | 36% 35% 46% 18% |
| 23 | AT | 99 | 14% 49% 46% |
| 23 | CT | 99 | 17% 49% 46% |
| 24 | AU | 24 | 96% 25% 67% 8% |
| 24 | CU | 24 | 79% 38% 54% 8% |
| 25 | BA | 2879 | 3% 48% 40% 9% |
| 25 | DA | 2879 | 3% 48% 39% 9% |
| 26 | BB | 119 | 41% 48% 11% |
| 26 | DB | 119 | 2% 39% 50% 11% |
| 27 | BD | 271 | 5% 41% 50% 9% |
| 27 | DD | 271 | 2% 41% 50% 9% |
| 28 | BE | 204 | 5% 50% 44% 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | DE | 204 | 2%, 49%, 44%, 8% |
| 29 | BF | 202 | 44%, 49%, 8% |
| 29 | DF | 202 | %, 43%, 50%, 8% |
| 30 | BG | 181 | 22%, 41%, 49%, 10% |
| 30 | DG | 181 | 16%, 40%, 50%, 10% |
| 31 | BH | 159 | 31%, 52%, 42%, 7% |
| 31 | DH | 159 | 4%, 50%, 43%, 6% |
| 32 | BI | 145 | 41%, 35%, 58%, 7% |
| 32 | DI | 145 | 10%, 36%, 57%, 8% |
| 33 | BK | 147 | 83%, 50%, 41%, 9% |
| 33 | DK | 147 | 82%, 49%, 45%, 6% |
| 34 | BN | 137 | 4%, 42%, 45%, 12% |
| 34 | DN | 137 | 44%, 44%, 12% |
| 35 | BO | 122 | 60%, 39% |
| 35 | DO | 122 | 59%, 39% |
| 36 | BP | 146 | 9%, 30%, 46%, 19%, 5% |
| 36 | DP | 146 | 10%, 29%, 48%, 18%, 5% |
| 37 | BQ | 134 | 5%, 43%, 51%, 6% |
| 37 | DQ | 134 | 5%, 45%, 49%, 5% |
| 38 | BR | 117 | %, 41%, 49%, 9% |
| 38 | DR | 117 | 3%, 43%, 48%, 9% |
| 39 | BS | 98 | 26%, 35%, 52%, 10% |
| 39 | DS | 98 | 14%, 37%, 48%, 12% |
| 40 | BT | 137 | 5%, 47%, 41%, 11% |
| 40 | DT | 137 | 10%, 45%, 44%, 11% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | BU | 117 | 5% 47% 45% 8% |
| 41 | DU | 117 | 3% 50% 43% 8% |
| 42 | BV | 101 | 2% 36% 50% 13% • |
| 42 | DV | 101 | 9% 32% 54% 13% • |
| 43 | BW | 112 | % 54% 40% 6% |
| 43 | DW | 112 | 53% 41% 6% |
| 44 | BX | 92 | 2% 38% 58% • |
| 44 | DX | 92 | % 39% 57% • |
| 45 | BY | 100 | 23% 38% 48% 12% • |
| 45 | DY | 100 | 15% 39% 46% 12% • |
| 46 | BZ | 187 | 9% 45% 51% • |
| 46 | DZ | 187 | 6% 47% 49% • |
| 47 | B0 | 76 | 3% 43% 47% 9% |
| 47 | D0 | 76 | 4% 46% 46% 8% |
| 48 | B1 | 88 | 6% 24% 57% 18% • |
| 48 | D1 | 88 | 5% 20% 58% 20% • |
| 49 | B2 | 62 | 10% 31% 55% 11% • |
| 49 | D2 | 62 | 11% 31% 52% 15% • |
| 50 | B3 | 59 | 10% 44% 51% 5% |
| 50 | D3 | 59 | 5% 47% 47% 5% |
| 51 | B4 | 30 | 17% 53% 43% • |
| 51 | D4 | 30 | 37% 53% 43% • |
| 52 | B5 | 52 | 6% 58% 38% • • |
| 52 | D5 | 52 | 2% 56% 38% • • |
| 53 | B6 | 44 | 100% 32% 50% 18% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | D6 | 44 | 95%; 34%, 48%, 18% |
| 54 | B7 | 48 | 12%; 58%, 38%, · |
| 54 | D7 | 48 | 6%; 58%, 38%, · |
| 55 | B8 | 63 | 3%; 29%, 52%, 16%, · |
| 55 | D8 | 63 | 5%; 29%, 52%, 16%, · |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1607 | - | - | - | X |
| 56 | MG | AA | 1612 | - | - | - | X |
| 56 | MG | AA | 1619 | - | - | - | X |
| 56 | MG | AA | 1622 | - | - | - | X |
| 56 | MG | AA | 1625 | - | - | - | X |
| 56 | MG | AA | 1629 | - | - | - | X |
| 56 | MG | AA | 1631 | - | - | - | X |
| 56 | MG | AA | 1632 | - | - | - | X |
| 56 | MG | AA | 1639 | - | - | - | X |
| 56 | MG | AA | 1672 | - | - | - | X |
| 56 | MG | AA | 1675 | - | - | - | X |
| 56 | MG | AA | 1686 | - | - | - | X |
| 56 | MG | AA | 1699 | - | - | - | X |
| 56 | MG | AA | 1702 | - | - | - | X |
| 56 | MG | AA | 1714 | - | - | - | X |
| 56 | MG | AA | 1725 | - | - | - | X |
| 56 | MG | AA | 1726 | - | - | - | X |
| 56 | MG | AA | 1727 | - | - | - | X |
| 56 | MG | AA | 1742 | - | - | - | X |
| 56 | MG | AA | 1744 | - | - | - | X |
| 56 | MG | AA | 1764 | - | - | - | X |
| 56 | MG | AA | 1765 | - | - | - | X |
| 56 | MG | AA | 1767 | - | - | - | X |
| 56 | MG | AA | 1772 | - | - | - | X |
| 56 | MG | AA | 1780 | - | - | - | X |
| 56 | MG | AA | 1782 | - | - | - | X |
| 56 | MG | AA | 1783 | - | - | - | X |
| 56 | MG | AA | 1786 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1790 | - | - | - | X |
| 56 | MG | AA | 1796 | - | - | - | X |
| 56 | MG | AA | 1804 | - | - | - | X |
| 56 | MG | AA | 1824 | - | - | - | X |
| 56 | MG | AA | 1825 | - | - | - | X |
| 56 | MG | AA | 1829 | - | - | - | X |
| 56 | MG | AA | 1831 | - | - | - | X |
| 56 | MG | AA | 1835 | - | - | - | X |
| 56 | MG | AA | 1839 | - | - | - | X |
| 56 | MG | AA | 1846 | - | - | - | X |
| 56 | MG | AA | 1854 | - | - | - | X |
| 56 | MG | AA | 1860 | - | - | - | X |
| 56 | MG | AA | 1874 | - | - | - | X |
| 56 | MG | AA | 1879 | - | - | - | X |
| 56 | MG | AA | 1897 | - | - | - | X |
| 56 | MG | AA | 1934 | - | - | - | X |
| 56 | MG | AA | 1941 | - | - | - | X |
| 56 | MG | AA | 1945 | - | - | - | X |
| 56 | MG | AA | 1947 | - | - | - | X |
| 56 | MG | AA | 1950 | - | - | - | X |
| 56 | MG | AA | 1951 | - | - | - | X |
| 56 | MG | AA | 1957 | - | - | - | X |
| 56 | MG | AA | 1979 | - | - | - | X |
| 56 | MG | AC | 301 | - | - | - | X |
| 56 | MG | AG | 201 | - | - | - | X |
| 56 | MG | AT | 203 | - | - | - | X |
| 56 | MG | AW | 102 | - | - | - | X |
| 56 | MG | AW | 104 | - | - | - | X |
| 56 | MG | AW | 107 | - | - | - | X |
| 56 | MG | AW | 109 | - | - | - | X |
| 56 | MG | AW | 112 | - | - | - | X |
| 56 | MG | AY | 401 | - | - | - | X |
| 56 | MG | AY | 403 | - | - | - | X |
| 56 | MG | B0 | 102 | - | - | - | X |
| 56 | MG | BA | 2917 | - | - | - | X |
| 56 | MG | BA | 2918 | - | - | - | X |
| 56 | MG | BA | 2920 | - | - | - | X |
| 56 | MG | BA | 2922 | - | - | - | X |
| 56 | MG | BA | 2925 | - | - | - | X |
| 56 | MG | BA | 2926 | - | - | - | X |
| 56 | MG | BA | 2929 | - | - | - | X |
| 56 | MG | BA | 2930 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 2934 | - | - | - | X |
| 56 | MG | BA | 2935 | - | - | - | X |
| 56 | MG | BA | 2939 | - | - | - | X |
| 56 | MG | BA | 2943 | - | - | - | X |
| 56 | MG | BA | 2946 | - | - | - | X |
| 56 | MG | BA | 2949 | - | - | - | X |
| 56 | MG | BA | 2950 | - | - | - | X |
| 56 | MG | BA | 2959 | - | - | - | X |
| 56 | MG | BA | 2972 | - | - | - | X |
| 56 | MG | BA | 2973 | - | - | - | X |
| 56 | MG | BA | 2976 | - | - | - | X |
| 56 | MG | BA | 2992 | - | - | - | X |
| 56 | MG | BA | 2994 | - | - | - | X |
| 56 | MG | BA | 3003 | - | - | - | X |
| 56 | MG | BA | 3004 | - | - | - | X |
| 56 | MG | BA | 3011 | - | - | - | X |
| 56 | MG | BA | 3012 | - | - | - | X |
| 56 | MG | BA | 3020 | - | - | - | X |
| 56 | MG | BA | 3022 | - | - | - | X |
| 56 | MG | BA | 3032 | - | - | - | X |
| 56 | MG | BA | 3043 | - | - | - | X |
| 56 | MG | BA | 3053 | - | - | - | X |
| 56 | MG | BA | 3064 | - | - | - | X |
| 56 | MG | BA | 3073 | - | - | - | X |
| 56 | MG | BA | 3078 | - | - | - | X |
| 56 | MG | BA | 3084 | - | - | - | X |
| 56 | MG | BA | 3085 | - | - | - | X |
| 56 | MG | BA | 3092 | - | - | - | X |
| 56 | MG | BA | 3093 | - | - | - | X |
| 56 | MG | BA | 3095 | - | - | - | X |
| 56 | MG | BA | 3097 | - | - | - | X |
| 56 | MG | BA | 3098 | - | - | - | X |
| 56 | MG | BA | 3119 | - | - | - | X |
| 56 | MG | BA | 3121 | - | - | - | X |
| 56 | MG | BA | 3128 | - | - | - | X |
| 56 | MG | BA | 3130 | - | - | - | X |
| 56 | MG | BA | 3139 | - | - | - | X |
| 56 | MG | BA | 3141 | - | - | - | X |
| 56 | MG | BA | 3143 | - | - | - | X |
| 56 | MG | BA | 3147 | - | - | - | X |
| 56 | MG | BA | 3156 | - | - | - | X |
| 56 | MG | BA | 3157 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3168 | - | - | - | X |
| 56 | MG | BA | 3173 | - | - | - | X |
| 56 | MG | BA | 3175 | - | - | - | X |
| 56 | MG | BA | 3180 | - | - | - | X |
| 56 | MG | BA | 3182 | - | - | - | X |
| 56 | MG | BA | 3185 | - | - | - | X |
| 56 | MG | BA | 3186 | - | - | - | X |
| 56 | MG | BA | 3188 | - | - | - | X |
| 56 | MG | BA | 3189 | - | - | - | X |
| 56 | MG | BA | 3205 | - | - | - | X |
| 56 | MG | BA | 3211 | - | - | - | X |
| 56 | MG | BA | 3213 | - | - | - | X |
| 56 | MG | BA | 3218 | - | - | - | X |
| 56 | MG | BA | 3224 | - | - | - | X |
| 56 | MG | BA | 3229 | - | - | - | X |
| 56 | MG | BA | 3230 | - | - | - | X |
| 56 | MG | BA | 3237 | - | - | - | X |
| 56 | MG | BA | 3239 | - | - | - | X |
| 56 | MG | BA | 3244 | - | - | - | X |
| 56 | MG | BA | 3247 | - | - | - | X |
| 56 | MG | BA | 3248 | - | - | - | X |
| 56 | MG | BA | 3252 | - | - | - | X |
| 56 | MG | BA | 3256 | - | - | - | X |
| 56 | MG | BA | 3257 | - | - | - | X |
| 56 | MG | BA | 3261 | - | - | - | X |
| 56 | MG | BA | 3264 | - | - | - | X |
| 56 | MG | BA | 3267 | - | - | - | X |
| 56 | MG | BA | 3270 | - | - | - | X |
| 56 | MG | BA | 3275 | - | - | - | X |
| 56 | MG | BA | 3278 | - | - | - | X |
| 56 | MG | BA | 3284 | - | - | - | X |
| 56 | MG | BA | 3297 | - | - | - | X |
| 56 | MG | BA | 3299 | - | - | - | X |
| 56 | MG | BA | 3332 | - | - | - | X |
| 56 | MG | BA | 3369 | - | - | - | X |
| 56 | MG | BA | 3377 | - | - | - | X |
| 56 | MG | BA | 3403 | - | - | - | X |
| 56 | MG | BA | 3407 | - | - | - | X |
| 56 | MG | BA | 3414 | - | - | - | X |
| 56 | MG | BA | 3435 | - | - | - | X |
| 56 | MG | BA | 3450 | - | - | - | X |
| 56 | MG | BA | 3462 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3465 | - | - | - | X |
| 56 | MG | BA | 3479 | - | - | - | X |
| 56 | MG | BA | 3482 | - | - | - | X |
| 56 | MG | BA | 3496 | - | - | - | X |
| 56 | MG | BA | 3514 | - | - | - | X |
| 56 | MG | BA | 3517 | - | - | - | X |
| 56 | MG | BA | 3536 | - | - | - | X |
| 56 | MG | BA | 3540 | - | - | - | X |
| 56 | MG | BA | 3546 | - | - | - | X |
| 56 | MG | BA | 3548 | - | - | - | X |
| 56 | MG | BA | 3553 | - | - | - | X |
| 56 | MG | BA | 3563 | - | - | - | X |
| 56 | MG | BA | 3569 | - | - | - | X |
| 56 | MG | BA | 3577 | - | - | - | X |
| 56 | MG | BA | 3583 | - | - | - | X |
| 56 | MG | BA | 3584 | - | - | - | X |
| 56 | MG | BA | 3588 | - | - | - | X |
| 56 | MG | BA | 3591 | - | - | - | X |
| 56 | MG | BA | 3597 | - | - | - | X |
| 56 | MG | BA | 3599 | - | - | - | X |
| 56 | MG | BA | 3600 | - | - | - | X |
| 56 | MG | BA | 3602 | - | - | - | X |
| 56 | MG | BA | 3612 | - | - | - | X |
| 56 | MG | BA | 3613 | - | - | - | X |
| 56 | MG | BA | 3616 | - | - | - | X |
| 56 | MG | BA | 3618 | - | - | - | X |
| 56 | MG | BA | 3622 | - | - | - | X |
| 56 | MG | BA | 3628 | - | - | - | X |
| 56 | MG | BA | 3629 | - | - | - | X |
| 56 | MG | BA | 3639 | - | - | - | X |
| 56 | MG | BA | 3641 | - | - | - | X |
| 56 | MG | BA | 3650 | - | - | - | X |
| 56 | MG | BA | 3655 | - | - | - | X |
| 56 | MG | BA | 3661 | - | - | - | X |
| 56 | MG | BA | 3672 | - | - | - | X |
| 56 | MG | BA | 3676 | - | - | - | X |
| 56 | MG | BA | 3713 | - | - | - | X |
| 56 | MG | BB | 208 | - | - | - | X |
| 56 | MG | BB | 211 | - | - | - | X |
| 56 | MG | BB | 216 | - | - | - | X |
| 56 | MG | BB | 223 | - | - | - | X |
| 56 | MG | BE | 301 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | CA | 1607 | - | - | - | X |
| 56 | MG | CA | 1613 | - | - | - | X |
| 56 | MG | CA | 1614 | - | - | - | X |
| 56 | MG | CA | 1626 | - | - | - | X |
| 56 | MG | CA | 1631 | - | - | - | X |
| 56 | MG | CA | 1644 | - | - | - | X |
| 56 | MG | CA | 1645 | - | - | - | X |
| 56 | MG | CA | 1647 | - | - | - | X |
| 56 | MG | CA | 1658 | - | - | - | X |
| 56 | MG | CA | 1663 | - | - | - | X |
| 56 | MG | CA | 1665 | - | - | - | X |
| 56 | MG | CA | 1669 | - | - | - | X |
| 56 | MG | CA | 1675 | - | - | - | X |
| 56 | MG | CA | 1677 | - | - | - | X |
| 56 | MG | CA | 1678 | - | - | - | X |
| 56 | MG | CA | 1681 | - | - | - | X |
| 56 | MG | CA | 1683 | - | - | - | X |
| 56 | MG | CA | 1693 | - | - | - | X |
| 56 | MG | CA | 1699 | - | - | - | X |
| 56 | MG | CA | 1704 | - | - | - | X |
| 56 | MG | CA | 1710 | - | - | - | X |
| 56 | MG | CA | 1719 | - | - | - | X |
| 56 | MG | CA | 1720 | - | - | - | X |
| 56 | MG | CA | 1725 | - | - | - | X |
| 56 | MG | CA | 1732 | - | - | - | X |
| 56 | MG | CA | 1735 | - | - | - | X |
| 56 | MG | CA | 1737 | - | - | - | X |
| 56 | MG | CA | 1747 | - | - | - | X |
| 56 | MG | CA | 1748 | - | - | - | X |
| 56 | MG | CA | 1752 | - | - | - | X |
| 56 | MG | CA | 1772 | - | - | - | X |
| 56 | MG | CA | 1780 | - | - | - | X |
| 56 | MG | CA | 1790 | - | - | - | X |
| 56 | MG | CA | 1792 | - | - | - | X |
| 56 | MG | CA | 1800 | - | - | - | X |
| 56 | MG | CA | 1807 | - | - | - | X |
| 56 | MG | CA | 1808 | - | - | - | X |
| 56 | MG | CA | 1809 | - | - | - | X |
| 56 | MG | CA | 1810 | - | - | - | X |
| 56 | MG | CA | 1812 | - | - | - | X |
| 56 | MG | CA | 1816 | - | - | - | X |
| 56 | MG | CA | 1820 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | CA | 1833 | - | - | - | X |
| 56 | MG | CA | 1840 | - | - | - | X |
| 56 | MG | CA | 1842 | - | - | - | X |
| 56 | MG | CA | 1854 | - | - | - | X |
| 56 | MG | CA | 1874 | - | - | - | X |
| 56 | MG | CA | 1877 | - | - | - | X |
| 56 | MG | CA | 1882 | - | - | - | X |
| 56 | MG | CA | 1884 | - | - | - | X |
| 56 | MG | CA | 1887 | - | - | - | X |
| 56 | MG | CA | 1900 | - | - | - | X |
| 56 | MG | CA | 1902 | - | - | - | X |
| 56 | MG | CA | 1907 | - | - | - | X |
| 56 | MG | CA | 1911 | - | - | - | X |
| 56 | MG | CA | 1912 | - | - | - | X |
| 56 | MG | CA | 1926 | - | - | - | X |
| 56 | MG | CD | 302 | - | - | - | X |
| 56 | MG | CM | 201 | - | - | - | X |
| 56 | MG | CW | 102 | - | - | - | X |
| 56 | MG | CW | 105 | - | - | - | X |
| 56 | MG | CY | 401 | - | - | - | X |
| 56 | MG | D7 | 101 | - | - | - | X |
| 56 | MG | DA | 2903 | - | - | - | X |
| 56 | MG | DA | 2911 | - | - | - | X |
| 56 | MG | DA | 2914 | - | - | - | X |
| 56 | MG | DA | 2915 | - | - | - | X |
| 56 | MG | DA | 2916 | - | - | - | X |
| 56 | MG | DA | 2917 | - | - | - | X |
| 56 | MG | DA | 2930 | - | - | - | X |
| 56 | MG | DA | 2936 | - | - | - | X |
| 56 | MG | DA | 2937 | - | - | - | X |
| 56 | MG | DA | 2948 | - | - | - | X |
| 56 | MG | DA | 2949 | - | - | - | X |
| 56 | MG | DA | 2964 | - | - | - | X |
| 56 | MG | DA | 2972 | - | - | - | X |
| 56 | MG | DA | 2975 | - | - | - | X |
| 56 | MG | DA | 2989 | - | - | - | X |
| 56 | MG | DA | 3001 | - | - | - | X |
| 56 | MG | DA | 3003 | - | - | - | X |
| 56 | MG | DA | 3004 | - | - | - | X |
| 56 | MG | DA | 3008 | - | - | - | X |
| 56 | MG | DA | 3009 | - | - | - | X |
| 56 | MG | DA | 3016 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3030 | - | - | - | X |
| 56 | MG | DA | 3033 | - | - | - | X |
| 56 | MG | DA | 3044 | - | - | - | X |
| 56 | MG | DA | 3052 | - | - | - | X |
| 56 | MG | DA | 3054 | - | - | - | X |
| 56 | MG | DA | 3062 | - | - | - | X |
| 56 | MG | DA | 3066 | - | - | - | X |
| 56 | MG | DA | 3070 | - | - | - | X |
| 56 | MG | DA | 3072 | - | - | - | X |
| 56 | MG | DA | 3073 | - | - | - | X |
| 56 | MG | DA | 3086 | - | - | - | X |
| 56 | MG | DA | 3092 | - | - | - | X |
| 56 | MG | DA | 3097 | - | - | - | X |
| 56 | MG | DA | 3107 | - | - | - | X |
| 56 | MG | DA | 3119 | - | - | - | X |
| 56 | MG | DA | 3188 | - | - | - | X |
| 56 | MG | DA | 3243 | - | - | - | X |
| 56 | MG | DA | 3248 | - | - | - | X |
| 56 | MG | DA | 3270 | - | - | - | X |
| 56 | MG | DA | 3287 | - | - | - | X |
| 56 | MG | DA | 3308 | - | - | - | X |
| 56 | MG | DA | 3325 | - | - | - | X |
| 56 | MG | DA | 3326 | - | - | - | X |
| 56 | MG | DA | 3338 | - | - | - | X |
| 56 | MG | DA | 3343 | - | - | - | X |
| 56 | MG | DA | 3348 | - | - | - | X |
| 56 | MG | DA | 3351 | - | - | - | X |
| 56 | MG | DA | 3375 | - | - | - | X |
| 56 | MG | DA | 3381 | - | - | - | X |
| 56 | MG | DA | 3385 | - | - | - | X |
| 56 | MG | DA | 3398 | - | - | - | X |
| 56 | MG | DA | 3403 | - | - | - | X |
| 56 | MG | DA | 3427 | - | - | - | X |
| 56 | MG | DA | 3428 | - | - | - | X |
| 56 | MG | DA | 3484 | - | - | - | X |
| 56 | MG | DA | 3498 | - | - | - | X |
| 56 | MG | DA | 3502 | - | - | - | X |
| 56 | MG | DA | 3510 | - | - | - | X |
| 56 | MG | DA | 3516 | - | - | - | X |
| 56 | MG | DA | 3517 | - | - | - | X |
| 56 | MG | DA | 3519 | - | - | - | X |
| 56 | MG | DA | 3531 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3541 | - | - | - | X |
| 56 | MG | DA | 3544 | - | - | - | X |
| 56 | MG | DA | 3548 | - | - | - | X |
| 56 | MG | DA | 3568 | - | - | - | X |
| 56 | MG | DA | 3577 | - | - | - | X |
| 56 | MG | DA | 3586 | - | - | - | X |
| 56 | MG | DA | 3611 | - | - | - | X |
| 56 | MG | DB | 206 | - | - | - | X |
| 56 | MG | DB | 209 | - | - | - | X |
| 56 | MG | DB | 218 | - | - | - | X |
| 56 | MG | DF | 301 | - | - | - | X |
| 56 | MG | DV | 201 | - | - | - | X |
| 56 | MG | DW | 201 | - | - | - | X |

# 2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 294074 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 (1504-MER).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | AA | 1504 | 32332 | 14391 | 5994 | 10444 | 1503 | 0 | 0 | 0 |
| 1 | CA | 1504 | 32332 | 14391 | 5994 | 10444 | 1503 | 0 | 0 | 0 |

- Molecule 2 is a RNA chain called messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 2 | AV | 10 | 214 | 98 | 44 | 63 | 9 | 0 | 0 | 0 |
| 2 | CV | 10 | 214 | 98 | 44 | 63 | 9 | 0 | 0 | 0 |

- Molecule 3 is a RNA chain called P-site tRNA-fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 3 | AW | 77 | 1640 | 732 | 297 | 535 | 76 | 0 | 0 | 0 |
| 3 | CW | 77 | 1640 | 732 | 297 | 535 | 76 | 0 | 0 | 0 |

- Molecule 4 is a protein called Bacterial peptide chain release factor 2 (RF-2).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | AY | 362 | 2874 | 1794 | 517 | 555 | 8 | 0 | 0 | 0 |
| 4 | CY | 362 | 2874 | 1794 | 517 | 555 | 8 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AY | 253 | PRO | GLN | engineered mutation | UNP Q72GJ6 |
| CY | 253 | PRO | GLN | engineered mutation | UNP Q72GJ6 |

- Molecule 5 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | AB | 234 | 1901 | 1213 | 341 | 342 | 5 | 0 | 0 | 0 |
| 5 | CB | 234 | 1901 | 1213 | 341 | 342 | 5 | 0 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | AC | 206 | 1613 | 1016 | 314 | 282 | 1 | 0 | 0 | 0 |
| 6 | CC | 206 | 1613 | 1016 | 314 | 282 | 1 | 0 | 0 | 0 |

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 8 | AE | 151 | 1156 | 729 | 218 | 205 | 4 | 0 | 0 | 0 |
| 8 | CE | 151 | 1156 | 729 | 218 | 205 | 4 | 0 | 0 | 0 |

- Molecule 9 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 9 | AF | 101 | 843 | 531 | 155 | 154 | 3 | 0 | 0 | 0 |
| 9 | CF | 101 | 843 | 531 | 155 | 154 | 3 | 0 | 0 | 0 |

- Molecule 10 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | AG | 155 | 1257 | 781 | 252 | 218 | 6 | 0 | 0 | 0 |
| 10 | CG | 155 | 1257 | 781 | 252 | 218 | 6 | 0 | 0 | 0 |

- Molecule 11 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 11 | AH | 138 | 1116 | 705 | 215 | 193 | 3 | 0 | 0 | 0 |
| 11 | CH | 138 | 1116 | 705 | 215 | 193 | 3 | 0 | 0 | 0 |

- Molecule 12 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 12 | AI | 127 | 1011 | 639 | 198 | 174 | 0 | 0 | 0 |
| 12 | CI | 127 | 1011 | 639 | 198 | 174 | 0 | 0 | 0 |

- Molecule 13 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 13 | AJ | 98 | 795 | 499 | 156 | 139 | 1 | 0 | 0 | 0 |
| 13 | CJ | 98 | 795 | 499 | 156 | 139 | 1 | 0 | 0 | 0 |

- Molecule 14 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 14 | AK | 114 | 843 | 522 | 159 | 159 | 3 | 0 | 0 | 0 |
| 14 | CK | 114 | 843 | 522 | 159 | 159 | 3 | 0 | 0 | 0 |

- Molecule 15 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 15 | AL | 122 | 957 | 603 | 193 | 160 | 1 | 0 | 0 | 0 |
| 15 | CL | 122 | 957 | 603 | 193 | 160 | 1 | 0 | 0 | 0 |

- Molecule 16 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 16 | AM | 117 | 934 | 577 | 192 | 163 | 2 | 0 | 0 | 0 |
| 16 | CM | 117 | 934 | 577 | 192 | 163 | 2 | 0 | 0 | 0 |

- Molecule 17 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 17 | AN | 60 | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |
| 17 | CN | 60 | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |

- Molecule 18 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 18 | AO | 88 | 734 | 459 | 147 | 126 | 2 | 0 | 0 | 0 |
| 18 | CO | 88 | 734 | 459 | 147 | 126 | 2 | 0 | 0 | 0 |

- Molecule 19 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 19 | AP | 83 | 701 | 443 | 139 | 118 | 1 | 0 | 0 | 0 |
| 19 | CP | 83 | 701 | 443 | 139 | 118 | 1 | 0 | 0 | 0 |

- Molecule 20 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 20 | AQ | 99 | 824 | 528 | 152 | 142 | 2 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 20 | CQ | 99 | 824 | 528 | 152 | 142 | 2 | 0 | 0 | 0 |

- Molecule 21 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 21 | AR | 70 | 574 | 367 | 112 | 95 | 0 | 0 | 0 |
| 21 | CR | 70 | 574 | 367 | 112 | 95 | 0 | 0 | 0 |

- Molecule 22 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 22 | AS | 78 | 630 | 403 | 114 | 111 | 2 | 0 | 0 | 0 |
| 22 | CS | 78 | 630 | 403 | 114 | 111 | 2 | 0 | 0 | 0 |

- Molecule 23 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 23 | AT | 99 | 762 | 469 | 162 | 129 | 2 | 0 | 0 | 0 |
| 23 | CT | 99 | 762 | 469 | 162 | 129 | 2 | 0 | 0 | 0 |

- Molecule 24 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 24 | AU | 24 | 209 | 128 | 50 | 31 | 0 | 0 | 0 |
| 24 | CU | 24 | 209 | 128 | 50 | 31 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 25 | BA | 2789 | 60059 | 26734 | 11225 | 19312 | 2788 | 0 | 0 | 0 |
| 25 | DA | 2789 | 60059 | 26734 | 11225 | 19312 | 2788 | 0 | 0 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BA | 276 | C | A | conflict | GB AE017221.1 |
| BA | 277 | A | C | conflict | GB AE017221.1 |
| BA | 1141A | U | C | conflict | GB AE017221.1 |
| BA | 2825 | U | G | conflict | GB AE017221.1 |
| DA | 276 | C | A | conflict | GB AE017221.1 |
| DA | 277 | A | C | conflict | GB AE017221.1 |
| DA | 1141A | U | C | conflict | GB AE017221.1 |
| DA | 2825 | U | G | conflict | GB AE017221.1 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 26 | BB | 119 | 2551 | 1136 | 471 | 826 | 118 | 0 | 0 | 0 |
| 26 | DB | 119 | 2551 | 1136 | 471 | 826 | 118 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 27 | BD | 271 | 2105 | 1329 | 416 | 357 | 3 | 0 | 0 | 0 |
| 27 | DD | 271 | 2105 | 1329 | 416 | 357 | 3 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 28 | BE | 204 | 1564 | 988 | 299 | 271 | 6 | 0 | 0 | 0 |
| 28 | DE | 204 | 1564 | 988 | 299 | 271 | 6 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 29 | BF | 202 | 1587 | 1011 | 297 | 276 | 3 | 0 | 0 | 0 |
| 29 | DF | 202 | 1587 | 1011 | 297 | 276 | 3 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 30 | BG | 181 | 1475 | 943 | 268 | 260 | 4 | 0 | 0 | 0 |
| 30 | DG | 181 | 1475 | 943 | 268 | 260 | 4 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 31 | BH | 159 | 1223 | 773 | 228 | 221 | 1 | 0 | 0 | 0 |
| 31 | DH | 159 | 1223 | 773 | 228 | 221 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 32 | BI | 145 | 1133 | 724 | 200 | 208 | 1 | 0 | 0 | 0 |
| 32 | DI | 145 | 1133 | 724 | 200 | 208 | 1 | 0 | 0 | 0 |

- Molecule 33 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 33 | BK | 147 | 1088 | 692 | 191 | 199 | 6 | 0 | 0 | 0 |
| 33 | DK | 147 | 1088 | 692 | 191 | 199 | 6 | 0 | 0 | 0 |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 34 | BN | 137 | 1097 | 707 | 205 | 182 | 3 | 0 | 0 | 0 |
| 34 | DN | 137 | 1097 | 707 | 205 | 182 | 3 | 0 | 0 | 0 |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 35 | BO | 122 | 932 | 587 | 171 | 170 | 4 | 0 | 0 | 0 |
| 35 | DO | 122 | 932 | 587 | 171 | 170 | 4 | 0 | 0 | 0 |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 36 | BP | 146 | 1114 | 692 | 227 | 193 | 2 | 0 | 0 | 0 |
| 36 | DP | 146 | 1114 | 692 | 227 | 193 | 2 | 0 | 0 | 0 |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 37 | BQ | 134 | 1065 | 680 | 201 | 179 | 5 | 0 | 0 | 0 |
| 37 | DQ | 134 | 1065 | 680 | 201 | 179 | 5 | 0 | 0 | 0 |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 38 | BR | 117 | 960 | 599 | 202 | 159 | 0 | 0 | 0 |
| 38 | DR | 117 | 960 | 599 | 202 | 159 | 0 | 0 | 0 |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 39 | BS | 98 | 771 | 486 | 154 | 131 | 0 | 0 | 0 |
| 39 | DS | 98 | 771 | 486 | 154 | 131 | 0 | 0 | 0 |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 40 | BT | 137 | 1144 | 713 | 234 | 196 | 1 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 40 | DT | 137 | 1144 | 713 | 234 | 196 | 1 | 0 | 0 | 0 |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 41 | BU | 117 | 964 | 610 | 202 | 151 | 1 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 41 | DU | 117 | 964 | 610 | 202 | 151 | 1 | 0 | 0 | 0 |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 42 | BV | 101 | 779 | 501 | 142 | 135 | 1 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 42 | DV | 101 | 779 | 501 | 142 | 135 | 1 | 0 | 0 | 0 |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 43 | BW | 112 | 891 | 560 | 175 | 154 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 43 | DW | 112 | 891 | 560 | 175 | 154 | 2 | 0 | 0 | 0 |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 44 | BX | 92 | 726 | 471 | 131 | 124 | 0 | 0 | 0 |
| | | | Total | C | N | O | | | |
| 44 | DX | 92 | 726 | 471 | 131 | 124 | 0 | 0 | 0 |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 45 | BY | 100 | 776 | 500 | 148 | 124 | 4 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 45 | DY | 100 | 776 | 500 | 148 | 124 | 4 | 0 | 0 | 0 |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 46 | BZ | 187 | 1483 | 945 | 264 | 272 | 2 | 0 | 0 | 0 |
| 46 | DZ | 187 | 1483 | 945 | 264 | 272 | 2 | 0 | 0 | 0 |

- Molecule 47 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 47 | B0 | 76 | 605 | 376 | 126 | 102 | 1 | 0 | 0 | 0 |
| 47 | D0 | 76 | 605 | 376 | 126 | 102 | 1 | 0 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 48 | B1 | 88 | 695 | 435 | 141 | 119 | 0 | 0 | 0 |
| 48 | D1 | 88 | 695 | 435 | 141 | 119 | 0 | 0 | 0 |

- Molecule 49 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 49 | B2 | 62 | 521 | 325 | 102 | 92 | 2 | 0 | 0 | 0 |
| 49 | D2 | 62 | 521 | 325 | 102 | 92 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 50 | B3 | 59 | 468 | 298 | 90 | 79 | 1 | 0 | 0 | 0 |
| 50 | D3 | 59 | 468 | 298 | 90 | 79 | 1 | 0 | 0 | 0 |

- Molecule 51 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 51 | B4 | 30 | 226 | 142 | 36 | 44 | 4 | 0 | 0 | 0 |
| 51 | D4 | 30 | 226 | 142 | 36 | 44 | 4 | 0 | 0 | 0 |

- Molecule 52 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 52 | B5 | 52 | 405 | 255 | 79 | 66 | 5 | 0 | 0 | 0 |
| 52 | D5 | 52 | 405 | 255 | 79 | 66 | 5 | 0 | 0 | 0 |

- Molecule 53 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 53 | B6 | 44 | 381 | 235 | 77 | 65 | 4 | 0 | 0 | 0 |
| 53 | D6 | 44 | 381 | 235 | 77 | 65 | 4 | 0 | 0 | 0 |

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 54 | B7 | 48 | 419 | 257 | 104 | 56 | 2 | 0 | 0 | 0 |
| 54 | D7 | 48 | 419 | 257 | 104 | 56 | 2 | 0 | 0 | 0 |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 55 | B8 | 63 | 508 | 326 | 101 | 79 | 2 | 0 | 0 | 0 |
| 55 | D8 | 63 | 508 | 326 | 101 | 79 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | AA | 393 | 393 | 393 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | AV | 1 | 1 | 1 | 0 | 0 |
| 56 | AW | 18 | 18 | 18 | 0 | 0 |
| 56 | AY | 3 | 3 | 3 | 0 | 0 |
| 56 | AC | 1 | 1 | 1 | 0 | 0 |
| 56 | AG | 1 | 1 | 1 | 0 | 0 |
| 56 | AO | 1 | 1 | 1 | 0 | 0 |
| 56 | AQ | 1 | 1 | 1 | 0 | 0 |
| 56 | AT | 3 | 3 | 3 | 0 | 0 |
| 56 | BA | 824 | 824 | 824 | 0 | 0 |
| 56 | BB | 23 | 23 | 23 | 0 | 0 |
| 56 | BD | 1 | 1 | 1 | 0 | 0 |
| 56 | BE | 1 | 1 | 1 | 0 | 0 |
| 56 | BF | 1 | 1 | 1 | 0 | 0 |
| 56 | BP | 1 | 1 | 1 | 0 | 0 |
| 56 | BT | 1 | 1 | 1 | 0 | 0 |
| 56 | BX | 2 | 2 | 2 | 0 | 0 |
| 56 | BY | 1 | 1 | 1 | 0 | 0 |
| 56 | B0 | 2 | 2 | 2 | 0 | 0 |
| 56 | B1 | 1 | 1 | 1 | 0 | 0 |
| 56 | B3 | 1 | 1 | 1 | 0 | 0 |
| 56 | B5 | 1 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 56 | B8 | 2 | 2 | 2 | 0 | 0 |
| 56 | CA | 326 | 326 | 326 | 0 | 0 |
| 56 | CV | 2 | 2 | 2 | 0 | 0 |
| 56 | CW | 16 | 16 | 16 | 0 | 0 |
| 56 | CY | 2 | 2 | 2 | 0 | 0 |
| 56 | CD | 1 | 1 | 1 | 0 | 0 |
| 56 | CM | 1 | 1 | 1 | 0 | 0 |
| 56 | CR | 1 | 1 | 1 | 0 | 0 |
| 56 | DA | 732 | 732 | 732 | 0 | 0 |
| 56 | DB | 20 | 20 | 20 | 0 | 0 |
| 56 | DD | 1 | 1 | 1 | 0 | 0 |
| 56 | DE | 1 | 1 | 1 | 0 | 0 |
| 56 | DF | 2 | 2 | 2 | 0 | 0 |
| 56 | DH | 1 | 1 | 1 | 0 | 0 |
| 56 | DI | 2 | 2 | 2 | 0 | 0 |
| 56 | DN | 1 | 1 | 1 | 0 | 0 |
| 56 | DP | 2 | 2 | 2 | 0 | 0 |
| 56 | DQ | 4 | 4 | 4 | 0 | 0 |
| 56 | DV | 1 | 1 | 1 | 0 | 0 |
| 56 | DW | 2 | 2 | 2 | 0 | 0 |
| 56 | DX | 1 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | D0 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | D1 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | D5 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | D7 | 2 | Total Mg<br>2 2 | 0 | 0 |

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

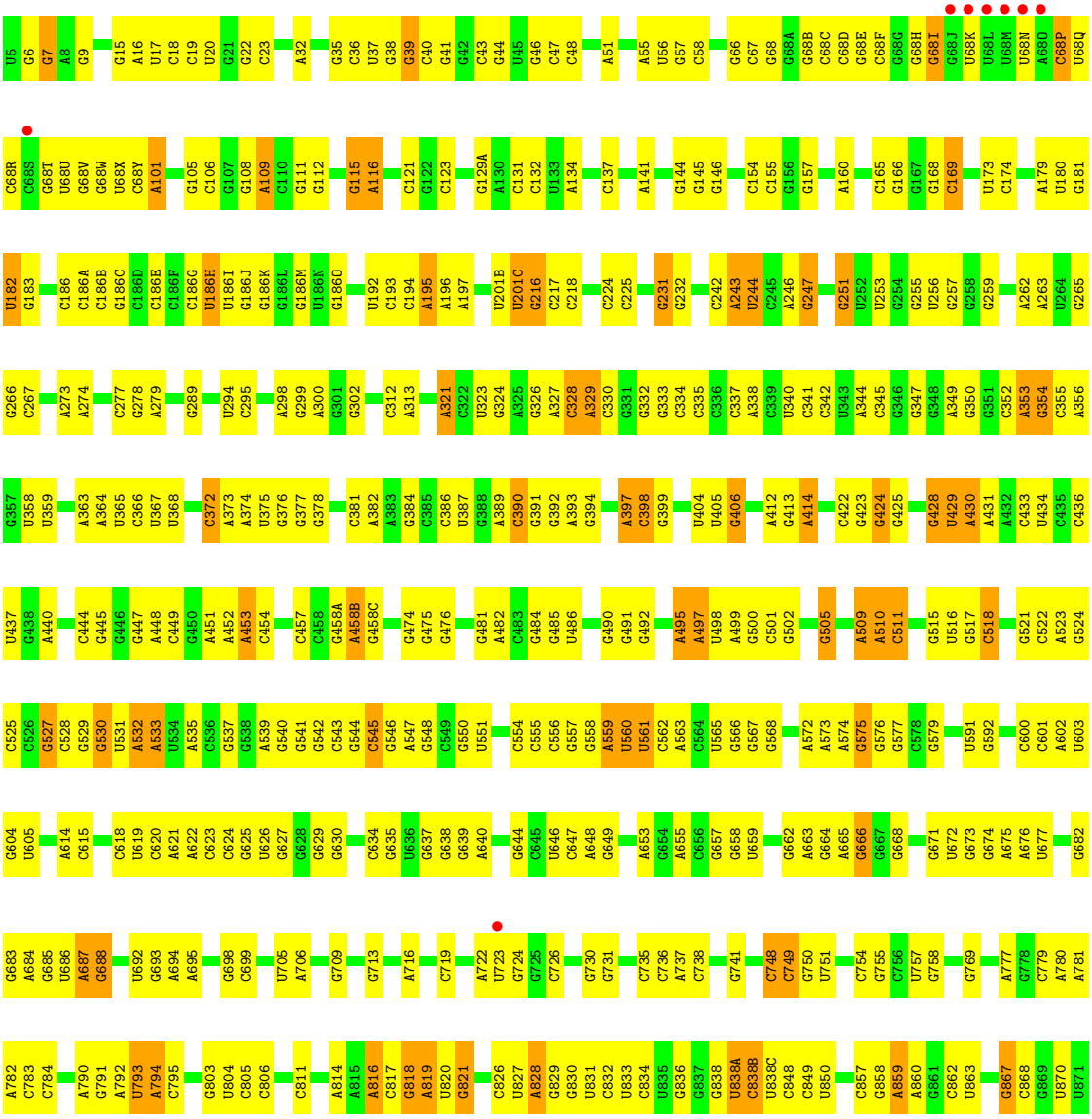
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | AD | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | AN | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | CD | 1 | Total Zn<br>1 1 | 0 | 0 |
| 57 | CN | 1 | Total Zn<br>1 1 | 0 | 0 |

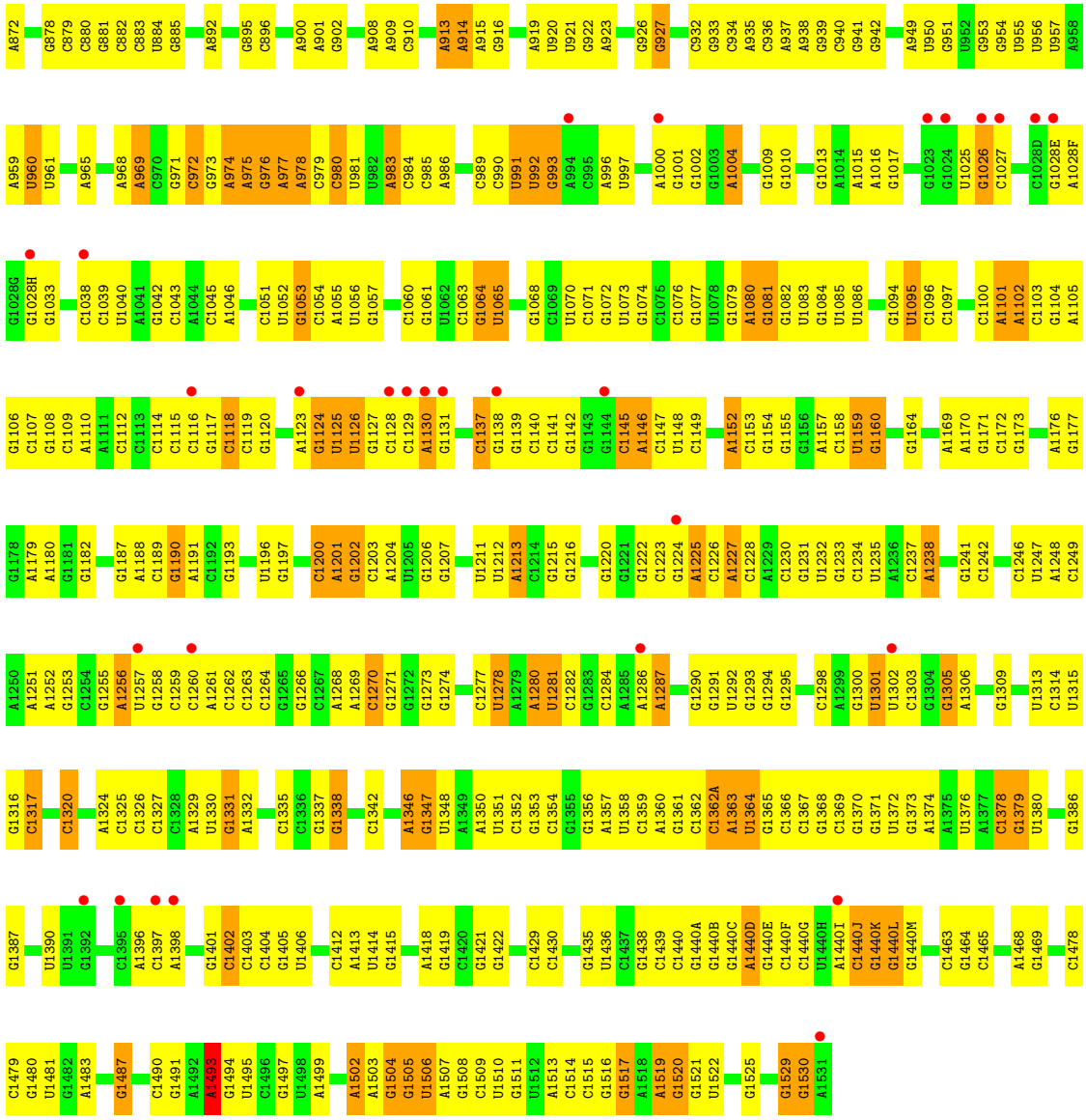
# 3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA (1504-MER)

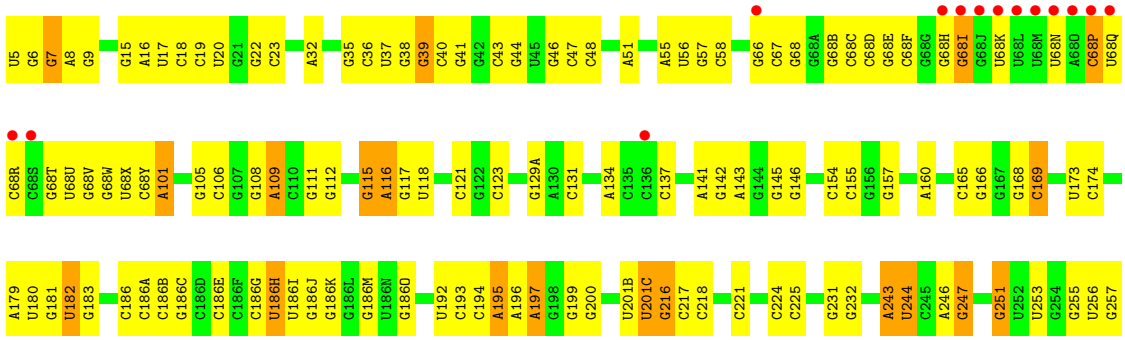
Chain AA: 2% 44% 46% 10%

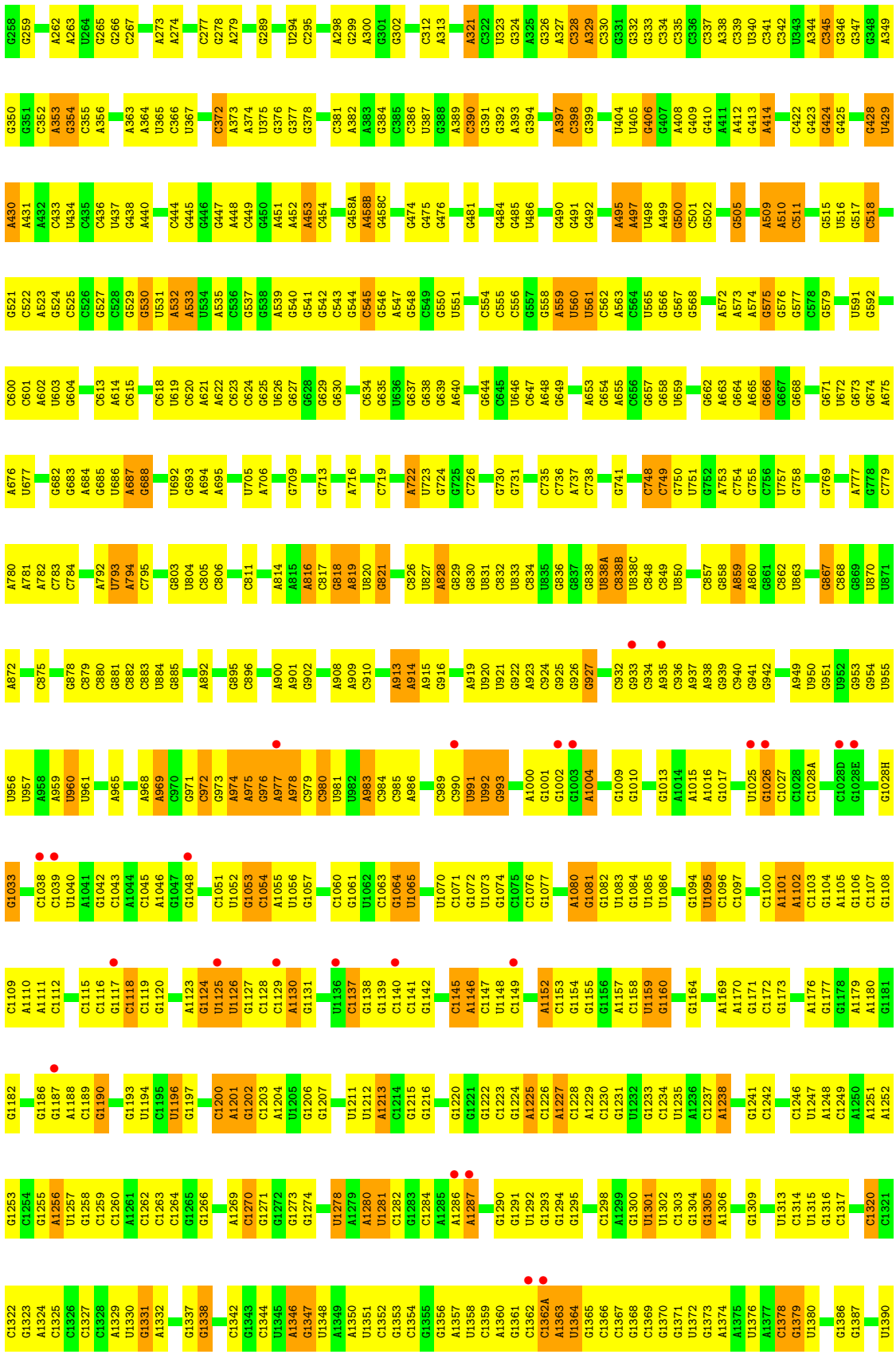


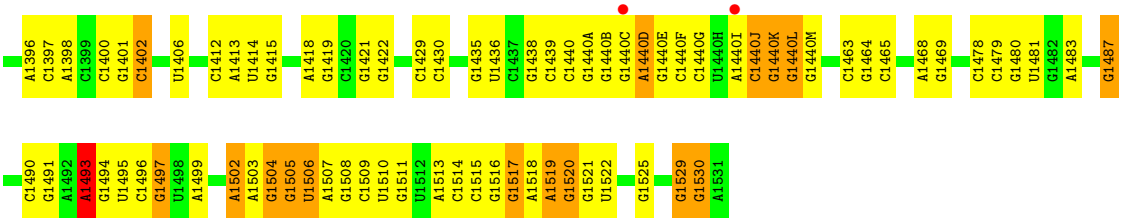


• Molecule 1: 16S rRNA (1504-MER)

Chain CA:




G258 G259 A262 A263 U264 G265 G266 C267 A273 A274 C277 G278 A279 G289 U294 C295 A298 G299 A300 G301 G302 C312 A313 A321 C322 U323 G324 A325 G326 A327 C328 A329 C330 G331 G332 G333 C334 C335 C336 C337 A338 C339 U340 C341 C342 U343 A344 C345 G346 G347 G348 A349
G350 G351 C352 A353 G354 C355 A356 A363 A364 U365 C366 U367 C372 A373 A374 U375 G376 G377 G378 C381 A382 A383 G384 C385 C386 U387 G388 A389 C390 G391 G392 A393 G394 A397 C398 G399 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 C422 G423 G424 G425 G428 U429
A430 A431 A432 C433 U434 C435 C436 U437 G438 A440 C444 G445 G446 G447 A448 C449 C450 A451 A452 A453 C454 C458A A458B G458C G474 G475 G476 G481 G484 G485 U486 G490 G491 G492 A495 A497 U498 A499 G500 C501 G502 G505 A509 A510 C511 G515 U516 G517 C518
G521 C522 A523 G524 C525 C526 G527 G528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 C549 G550 U551 C554 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568 A572 A573 A574 G575 G576 G577 G578 G579 U591 G592
C600 C601 A602 U603 G604 C613 A614 G615 G618 U619 G620 A621 A622 G623 C624 G625 U626 G627 G628 G629 G630 C634 G635 U636 G637 G638 G639 A640 G644 C645 U646 C647 A648 G649 A653 G654 A655 C656 G657 G658 U659 G662 A663 G664 A665 G666 G667 G668 G671 U672 G673 G674 A675
A676 U677 G682 G683 A684 G685 U686 A687 G688 U692 G693 A694 A695 U705 A706 G709 G713 A716 C719 A722 U723 G724 G725 C726 G730 G731 C735 C736 A737 C738 G741 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 G769 A777 G778 C779
A780 A781 A782 C783 C784 A792 U793 A794 C795 G803 U804 C805 C806 C811 A814 A815 A816 C817 G818 A819 U820 G821 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U838A C838B U838C C848 C849 U850 C857 G858 A859 A860 G861 C862 U863 G867 C868 G869 U870 U871
A872 C875 G878 C879 C880 G881 C882 C883 U884 G885 A892 G895 C896 A900 A901 G902 A908 A909 C910 A913 A914 A915 G916 A919 U920 U921 G922 A923 C924 G925 G926 G927 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 A949 U950 G951 U952 G953 G954 U955
U956 U957 A958 A959 U960 U961 A965 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 C989 C990 U991 U992 G993 A1000 G1001 G1002 G1003 A1004 G1009 G1010 G1013 A1014 A1015 A1016 G1017 U1025 G1026 C1027 C1028 C1028A C1028D C1028E G1028H
G1033 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 C1051 U1052 G1053 C1054 A1055 U1056 G1057 C1060 G1061 U1062 C1063 G1064 U1065 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1094 U1095 C1096 C1097 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108
C1109 A1110 A1111 C1112 C1115 C1116 G1117 C1118 C1119 G1120 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 U1136 C1137 G1138 G1139 C1140 C1141 G1142 C1145 A1146 C1147 U1148 C1149 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 G1164 A1169 A1170 G1171 C1172 G1173 A1176 G1177 G1178 A1179 A1180 G1181
G1182 G1186 G1187 A1188 C1189 G1190 G1193 U1194 C1195 U1196 G1197 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 U1211 U1212 A1213 C1214 G1215 G1216 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 G1241 C1242 C1246 U1247 A1248 C1249 A1250 A1251 A1252
G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 G1265 G1266 A1269 C1270 G1271 G1272 G1273 G1274 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 G1290 G1291 U1292 G1293 G1294 G1295 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 G1309 U1313 C1314 U1315 G1316 C1317 C1320 C1321
C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 U1330 G1331 A1332 G1337 G1338 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 C1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1362A A1363 U1364 G1365 C1366 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 U1380 G1386 G1387 U1390

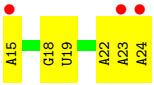



• Molecule 2: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')

Chain AV:

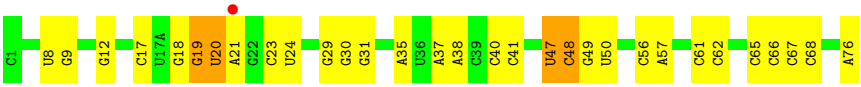
• Molecule 2: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')

Chain CV:




• Molecule 3: P-site tRNA-fMet

Chain AW:

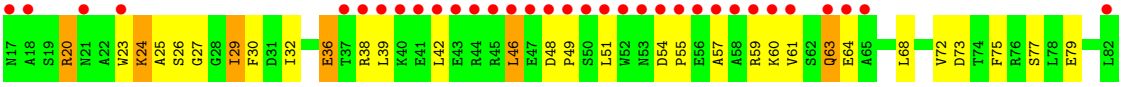


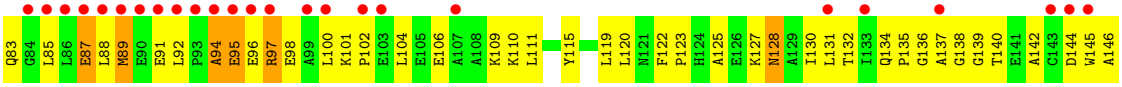

• Molecule 3: P-site tRNA-fMet

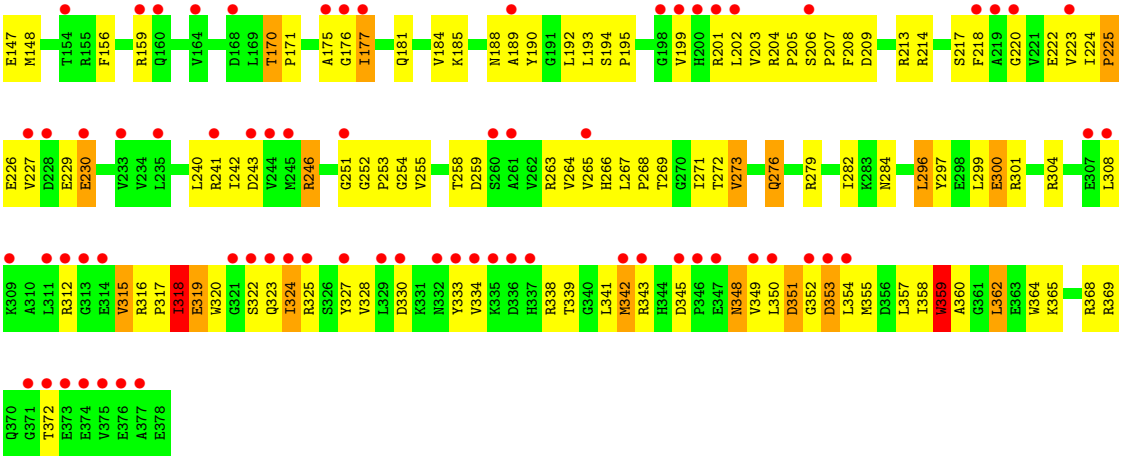
Chain CW:

• Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

Chain AY:

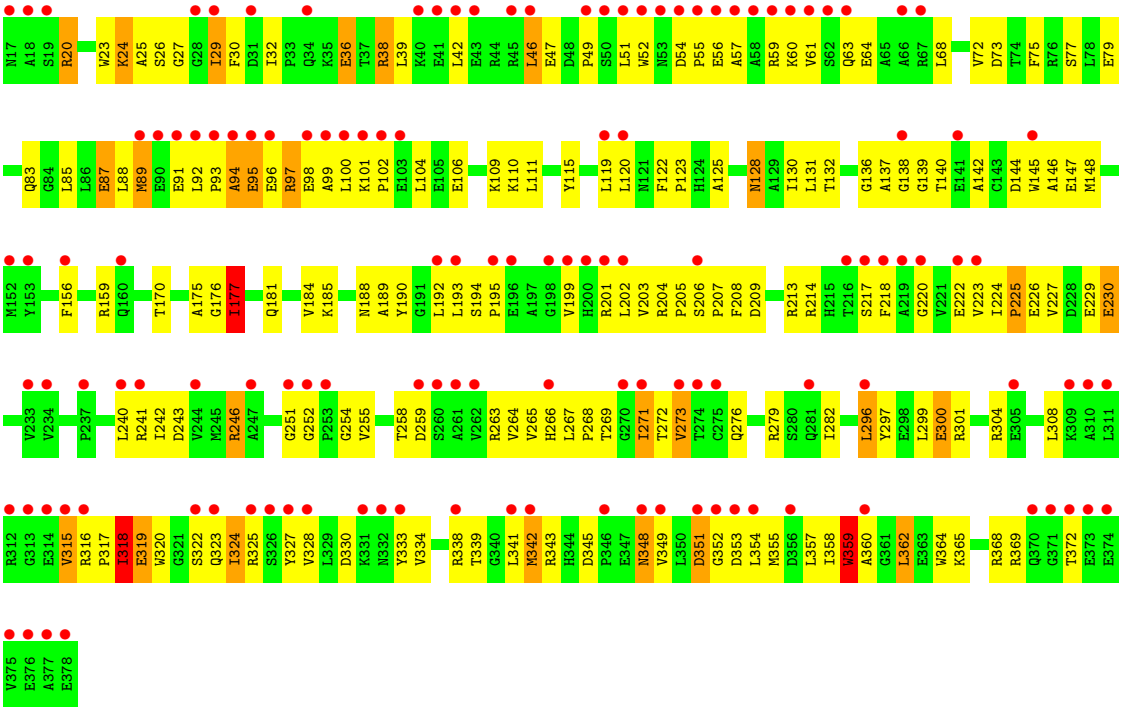




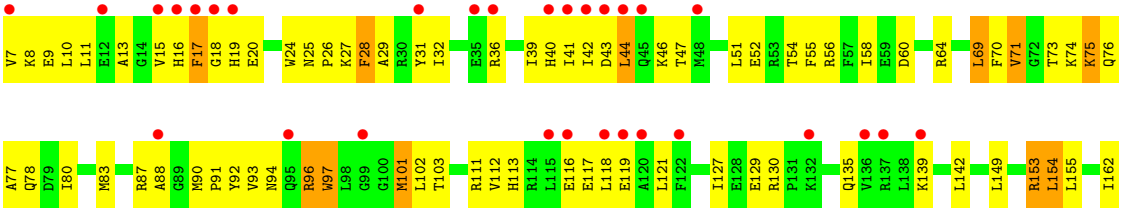

- Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

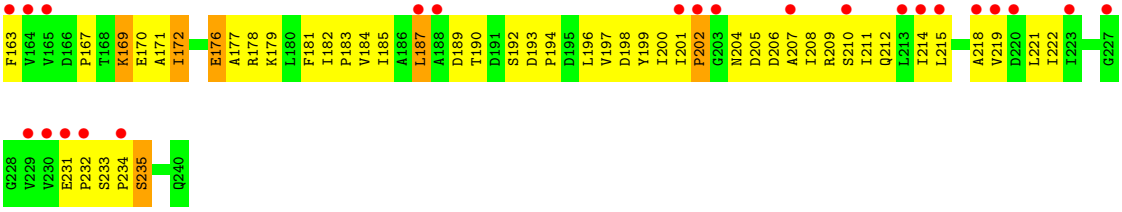
Chain CY:




- Molecule 5: 30S ribosomal protein S2

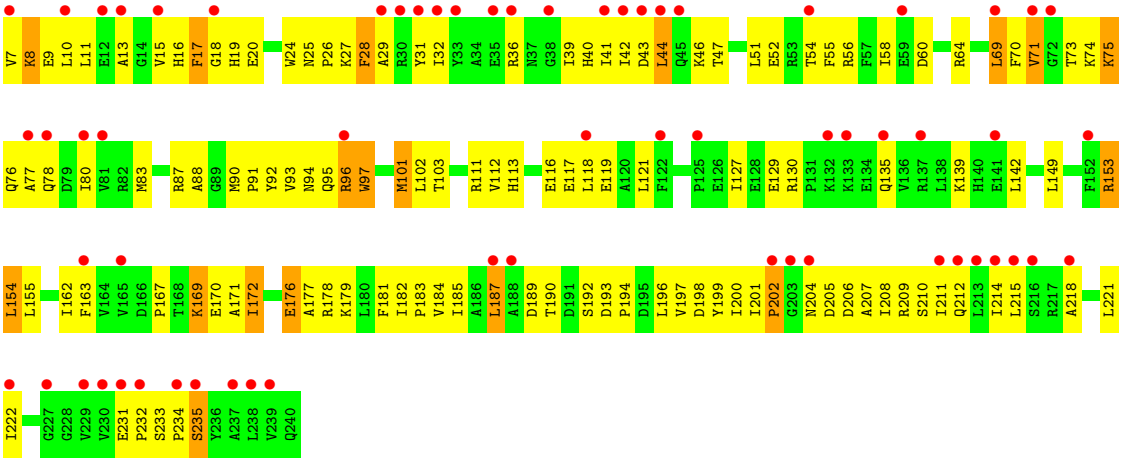
Chain AB:





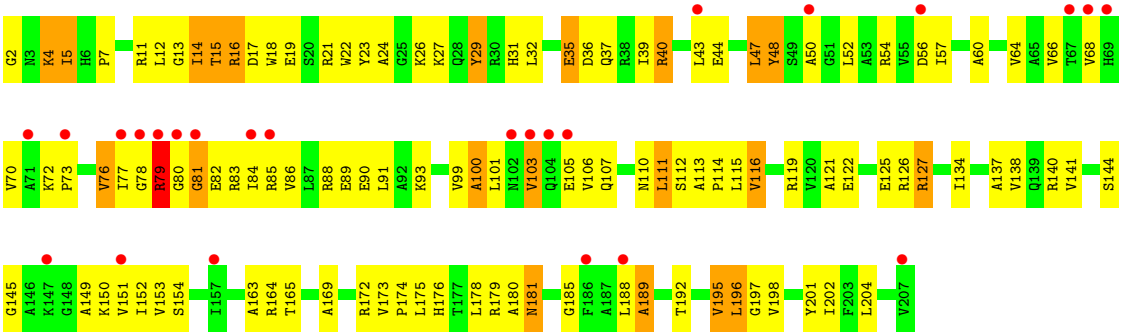

- Molecule 5: 30S ribosomal protein S2

Chain CB:



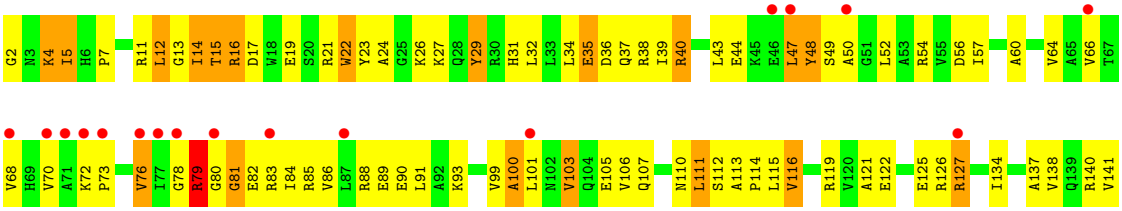

- Molecule 6: 30S ribosomal protein S3

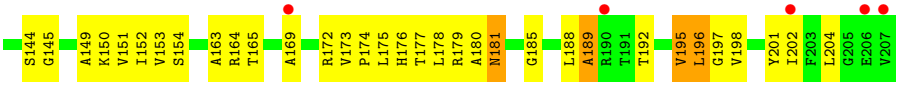
Chain AC:




- Molecule 6: 30S ribosomal protein S3

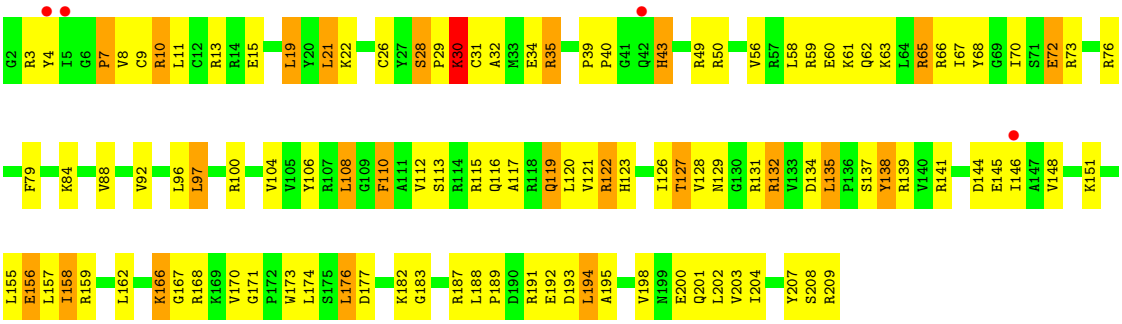
Chain CC:





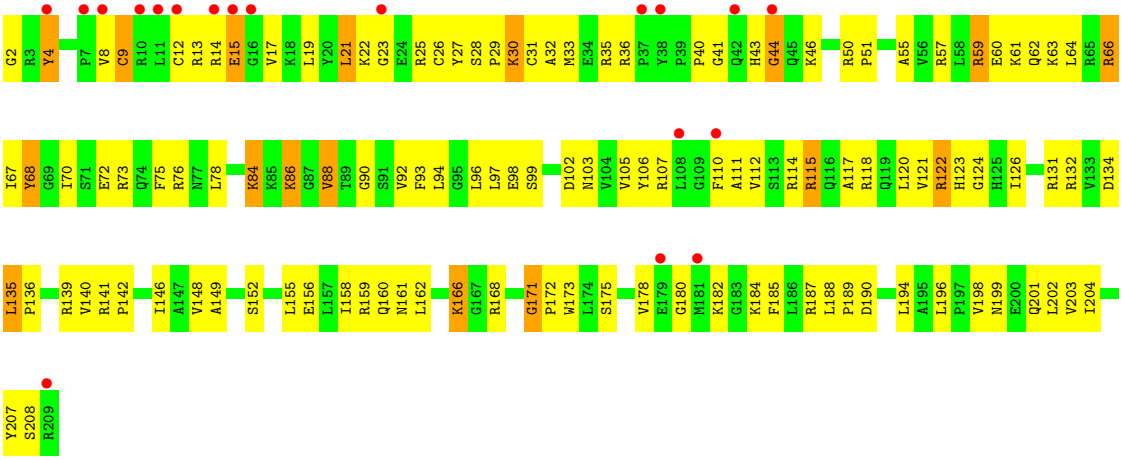

• Molecule 7: 30S ribosomal protein S4

Chain AD:



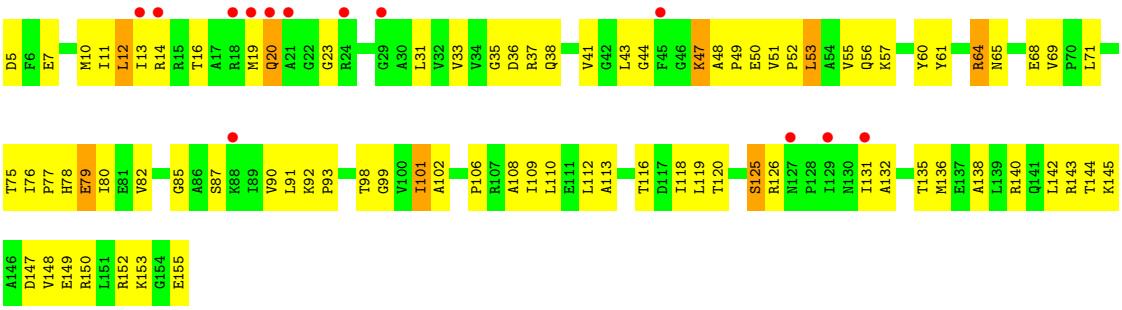

• Molecule 7: 30S ribosomal protein S4

Chain CD:



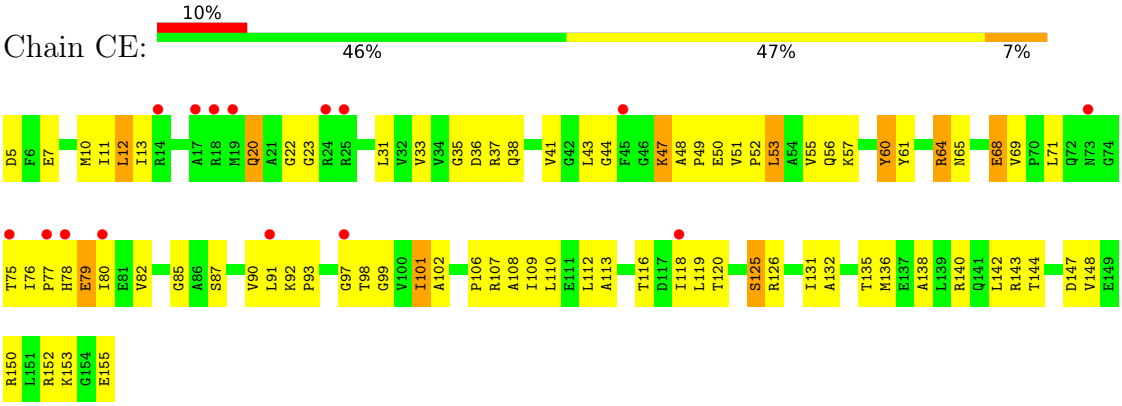

• Molecule 8: 30S ribosomal protein S5

Chain AE:



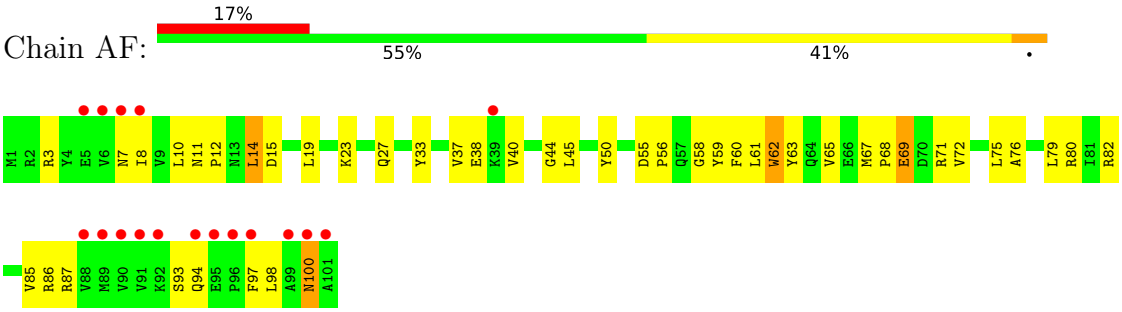

• Molecule 8: 30S ribosomal protein S5

Chain CE:



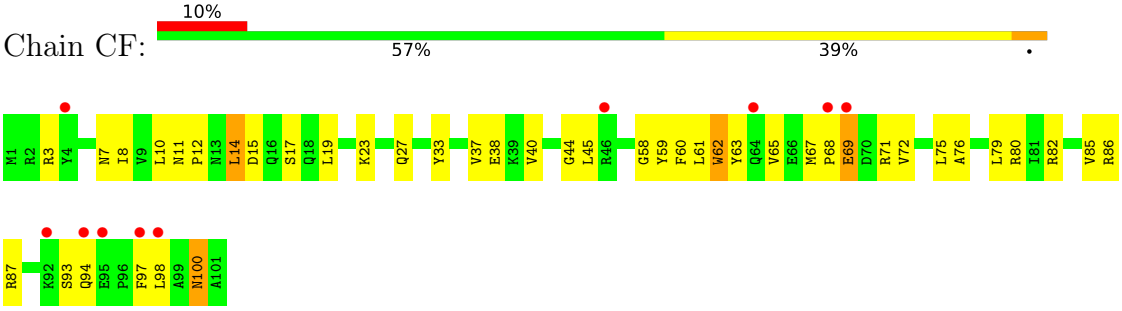

- Molecule 9: 30S ribosomal protein S6

Chain AF:



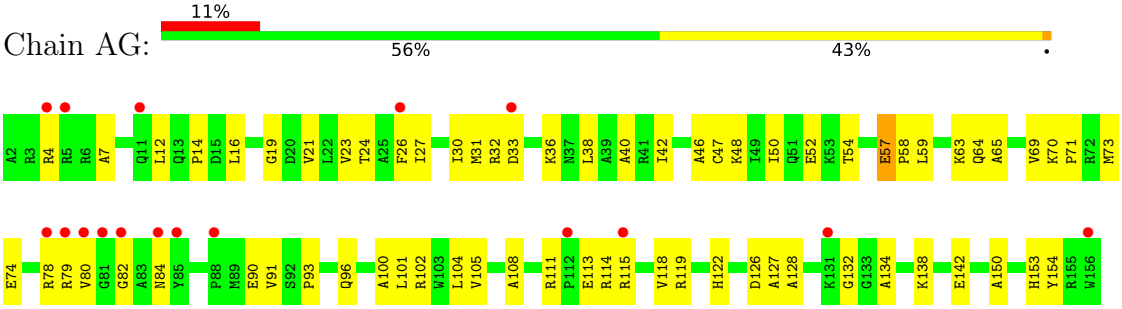

- Molecule 9: 30S ribosomal protein S6

Chain CF:



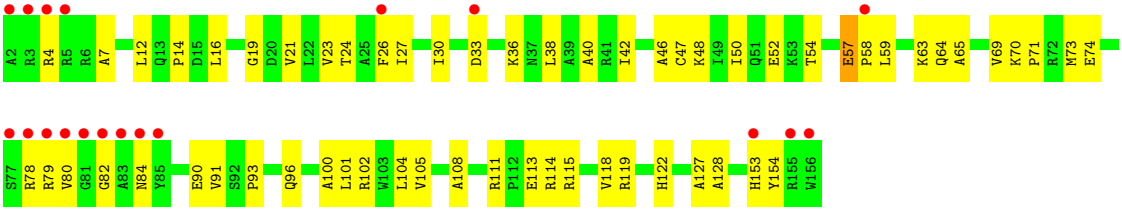

- Molecule 10: 30S ribosomal protein S7

Chain AG:



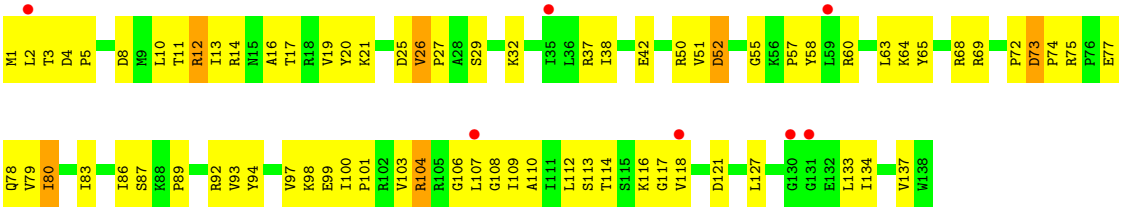

- Molecule 10: 30S ribosomal protein S7

Chain CG:



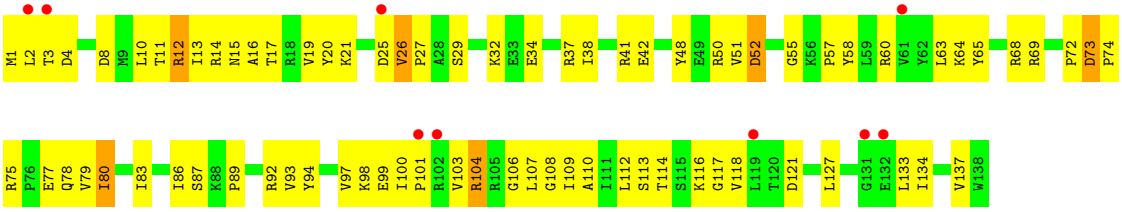

- Molecule 11: 30S ribosomal protein S8

Chain AH:



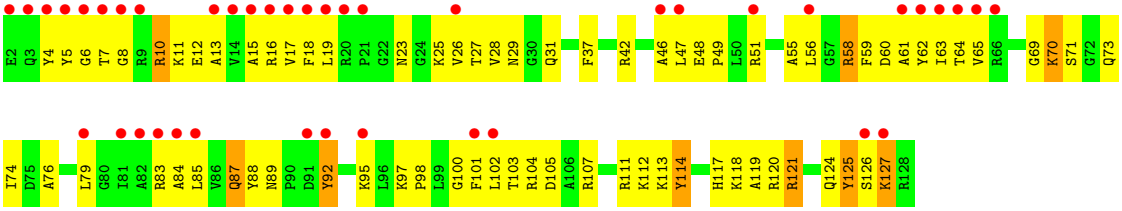

- Molecule 11: 30S ribosomal protein S8

Chain CH:



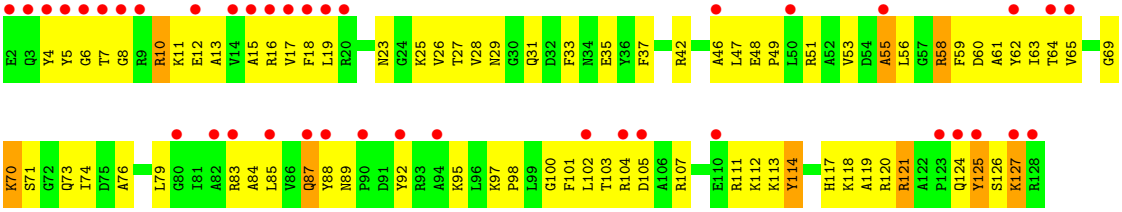

- Molecule 12: 30S ribosomal protein S9

Chain AI:



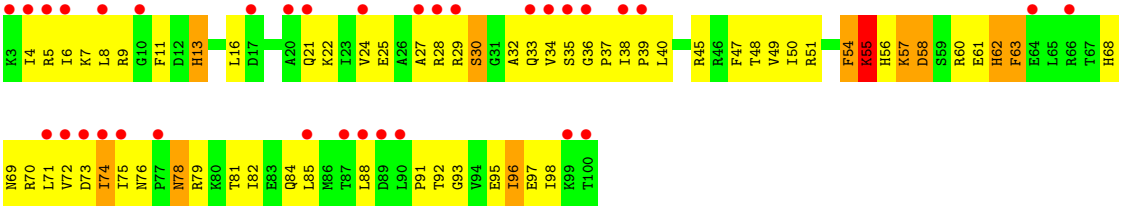

- Molecule 12: 30S ribosomal protein S9

Chain CI:



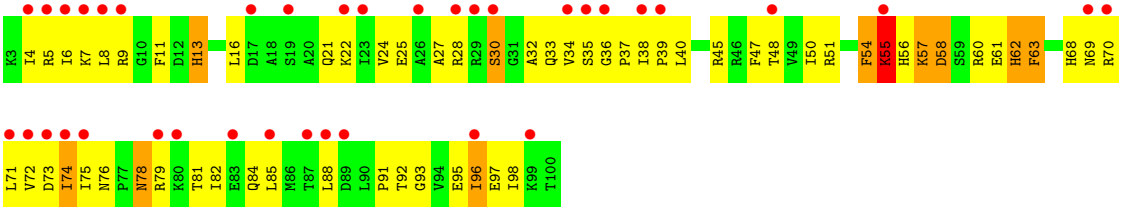
• Molecule 13: 30S ribosomal protein S10

Chain AJ:



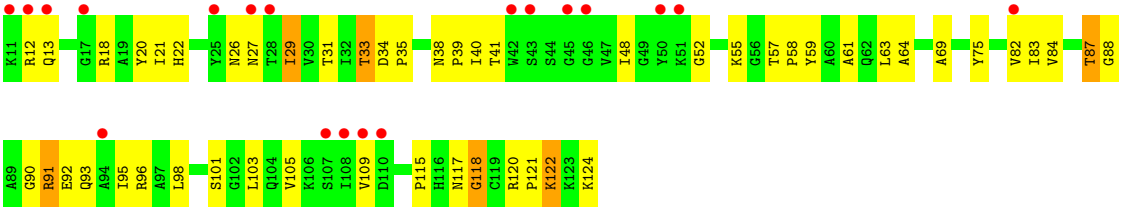

• Molecule 13: 30S ribosomal protein S10

Chain CJ:



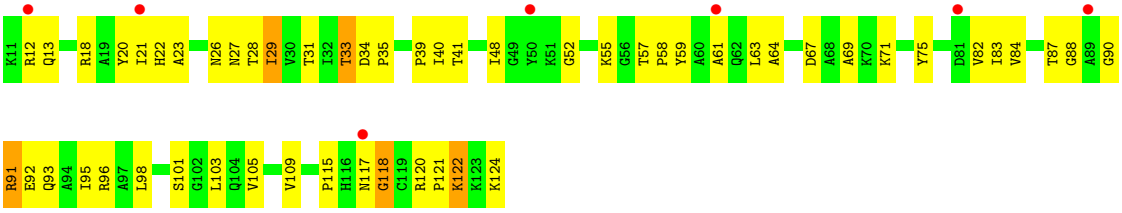

• Molecule 14: 30S ribosomal protein S11

Chain AK:



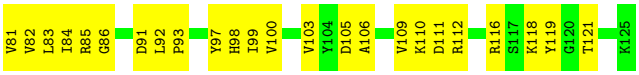

• Molecule 14: 30S ribosomal protein S11

Chain CK:



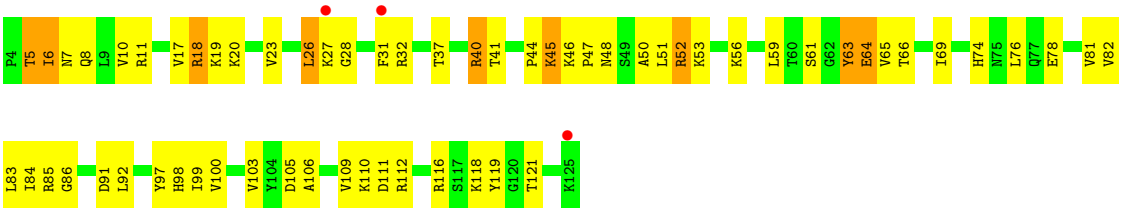

• Molecule 15: 30S ribosomal protein S12

Chain AL:



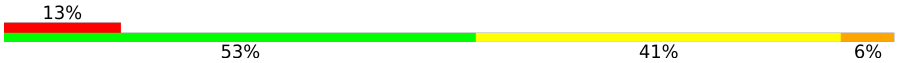

• Molecule 15: 30S ribosomal protein S12

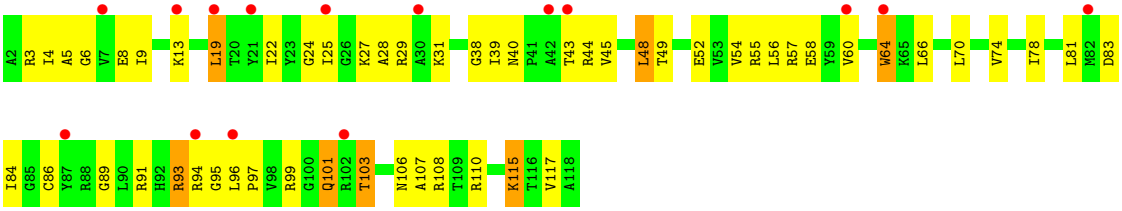
Chain CL:




• Molecule 16: 30S ribosomal protein S13

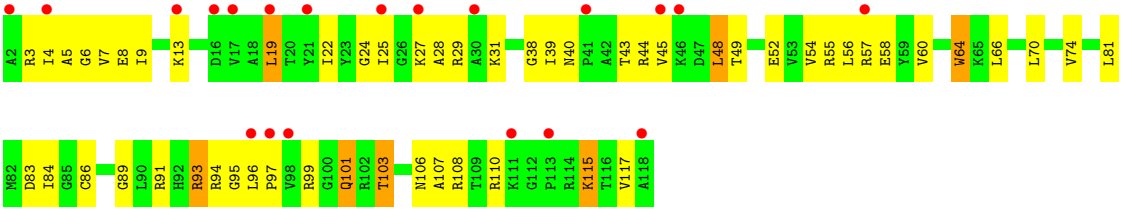
Chain AM:



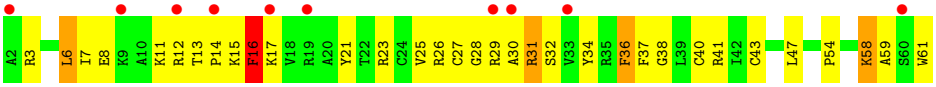

• Molecule 16: 30S ribosomal protein S13

Chain CM:




• Molecule 17: 30S ribosomal protein S14

Chain AN:




• Molecule 17: 30S ribosomal protein S14

Chain CN:

• Molecule 18: 30S ribosomal protein S15

Chain AO: 2% 56% 34% 10%

P2 I3 T4 K5 E6 E7 K8 I12 Q13 E14 F15 A16 R17 D21 T22 G23 S24 T25 E26 L31 R35 L39 S40 E41 H42 L43 K44 V45 H46 K47 R54 G55 L56 L57 M58 M59 V60 G61 R64 R65 R68 Y69 L70 Q71 E76 R77 Y78 I82 E83 K84 L85 G86 I87 R88 G89

• Molecule 18: 30S ribosomal protein S15

Chain CO: % 53% 35% 11%

P2 I3 T4 K5 E6 E7 K8 Q9 K10 V11 I12 Q13 E14 F15 A16 R17 D21 T22 G23 E26 L31 R35 L39 S40 E41 H42 L43 K44 V45 H46 K47 R54 G55 L56 L57 M58 M59 V60 G61 R64 R65 R68 Y69 L70 Q71 E76 R77 Y78 I82 E83 K84 L85 G86 I87 R88 G89

• Molecule 19: 30S ribosomal protein S16

Chain AP: 5% 41% 51% 8%

M1 I4 R5 L6 A7 R8 F9 G10 S11 K12 H13 N14 P15 H16 Y17 R18 I19 V20 V21 T22 R25 R26 K27 R28 D29 Y32 I33 E34 K35 I36 G37 Y38 K43 T44 T45 P46 D47 W48 L49 K50 V51 D52 V53 E54 R55 A56 R57 Y58 W59 L60 S61 V62 G63 A64 T67 D68 T69 V79 F80 R81 Q82 E83

• Molecule 19: 30S ribosomal protein S16

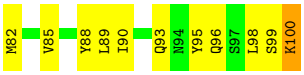
Chain CP: 31% 42% 51% 7%

M1 I4 R5 L6 A7 R8 F9 G10 S11 K12 H13 N14 P15 H16 Y17 R18 I19 V20 V21 T22 D23 A24 R25 R26 K27 R28 D29 Y32 I33 E34 K35 I36 G37 Y38 Y39 D40 P41 R42 K43 T44 T45 P46 D47 W48 L49 K50 V51 D52 V53 E54 R55 A56 R57 Y58 W59 L60 S61 V62 G63 A64 Q65 P66 T67 D68 T69 V79 F80 R81 Q82 E83

• Molecule 20: 30S ribosomal protein S17

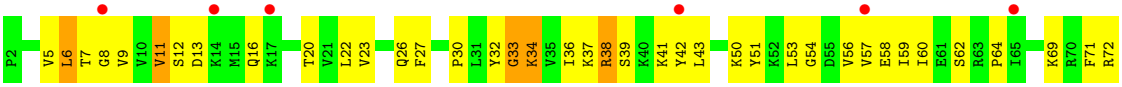
Chain AQ: 4% 48% 45% 6%

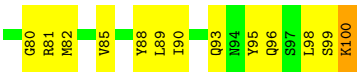
P2 V5 L6 T7 G8 V9 V10 V11 S12 D13 Q16 T20 V21 L22 V23 Q26 F27 P30 L31 Y32 G33 K34 V35 I36 K37 R38 S39 K40 K41 Y42 L43 A44 K50 Y51 K52 L53 G54 D55 V56 V57 E58 I59 I60 E61 S62 R63 P64 K69 R70 F71 G80 R81




• Molecule 20: 30S ribosomal protein S17

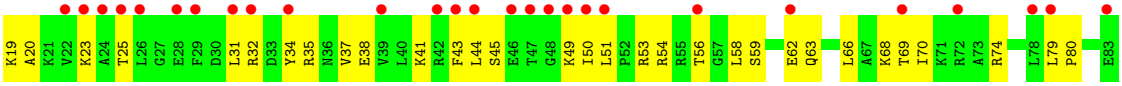
Chain CQ:



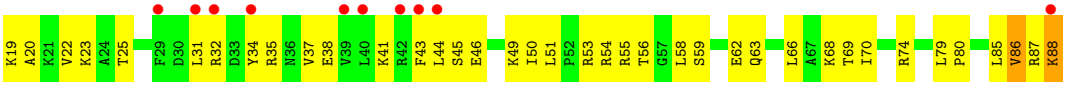

• Molecule 21: 30S ribosomal protein S18

Chain AR:



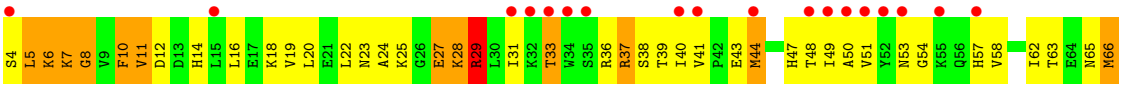
• Molecule 21: 30S ribosomal protein S18

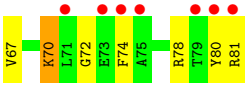
Chain CR:




• Molecule 22: 30S ribosomal protein S19

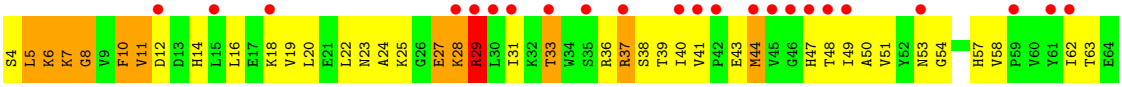
Chain AS:

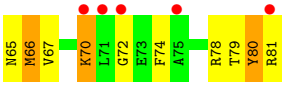



• Molecule 22: 30S ribosomal protein S19

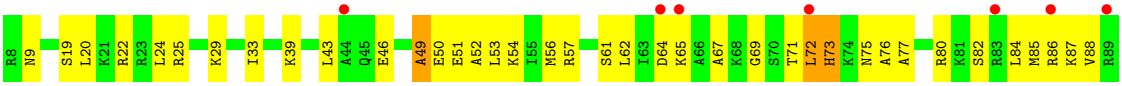
Chain CS:

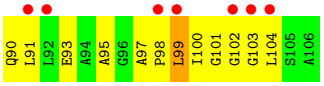





• Molecule 23: 30S ribosomal protein S20

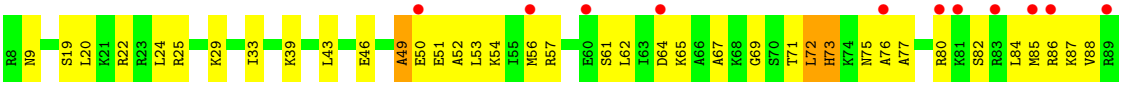
Chain AT:

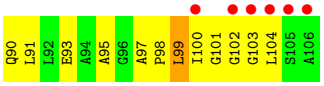



• Molecule 23: 30S ribosomal protein S20

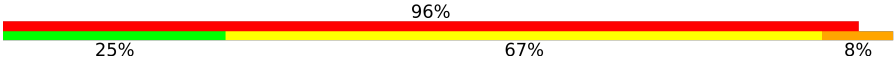
Chain CT:

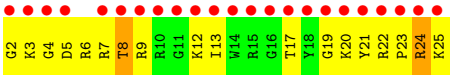



• Molecule 24: 30S ribosomal protein Thx

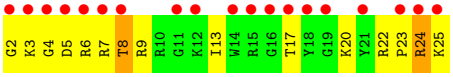
Chain AU:



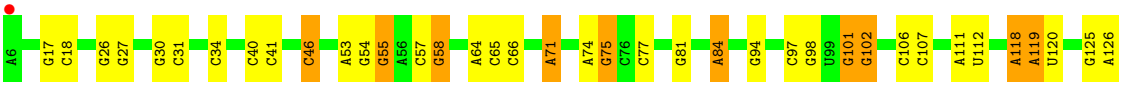

• Molecule 24: 30S ribosomal protein Thx

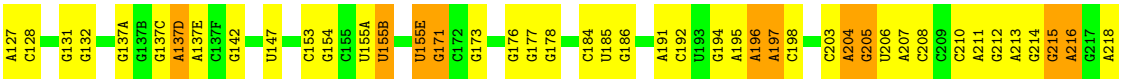
Chain CU:

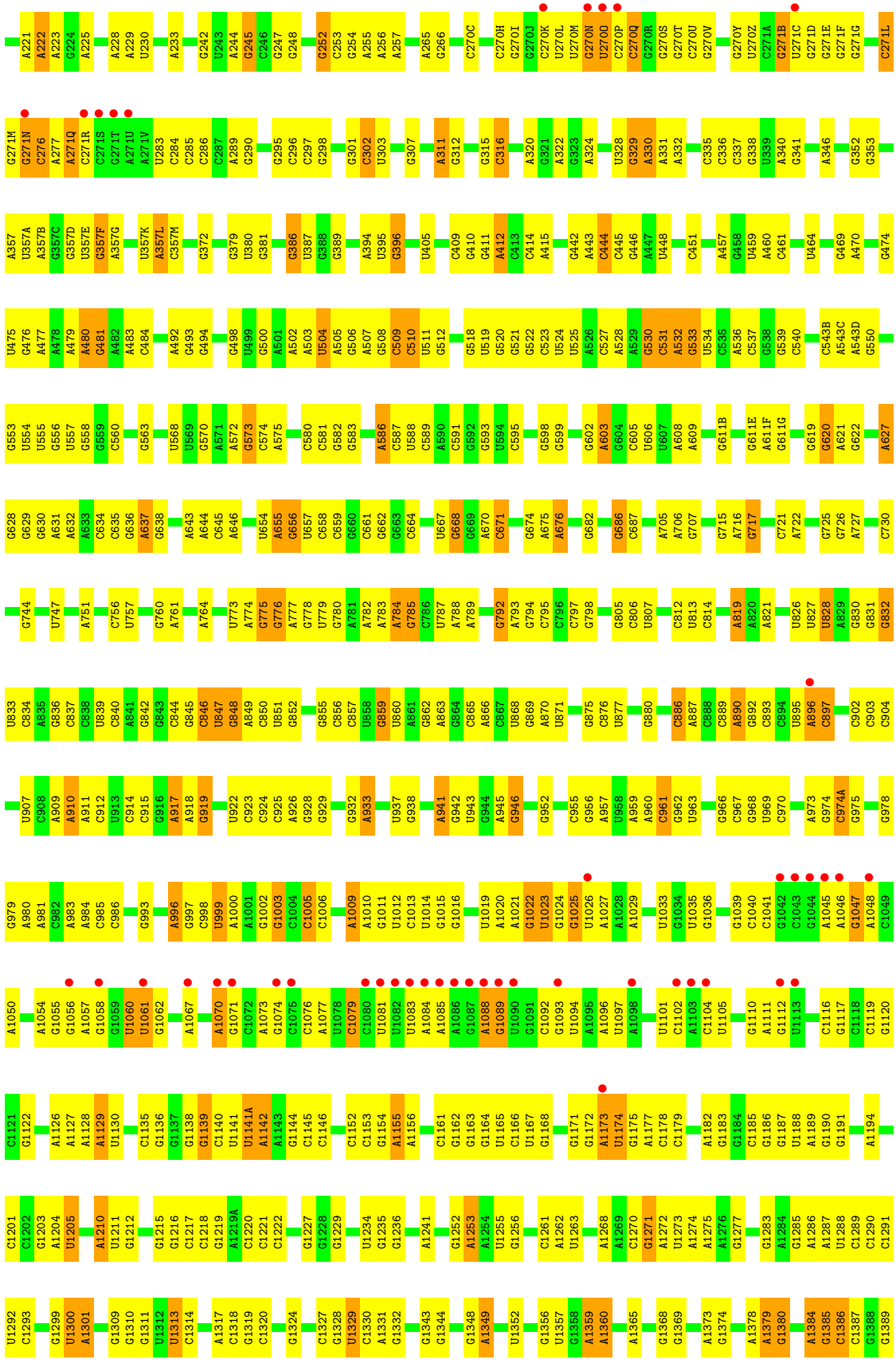



• Molecule 25: 23S ribosomal RNA

Chain BA:

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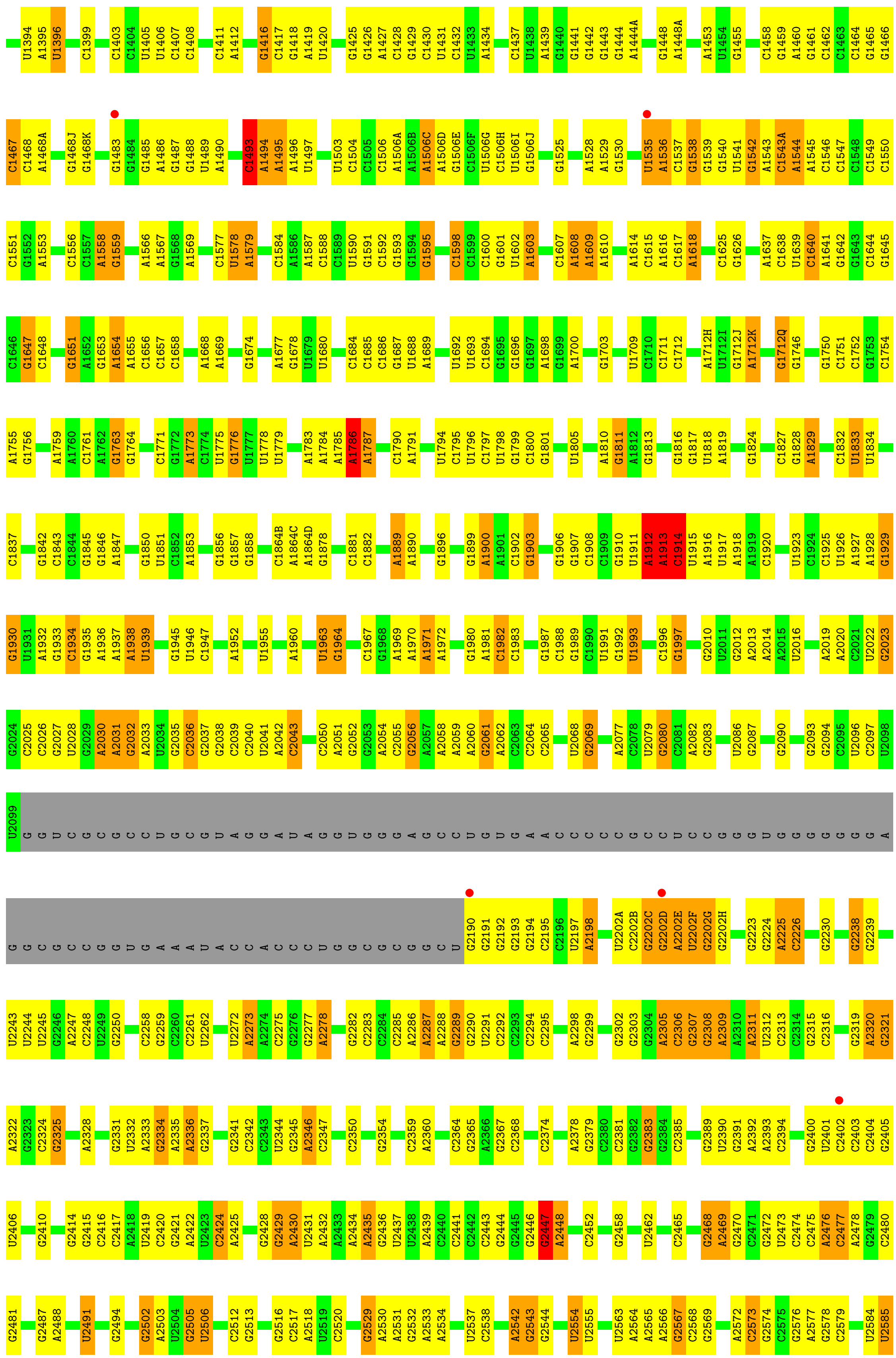
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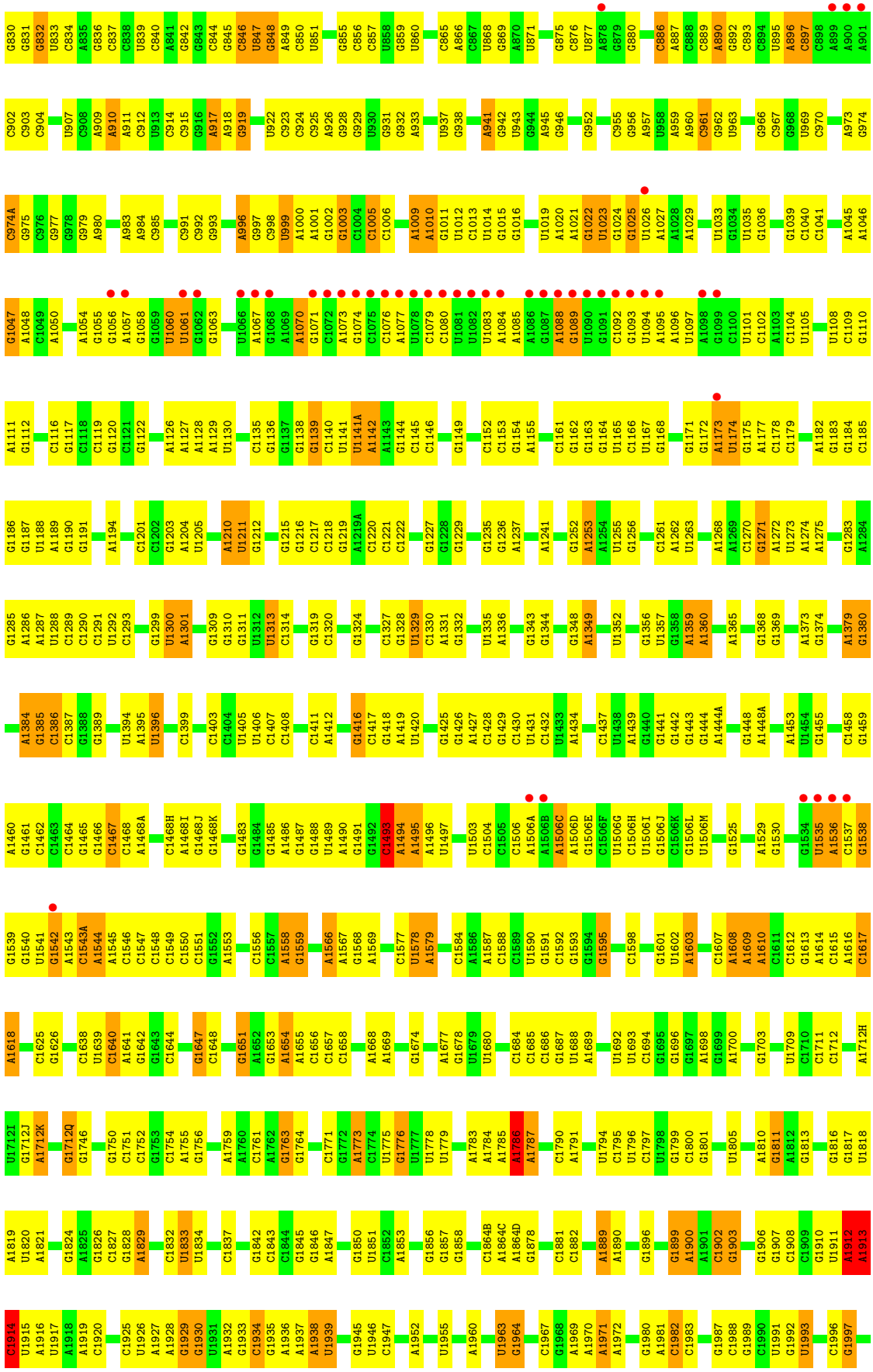
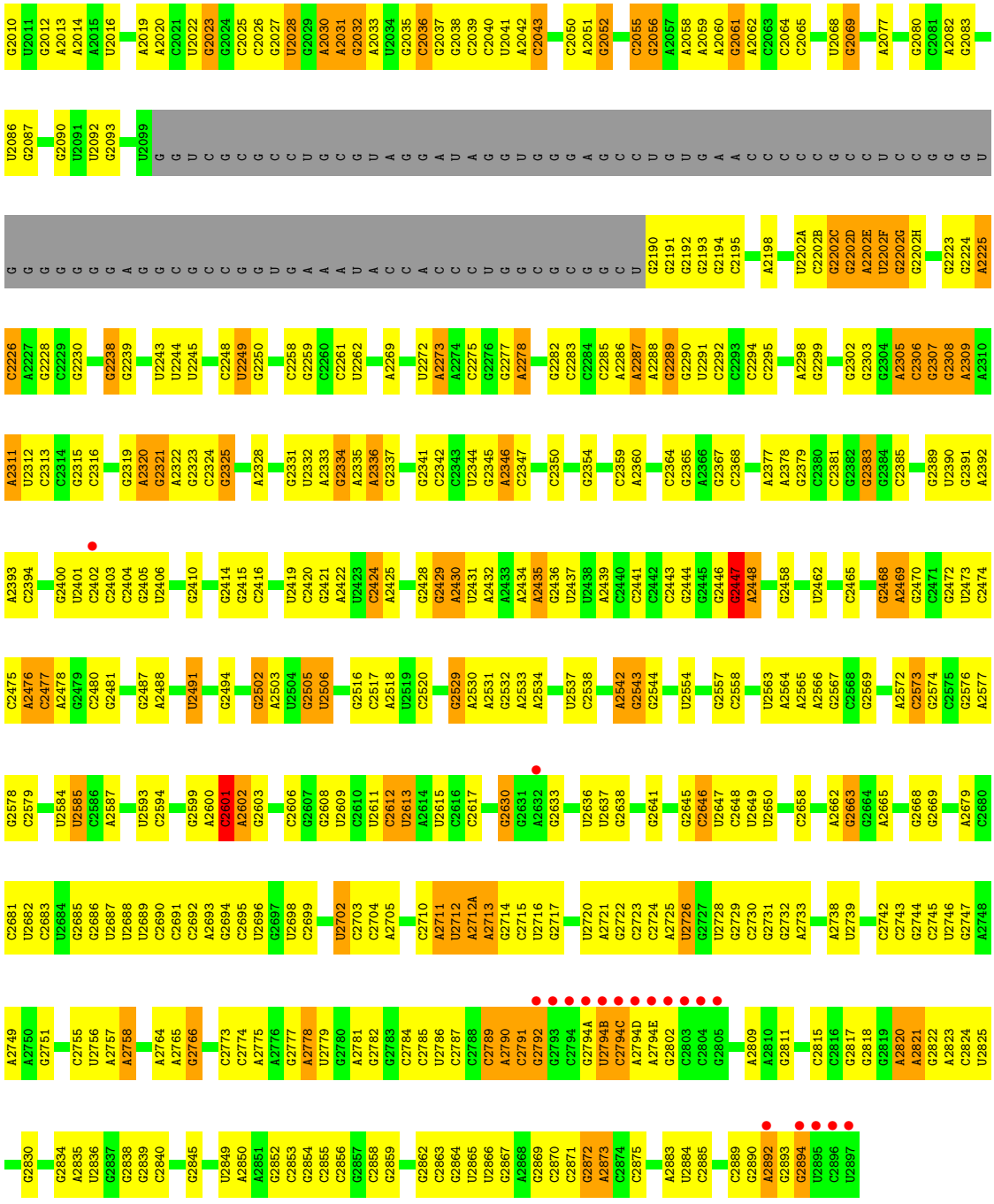
• Molecule 25: 23S ribosomal RNA

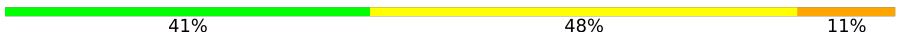
Chain DA:

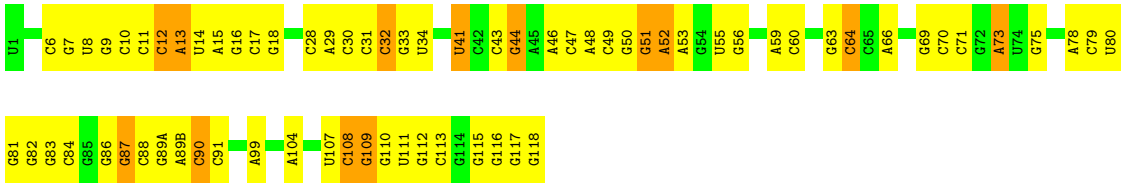




• Molecule 26: 5S ribosomal RNA

Chain BB:



• Molecule 26: 5S ribosomal RNA

Chain DB: 2% 39% 50% 11%

U1 C6 G7 U8 G9 C10 C11 C12 A13 U14 A15 G16 C17 G18 C27 C28 A29 C30 C31 C32 G33 U34 U41 C42 C43 G44 A45 A46 C47 A48 C49 G50 G51 A52 A53 G54 U55 G56 A59 C60 G61 C62 G63 C64 C65 A66 G69 C70 C71 G72 A73 U74 G75 A78

C79 U80 G81 G82 G83 C84 G85 G86 G87 C88 G89A A89B C90 C91 A99 G102 U103 A104 U107 C108 G109 G110 U111 G112 C113 G114 G115 G116 G117 G118

- Molecule 27: 50S ribosomal protein L2

Chain BD: 5% 41% 50% 9%

A2 K5 F6 K7 P8 P11 S12 R13 R14 F15 M16 T17 F21 I24 T25 K26 T27 E28 P29 E30 K31 S32 L33 V34 K35 P36 L37 K38 K39 T40 R43 N44 N45 Q46 G47 R48 I49 T50 V51 R52 H58 K59 R60 L61 Y62 R63 I64 F67 K68 R69 W70 D71 K72

V73 G74 I75 P76 A77 K78 V79 A80 A81 I82 E83 Y84 D85 P86 N87 R88 A93 L94 L95 H96 Y97 V98 D99 G100 E101 K102 R103 Y104 I105 I106 A107 P108 L111 Q112 V113 G114 Q115 Q116 V117 V118 A119 G120 P121 I125 Q126 V127 G128 N129 A130 L131 P132 L133 R134 F135 I136 P137 V138

V142 H143 A144 V145 E146 L147 E148 P149 K150 K151 G152 A153 K154 L155 A156 R157 A158 A159 G160 T161 Q166 G167 R168 E169 G170 D171 Y172 V173 I174 L175 R176 L177 E181 L182 R183 K184 V185 H186 G187 E188 C189 Y190 A191 T192 V193 N198 A199 D200 H201 I204 V205 L206 G207 K208 A209

G210 R211 S212 R218 P219 N227 P228 V229 D230 H231 P232 G235 G236 E237 G238 R239 A240 P241 R242 G243 R244 P245 P246 A247 S248 K255 G256 L257 K258 T259 R262 S267 I270 I271 A272

- Molecule 27: 50S ribosomal protein L2

Chain DD: 2% 41% 50% 9%

A2 V3 K4 K5 F6 K7 P8 P11 S12 R13 R14 F15 M16 T17 F21 S22 E23 I24 T25 K26 T27 E28 P29 E30 K31 S32 L33 V34 K35 P36 L37 K38 K39 T40 G41 G42 R43 G47 R48 I49 T50 V51 R52 G57 H58 K59 R60 L61 Y62 R63 I64 F67 W70 D71

K72 V73 G74 I75 P76 A77 K78 V79 A80 A81 I82 E83 Y84 D85 P86 N87 R88 A93 L94 L95 H96 Y97 V98 D99 K102 R103 Y104 I105 I106 A107 P108 L111 Q112 V113 G114 Q115 Q116 V117 V118 A119 G120 P121 I125 Q126 V127 G128 N129 A130 L131 P132 L133 R134 F135 I136 P137 V138

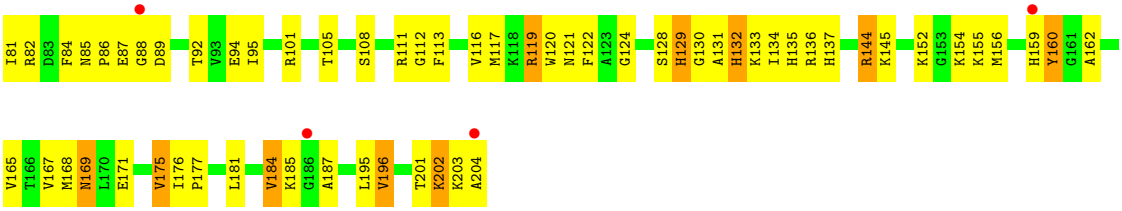
V142 H143 A144 V145 E146 L147 E148 P149 K150 K151 G152 A153 K154 L155 A156 R157 A158 A159 G160 T161 Q166 G167 R168 E169 G170 D171 Y172 V173 I174 L175 R176 L177 E181 L182 R183 K184 V185 H186 G187 E188 C189 Y190 A191 T192 V193 N198 A199 D200 H201 I204 G207 K208 A209 G210

R211 S212 G216 R217 R218 P219 N227 P228 V229 D230 H231 P232 G235 G236 E237 G238 R239 A240 P241 R242 G243 R244 P245 P246 A247 S248 K255 G256 L257 K261 R262 S267 I270 I271 A272

- Molecule 28: 50S ribosomal protein L3

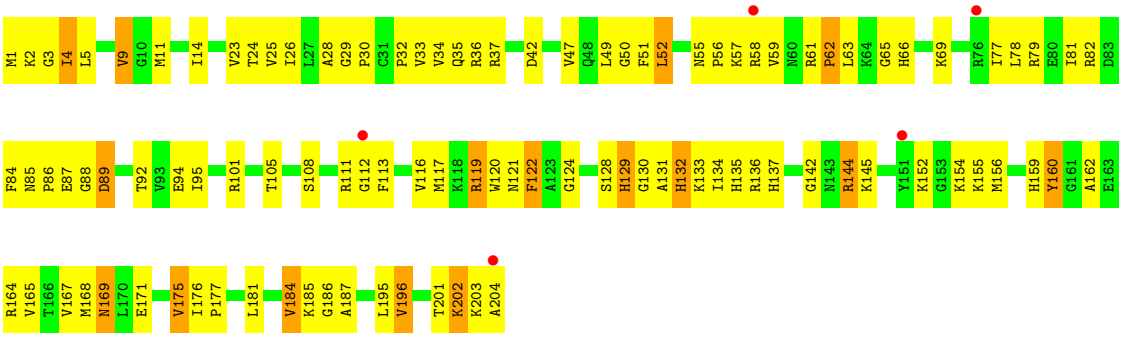
Chain BE: 5% 50% 44% 6%

M1 K2 G3 I4 L5 V9 G10 M11 I14 V23 T24 V25 I26 L27 A28 G29 P30 C31 P32 V33 V34 Q35 R36 R37 D42 V47 Q48 L49 G50 F51 L52 N55 P56 K57 R58 V59 M60 R61 P62 L63 K64 G65 H66 K69 E73 P74 V75 R76 I77 L78 R79 E80



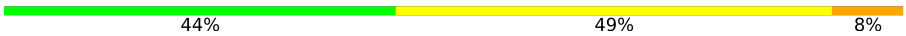

- Molecule 28: 50S ribosomal protein L3

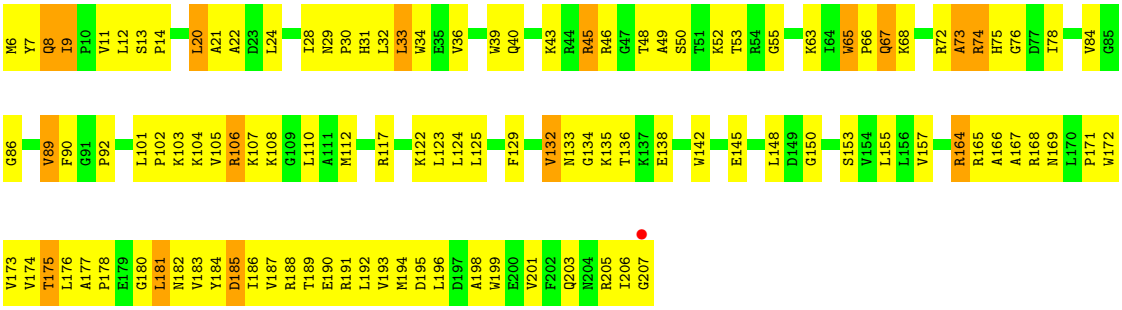
Chain DE:




- Molecule 29: 50S ribosomal protein L4

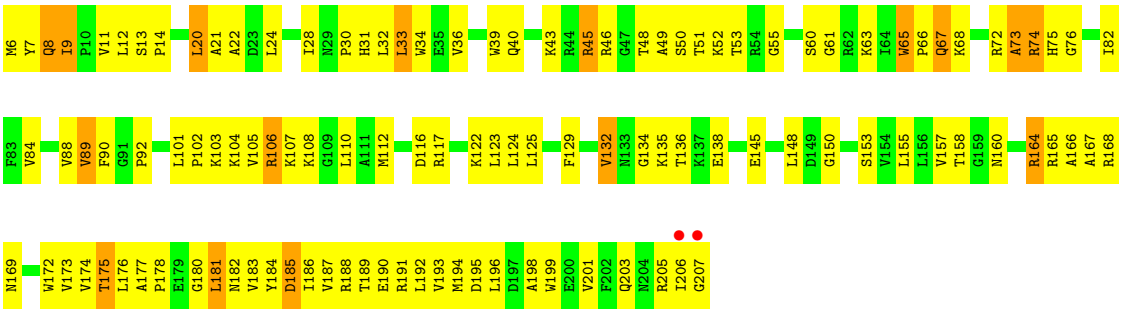
Chain BF:



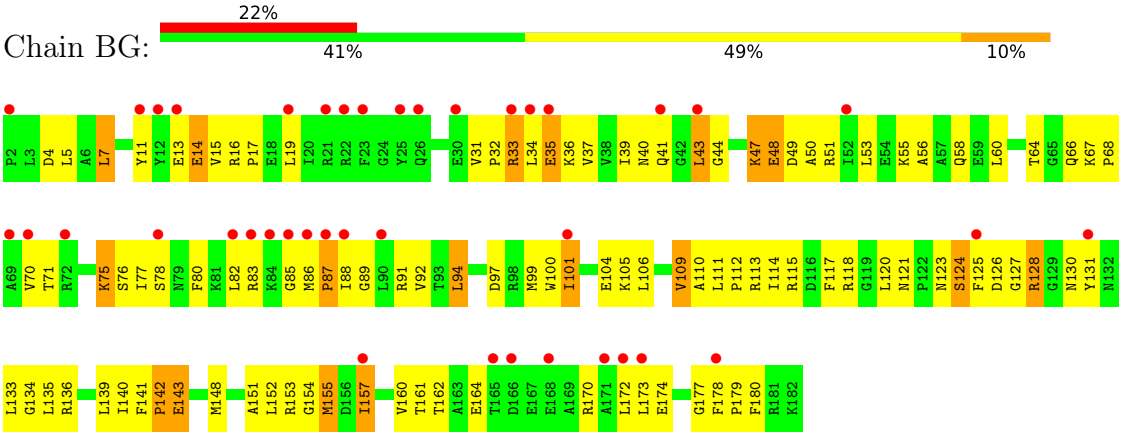

- Molecule 29: 50S ribosomal protein L4

Chain DF:



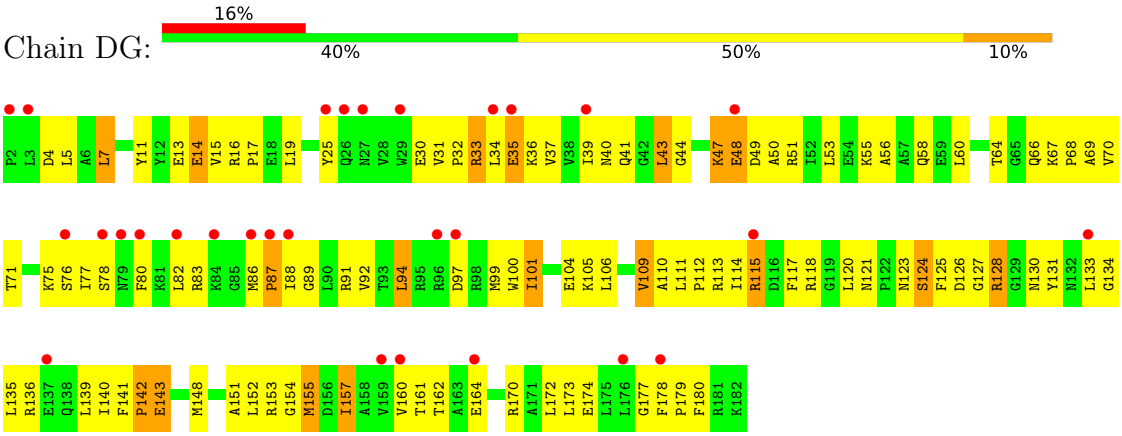

- Molecule 30: 50S ribosomal protein L5

Chain BG:



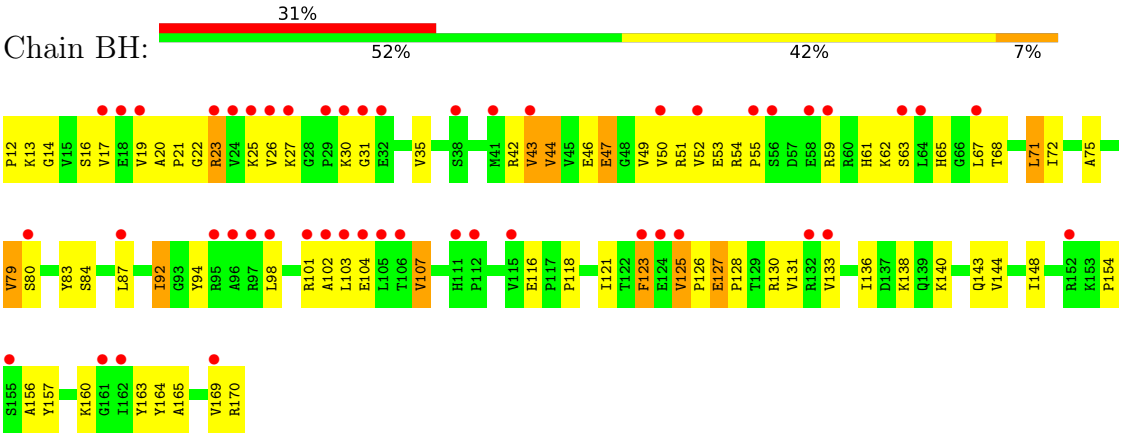

- Molecule 30: 50S ribosomal protein L5

Chain DG:



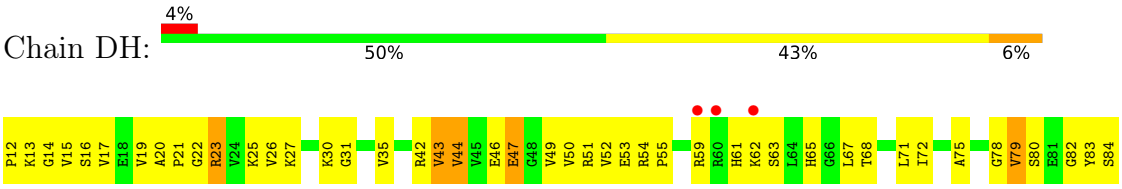

- Molecule 31: 50S ribosomal protein L6

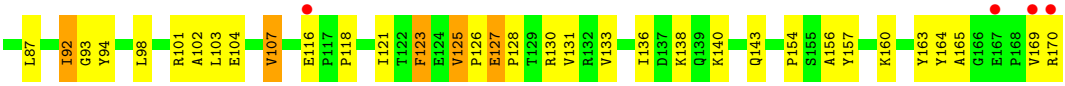
Chain BH:




- Molecule 31: 50S ribosomal protein L6

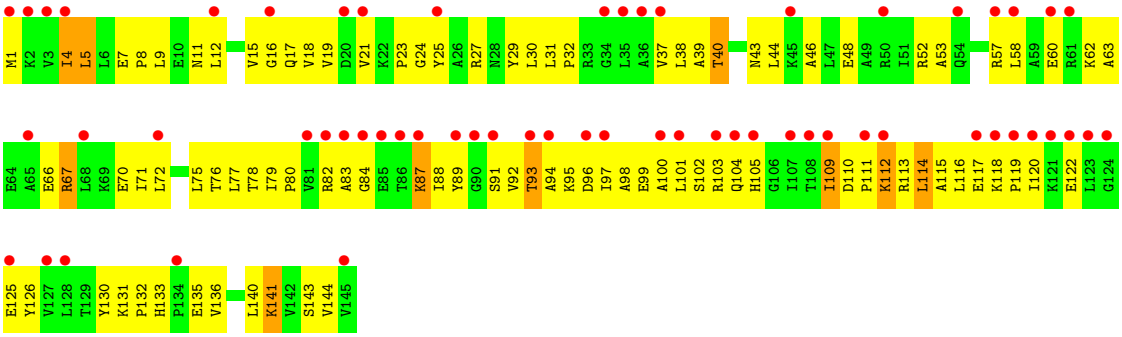
Chain DH:





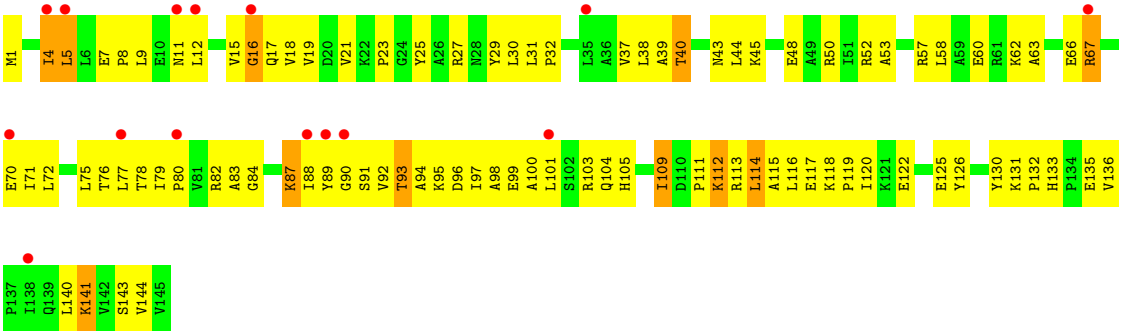

• Molecule 32: 50S ribosomal protein L9

Chain BI:



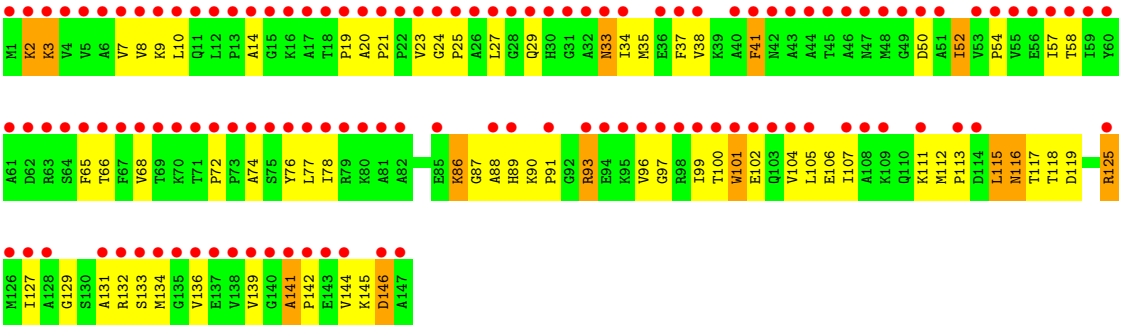

• Molecule 32: 50S ribosomal protein L9

Chain DI:



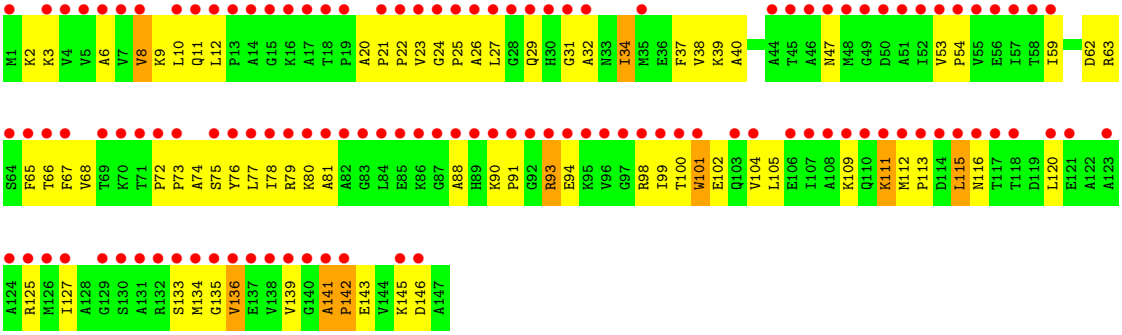

• Molecule 33: 50S ribosomal protein L11

Chain BK:



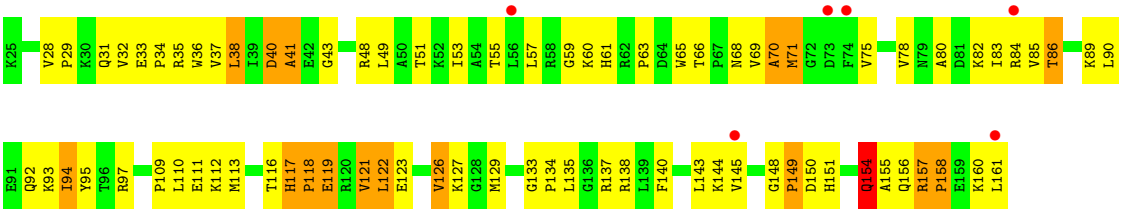

• Molecule 33: 50S ribosomal protein L11

Chain DK:




• Molecule 34: 50S ribosomal protein L13

Chain BN:




• Molecule 34: 50S ribosomal protein L13

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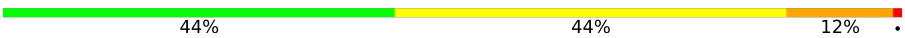
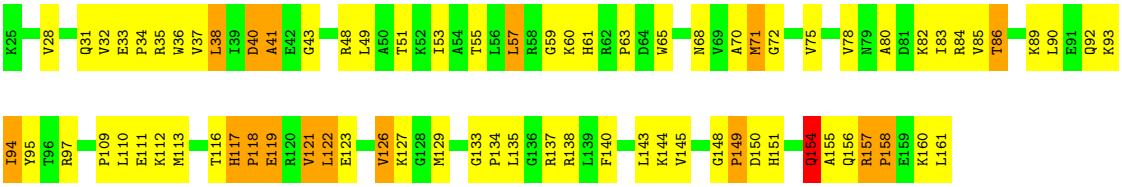


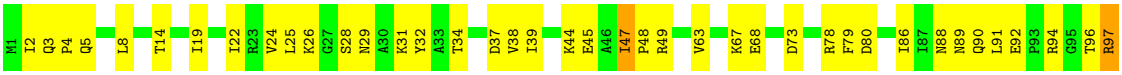



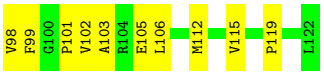

• Molecule 35: 50S ribosomal protein L14

Chain BO:

• Molecule 35: 50S ribosomal protein L14

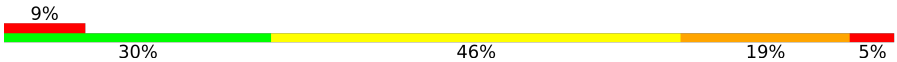
Chain DO:

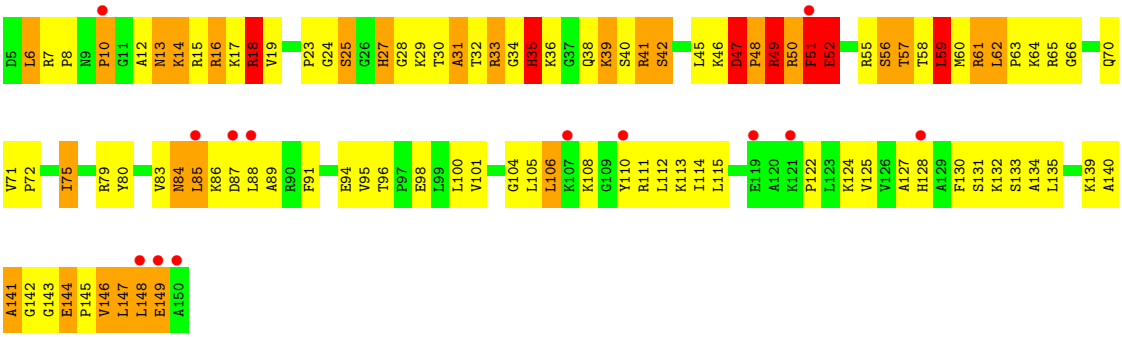





• Molecule 36: 50S ribosomal protein L15

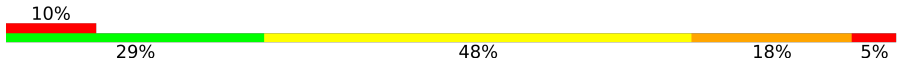
Chain BP:

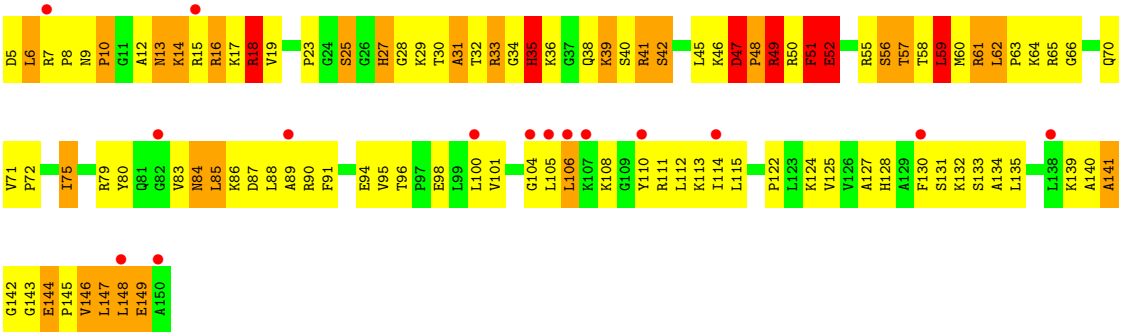



• Molecule 36: 50S ribosomal protein L15

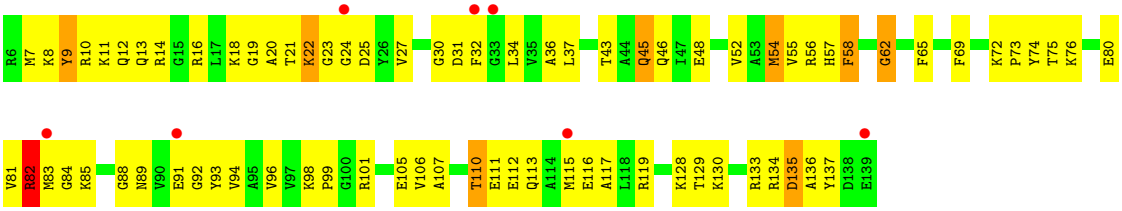
Chain DP:



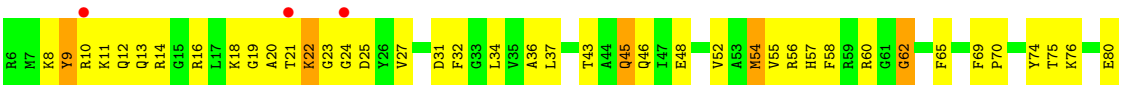

• Molecule 37: 50S ribosomal protein L16

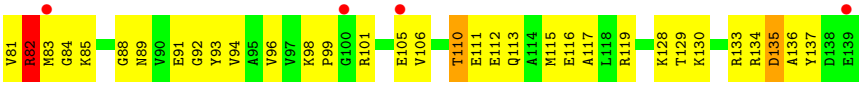
Chain BQ:




• Molecule 37: 50S ribosomal protein L16

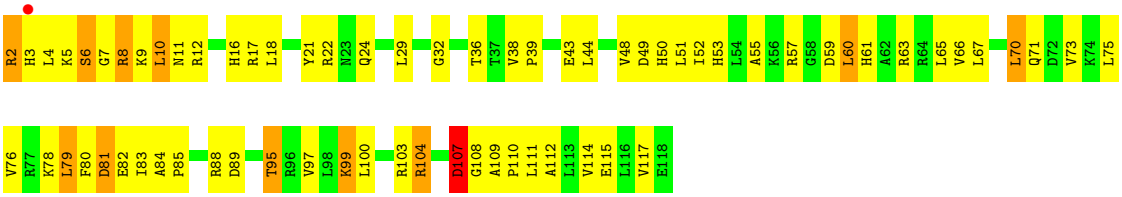
Chain DQ:





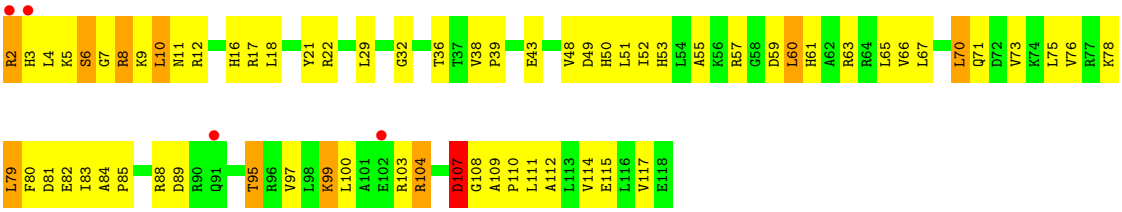

• Molecule 38: 50S ribosomal protein L17

Chain BR:



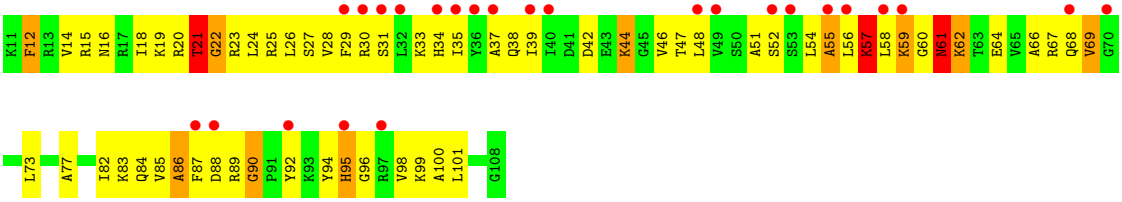

• Molecule 38: 50S ribosomal protein L17

Chain DR:



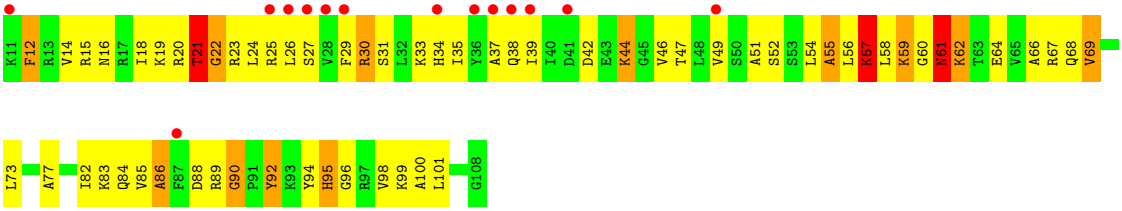

• Molecule 39: 50S ribosomal protein L18

Chain BS:



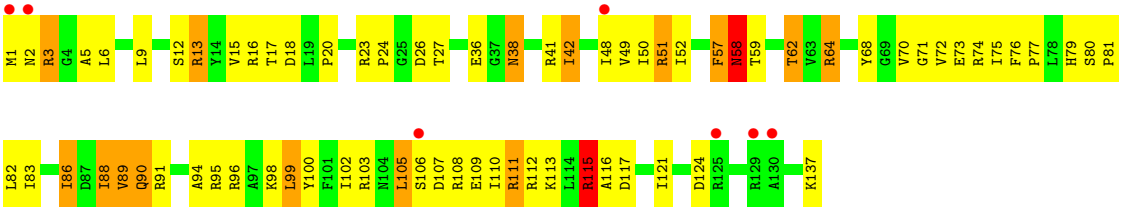

• Molecule 39: 50S ribosomal protein L18

Chain DS:



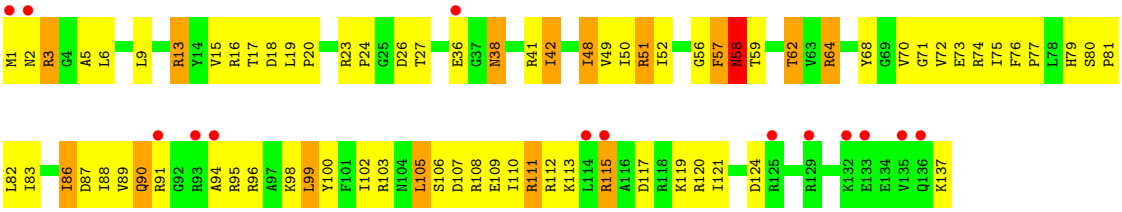

• Molecule 40: 50S ribosomal protein L19

Chain BT:



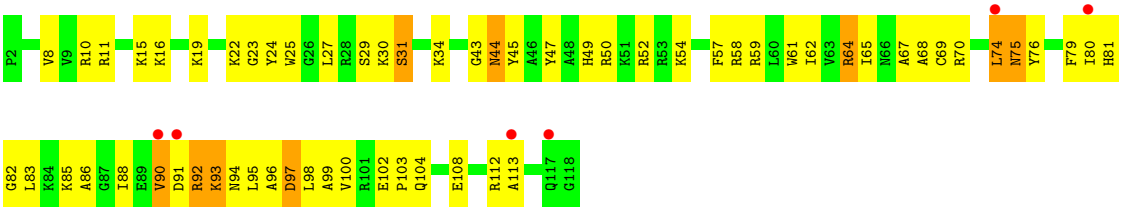

- Molecule 40: 50S ribosomal protein L19

Chain DT:



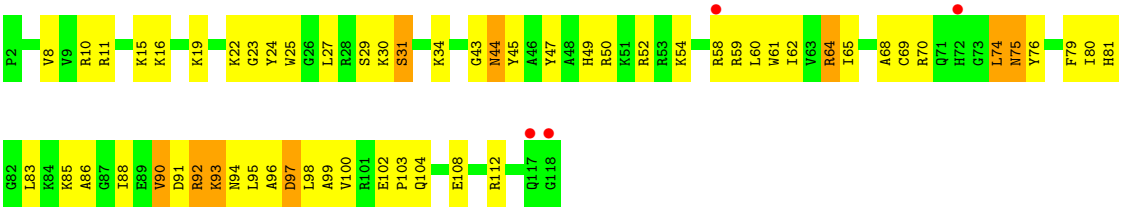

- Molecule 41: 50S ribosomal protein L20

Chain BU:



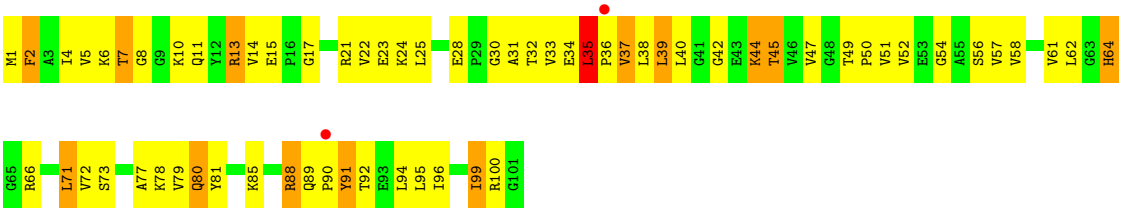

- Molecule 41: 50S ribosomal protein L20

Chain DU:



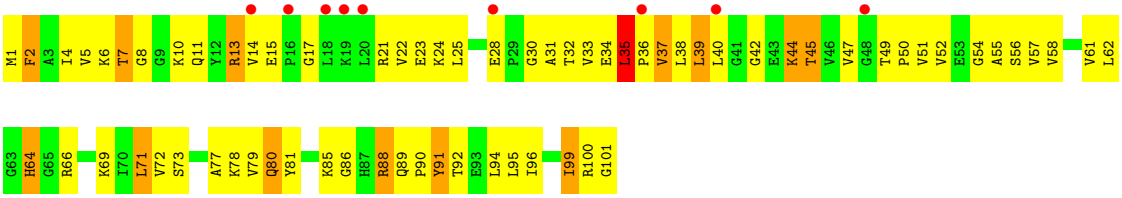

- Molecule 42: 50S ribosomal protein L21

Chain BV:



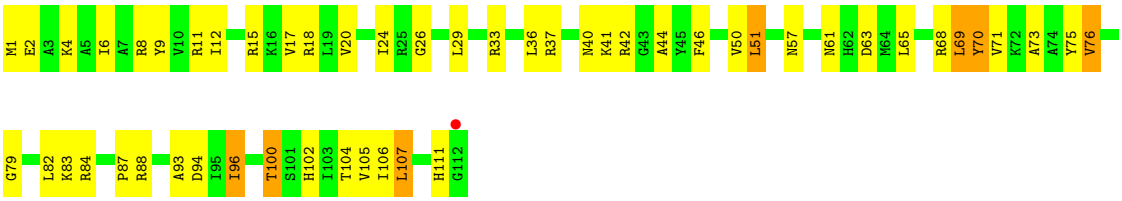
• Molecule 42: 50S ribosomal protein L21

Chain DV:



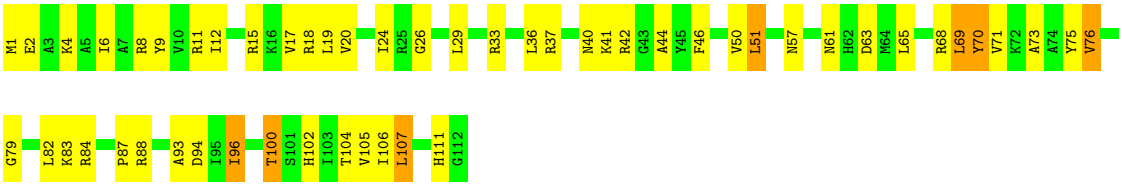

• Molecule 43: 50S ribosomal protein L22

Chain BW:



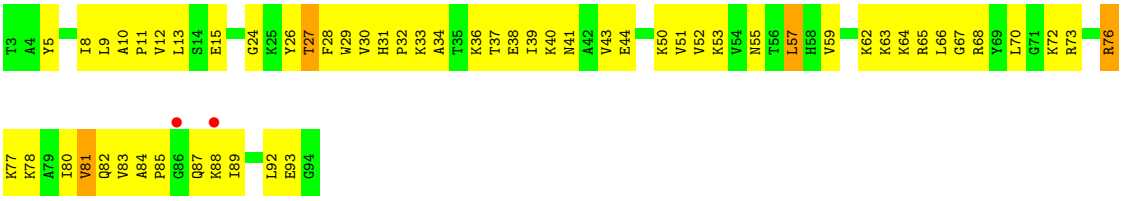

• Molecule 43: 50S ribosomal protein L22

Chain DW:



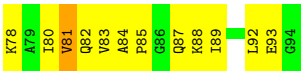

• Molecule 44: 50S ribosomal protein L23

Chain BX:



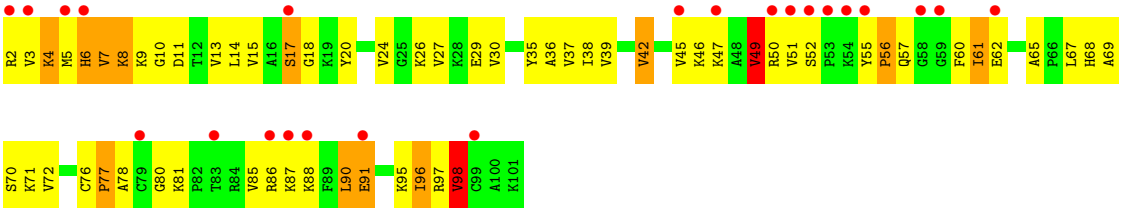

• Molecule 44: 50S ribosomal protein L23

Chain DX:



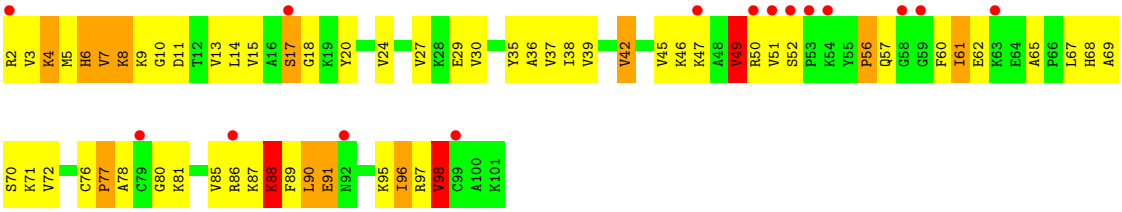

• Molecule 45: 50S ribosomal protein L24

Chain BY:



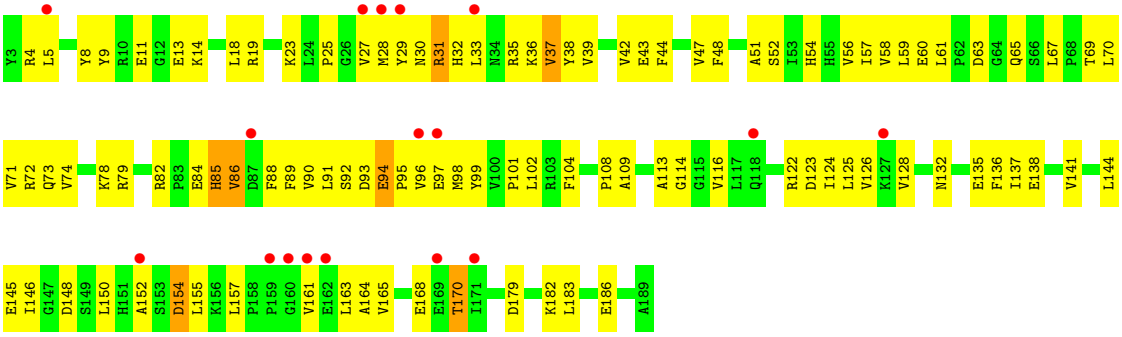

• Molecule 45: 50S ribosomal protein L24

Chain DY:



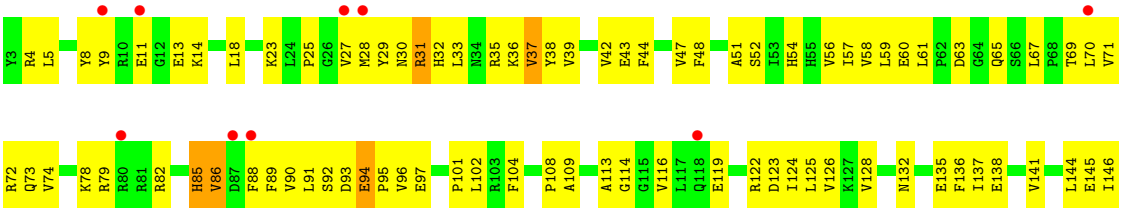

• Molecule 46: 50S ribosomal protein L25

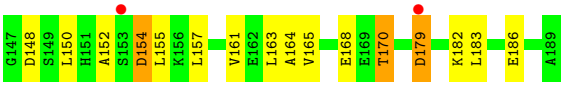
Chain BZ:




• Molecule 46: 50S ribosomal protein L25

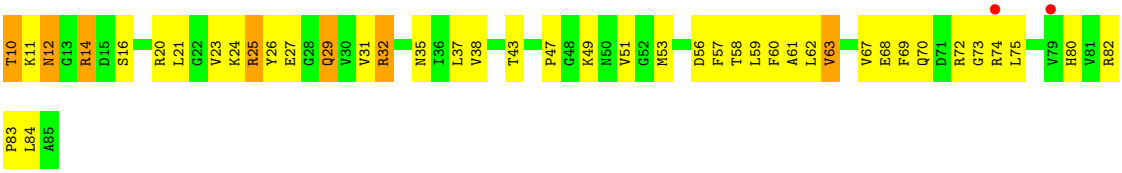
Chain DZ:





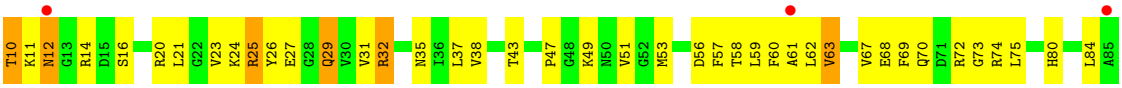

• Molecule 47: 50S ribosomal protein L27

Chain B0:



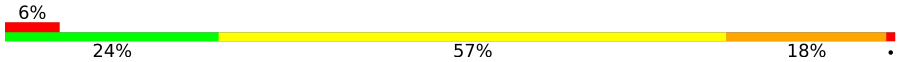

• Molecule 47: 50S ribosomal protein L27

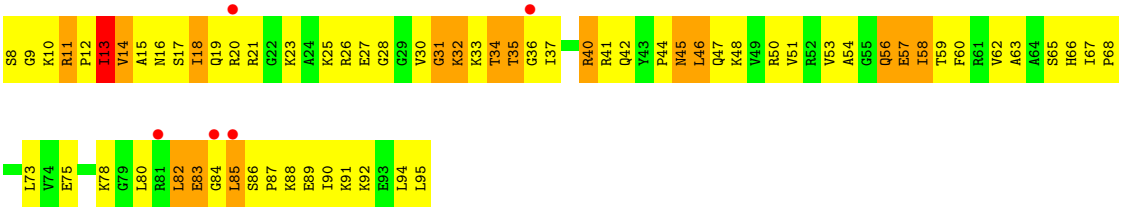
Chain D0:




• Molecule 48: 50S ribosomal protein L28

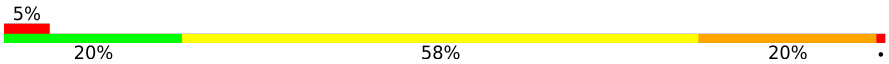
Chain B1:

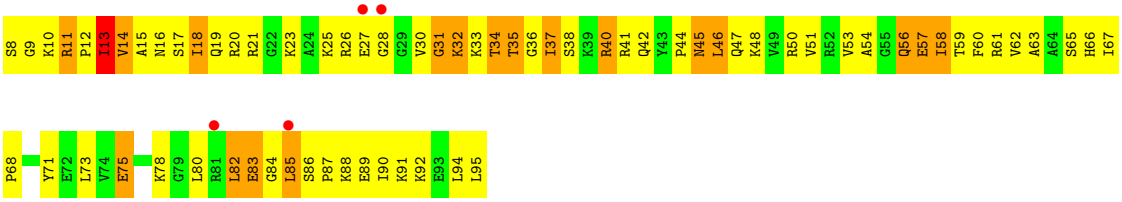



• Molecule 48: 50S ribosomal protein L28

Chain D1:



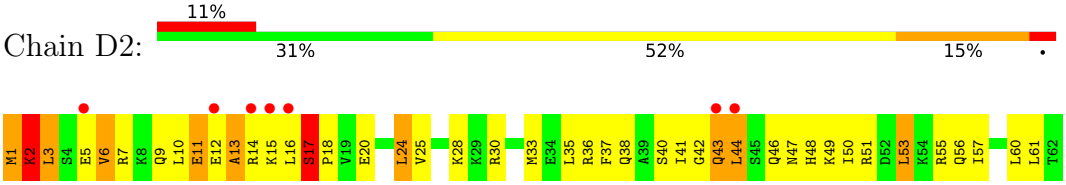




• Molecule 49: 50S ribosomal protein L29

Chain B2:

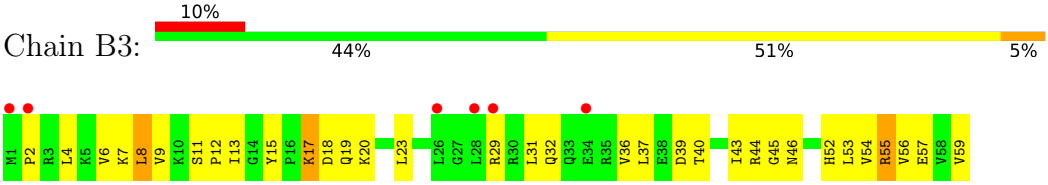
• Molecule 49: 50S ribosomal protein L29

Chain D2:



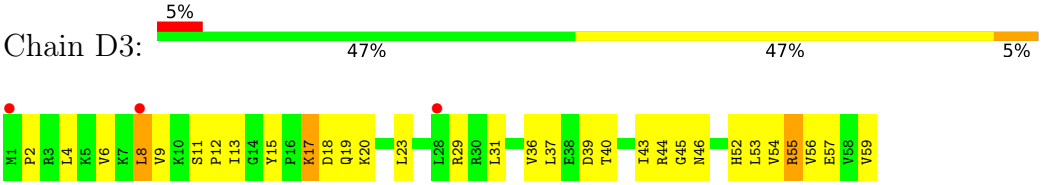

• Molecule 50: 50S ribosomal protein L30

Chain B3:



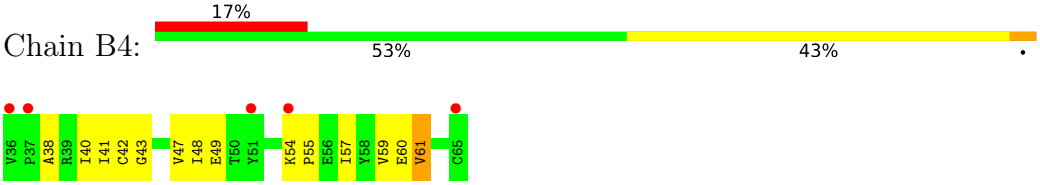

• Molecule 50: 50S ribosomal protein L30

Chain D3:



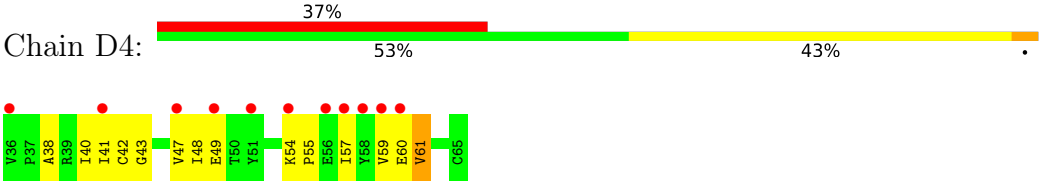

• Molecule 51: 50S ribosomal protein L31

Chain B4:



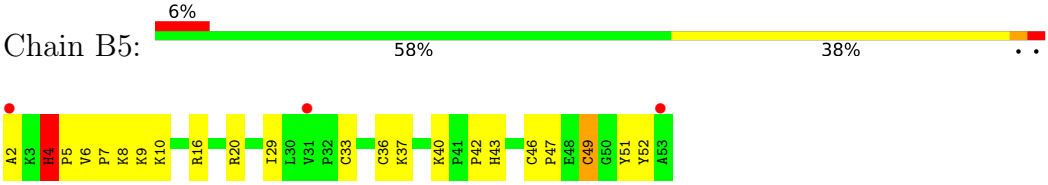

• Molecule 51: 50S ribosomal protein L31

Chain D4:



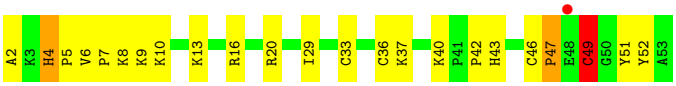

• Molecule 52: 50S ribosomal protein L32

Chain B5:



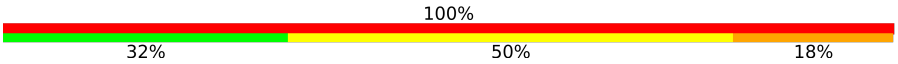

• Molecule 52: 50S ribosomal protein L32

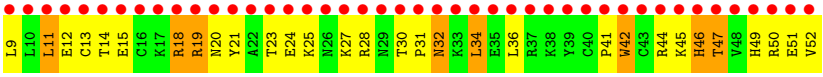
Chain D5:




• Molecule 53: 50S ribosomal protein L33

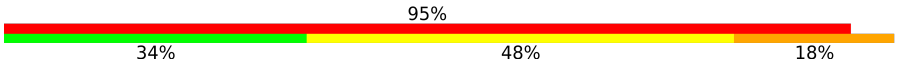
Chain B6:

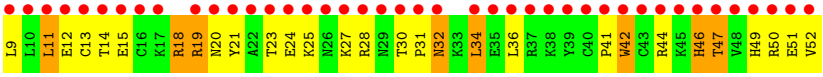



• Molecule 53: 50S ribosomal protein L33

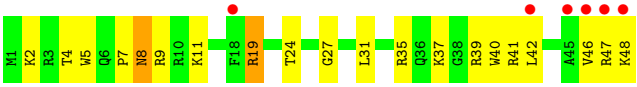
Chain D6:



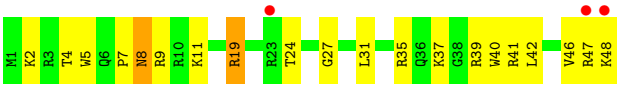

• Molecule 54: 50S ribosomal protein L34

Chain B7:



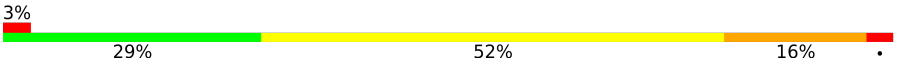

• Molecule 54: 50S ribosomal protein L34

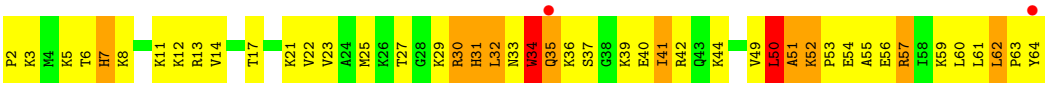
Chain D7:




• Molecule 55: 50S ribosomal protein L35

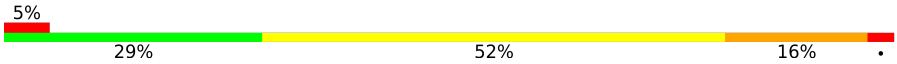
Chain B8:

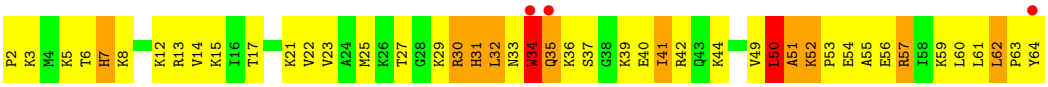



• Molecule 55: 50S ribosomal protein L35

Chain D8:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 212.07Å 454.40Å 618.45Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.67 – 3.40<br>49.78 – 3.35 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.7 (49.67-3.40)<br>99.7 (49.78-3.35) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.72 (at 3.33Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.6.4_486), CNS | Depositor |
| R, $R_{free}$ | 0.234 , 0.268<br>0.241 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 83.6 | Xtriage |
| Anisotropy | 0.218 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.27 , 97.0 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.44$, $< L^2 > = 0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 294074 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 109.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | AA | 0.27 | 2/36194 (0.0%) | 0.55 | 0/56493 |
| 1 | CA | 0.27 | 2/36194 (0.0%) | 0.54 | 0/56493 |
| 2 | AV | 0.26 | 0/241 | 0.53 | 0/374 |
| 2 | CV | 0.23 | 0/241 | 0.54 | 0/374 |
| 3 | AW | 0.25 | 0/1832 | 0.52 | 0/2855 |
| 3 | CW | 0.26 | 0/1832 | 0.53 | 0/2855 |
| 4 | AY | 0.21 | 0/2925 | 0.39 | 0/3953 |
| 4 | CY | 0.21 | 0/2925 | 0.39 | 0/3953 |
| 5 | AB | 0.22 | 0/1936 | 0.40 | 0/2609 |
| 5 | CB | 0.22 | 0/1936 | 0.39 | 0/2609 |
| 6 | AC | 0.22 | 0/1637 | 0.39 | 0/2205 |
| 6 | CC | 0.22 | 0/1637 | 0.39 | 0/2205 |
| 7 | AD | 0.25 | 0/1733 | 0.44 | 0/2318 |
| 7 | CD | 0.24 | 0/1733 | 0.41 | 0/2318 |
| 8 | AE | 0.24 | 0/1172 | 0.44 | 0/1576 |
| 8 | CE | 0.24 | 0/1172 | 0.43 | 0/1576 |
| 9 | AF | 0.23 | 0/856 | 0.42 | 0/1154 |
| 9 | CF | 0.24 | 0/856 | 0.43 | 0/1154 |
| 10 | AG | 0.22 | 0/1276 | 0.37 | 0/1709 |
| 10 | CG | 0.22 | 0/1276 | 0.37 | 0/1709 |
| 11 | AH | 0.23 | 0/1136 | 0.44 | 0/1527 |
| 11 | CH | 0.22 | 0/1136 | 0.43 | 0/1527 |
| 12 | AI | 0.23 | 0/1029 | 0.40 | 0/1378 |
| 12 | CI | 0.22 | 0/1029 | 0.40 | 0/1378 |
| 13 | AJ | 0.21 | 0/808 | 0.41 | 0/1085 |
| 13 | CJ | 0.21 | 0/808 | 0.41 | 0/1085 |
| 14 | AK | 0.24 | 0/857 | 0.43 | 0/1157 |
| 14 | CK | 0.24 | 0/857 | 0.43 | 0/1157 |
| 15 | AL | 0.27 | 0/973 | 0.47 | 0/1301 |
| 15 | CL | 0.26 | 0/973 | 0.47 | 0/1301 |
| 16 | AM | 0.20 | 0/944 | 0.40 | 0/1265 |
| 16 | CM | 0.20 | 0/944 | 0.40 | 0/1265 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | AN | 0.24 | 0/501 | 0.41 | 0/664 |
| 17 | CN | 0.25 | 0/501 | 0.39 | 0/664 |
| 18 | AO | 0.24 | 0/745 | 0.39 | 0/992 |
| 18 | CO | 0.24 | 0/745 | 0.39 | 0/992 |
| 19 | AP | 0.24 | 0/717 | 0.43 | 0/963 |
| 19 | CP | 0.22 | 0/717 | 0.43 | 0/963 |
| 20 | AQ | 0.25 | 0/837 | 0.41 | 0/1117 |
| 20 | CQ | 0.23 | 0/837 | 0.41 | 0/1117 |
| 21 | AR | 0.24 | 0/579 | 0.43 | 0/768 |
| 21 | CR | 0.24 | 0/579 | 0.43 | 0/768 |
| 22 | AS | 0.21 | 0/643 | 0.40 | 0/865 |
| 22 | CS | 0.22 | 0/643 | 0.40 | 0/865 |
| 23 | AT | 0.23 | 0/764 | 0.39 | 0/1006 |
| 23 | CT | 0.22 | 0/764 | 0.39 | 0/1006 |
| 24 | AU | 0.21 | 0/213 | 0.40 | 0/277 |
| 24 | CU | 0.21 | 0/213 | 0.41 | 0/277 |
| 25 | BA | 0.38 | 6/67268 (0.0%) | 0.67 | 12/105011 (0.0%) |
| 25 | DA | 0.42 | 6/67268 (0.0%) | 0.70 | 21/105011 (0.0%) |
| 26 | BB | 0.25 | 0/2853 | 0.55 | 0/4451 |
| 26 | DB | 0.26 | 0/2853 | 0.56 | 0/4451 |
| 27 | BD | 0.33 | 0/2155 | 0.53 | 0/2905 |
| 27 | DD | 0.35 | 0/2155 | 0.53 | 1/2905 (0.0%) |
| 28 | BE | 0.28 | 0/1597 | 0.49 | 0/2153 |
| 28 | DE | 0.29 | 0/1597 | 0.49 | 0/2153 |
| 29 | BF | 0.29 | 0/1622 | 0.48 | 0/2194 |
| 29 | DF | 0.31 | 0/1622 | 0.48 | 0/2194 |
| 30 | BG | 0.23 | 0/1500 | 0.42 | 0/2017 |
| 30 | DG | 0.23 | 0/1500 | 0.43 | 0/2017 |
| 31 | BH | 0.22 | 0/1246 | 0.44 | 0/1682 |
| 31 | DH | 0.24 | 0/1246 | 0.45 | 0/1682 |
| 32 | BI | 0.22 | 0/1148 | 0.42 | 0/1552 |
| 32 | DI | 0.23 | 0/1148 | 0.43 | 0/1552 |
| 33 | BK | 0.21 | 0/1108 | 0.40 | 0/1500 |
| 33 | DK | 0.20 | 0/1108 | 0.39 | 0/1500 |
| 34 | BN | 0.27 | 0/1124 | 0.46 | 0/1515 |
| 34 | DN | 0.29 | 0/1124 | 0.47 | 0/1515 |
| 35 | BO | 0.28 | 0/942 | 0.47 | 0/1268 |
| 35 | DO | 0.30 | 0/942 | 0.48 | 0/1268 |
| 36 | BP | 0.34 | 0/1131 | 0.62 | 1/1504 (0.1%) |
| 36 | DP | 0.36 | 0/1131 | 0.63 | 1/1504 (0.1%) |
| 37 | BQ | 0.30 | 0/1085 | 0.52 | 0/1449 |
| 37 | DQ | 0.31 | 0/1085 | 0.52 | 0/1449 |
| 38 | BR | 0.28 | 0/974 | 0.48 | 0/1302 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | DR | 0.29 | 0/974 | 0.49 | 0/1302 |
| 39 | BS | 0.24 | 0/779 | 0.44 | 0/1036 |
| 39 | DS | 0.25 | 0/779 | 0.44 | 0/1036 |
| 40 | BT | 0.27 | 0/1158 | 0.47 | 0/1544 |
| 40 | DT | 0.28 | 0/1158 | 0.48 | 0/1544 |
| 41 | BU | 0.31 | 0/982 | 0.47 | 0/1306 |
| 41 | DU | 0.32 | 0/982 | 0.46 | 0/1306 |
| 42 | BV | 0.28 | 0/790 | 0.49 | 0/1057 |
| 42 | DV | 0.29 | 0/790 | 0.49 | 0/1057 |
| 43 | BW | 0.30 | 0/902 | 0.47 | 0/1209 |
| 43 | DW | 0.29 | 0/902 | 0.47 | 0/1209 |
| 44 | BX | 0.30 | 0/740 | 0.46 | 0/993 |
| 44 | DX | 0.33 | 0/740 | 0.48 | 0/993 |
| 45 | BY | 0.28 | 0/789 | 0.49 | 0/1051 |
| 45 | DY | 0.30 | 0/789 | 0.49 | 0/1051 |
| 46 | BZ | 0.22 | 0/1515 | 0.42 | 0/2056 |
| 46 | DZ | 0.23 | 0/1515 | 0.42 | 0/2056 |
| 47 | B0 | 0.27 | 0/613 | 0.53 | 0/816 |
| 47 | D0 | 0.29 | 0/613 | 0.52 | 0/816 |
| 48 | B1 | 0.34 | 0/702 | 0.59 | 1/932 (0.1%) |
| 48 | D1 | 0.36 | 0/702 | 0.61 | 1/932 (0.1%) |
| 49 | B2 | 0.27 | 0/523 | 0.50 | 0/690 |
| 49 | D2 | 0.32 | 0/523 | 0.53 | 0/690 |
| 50 | B3 | 0.25 | 0/473 | 0.43 | 0/634 |
| 50 | D3 | 0.27 | 0/473 | 0.43 | 0/634 |
| 51 | B4 | 0.24 | 0/229 | 0.40 | 0/309 |
| 51 | D4 | 0.23 | 0/229 | 0.42 | 0/309 |
| 52 | B5 | 0.27 | 0/419 | 0.51 | 0/567 |
| 52 | D5 | 0.29 | 0/419 | 0.50 | 0/567 |
| 53 | B6 | 0.21 | 0/388 | 0.41 | 0/518 |
| 53 | D6 | 0.21 | 0/388 | 0.42 | 0/518 |
| 54 | B7 | 0.34 | 0/427 | 0.54 | 0/561 |
| 54 | D7 | 0.38 | 0/427 | 0.56 | 0/561 |
| 55 | B8 | 0.32 | 0/516 | 0.49 | 0/679 |
| 55 | D8 | 0.35 | 0/516 | 0.50 | 0/679 |
| All | All | 0.33 | 16/316492 (0.0%) | 0.59 | 38/472144 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 36 | BP | 0 | 1 |
| 36 | DP | 0 | 1 |
| 38 | BR | 0 | 1 |
| 38 | DR | 0 | 1 |
| 48 | B1 | 0 | 1 |
| 48 | D1 | 0 | 1 |
| 52 | B5 | 0 | 1 |
| All | All | 0 | 7 |

The worst 5 of 16 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | BA | 1913 | A | P-OP1 | -9.19 | 1.33 | 1.49 |
| 1 | AA | 1493 | A | P-OP2 | -9.00 | 1.33 | 1.49 |
| 25 | BA | 1912 | A | P-OP2 | -9.00 | 1.33 | 1.49 |
| 25 | DA | 1912 | A | P-OP1 | -8.94 | 1.33 | 1.49 |
| 1 | CA | 1493 | A | P-OP1 | -8.80 | 1.33 | 1.49 |

The worst 5 of 38 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | BA | 2061 | G | N1-C6-O6 | 8.50 | 125.00 | 119.90 |
| 25 | DA | 2447 | G | N1-C6-O6 | 6.34 | 123.71 | 119.90 |
| 25 | DA | 2061 | G | N1-C6-O6 | 6.02 | 123.51 | 119.90 |
| 25 | DA | 1899 | G | C2-N3-C4 | -6.02 | 108.89 | 111.90 |
| 25 | DA | 2447 | G | C6-C5-N7 | -5.97 | 126.82 | 130.40 |

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 48 | B1 | 26 | ARG | Peptide |
| 52 | B5 | 4 | HIS | Peptide |
| 36 | BP | 51 | PHE | Peptide |
| 38 | BR | 10 | LEU | Peptide |
| 36 | DP | 51 | PHE | Peptide |

## 5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | AA | 32332 | 0 | 16318 | 783 | 0 |
| 1 | CA | 32332 | 0 | 16318 | 798 | 0 |
| 2 | AV | 214 | 0 | 110 | 7 | 0 |
| 2 | CV | 214 | 0 | 110 | 8 | 0 |
| 3 | AW | 1640 | 0 | 837 | 26 | 0 |
| 3 | CW | 1640 | 0 | 837 | 24 | 0 |
| 4 | AY | 2874 | 0 | 2866 | 173 | 0 |
| 4 | CY | 2874 | 0 | 2866 | 164 | 0 |
| 5 | AB | 1901 | 0 | 1951 | 118 | 0 |
| 5 | CB | 1901 | 0 | 1951 | 119 | 0 |
| 6 | AC | 1613 | 0 | 1677 | 100 | 0 |
| 6 | CC | 1613 | 0 | 1677 | 101 | 0 |
| 7 | AD | 1703 | 0 | 1764 | 102 | 0 |
| 7 | CD | 1703 | 0 | 1765 | 121 | 0 |
| 8 | AE | 1156 | 0 | 1213 | 80 | 0 |
| 8 | CE | 1156 | 0 | 1213 | 80 | 0 |
| 9 | AF | 843 | 0 | 857 | 36 | 0 |
| 9 | CF | 843 | 0 | 857 | 36 | 0 |
| 10 | AG | 1257 | 0 | 1296 | 46 | 0 |
| 10 | CG | 1257 | 0 | 1296 | 42 | 0 |
| 11 | AH | 1116 | 0 | 1177 | 72 | 0 |
| 11 | CH | 1116 | 0 | 1177 | 77 | 0 |
| 12 | AI | 1011 | 0 | 1043 | 69 | 0 |
| 12 | CI | 1011 | 0 | 1043 | 70 | 0 |
| 13 | AJ | 795 | 0 | 840 | 74 | 0 |
| 13 | CJ | 795 | 0 | 840 | 72 | 0 |
| 14 | AK | 843 | 0 | 859 | 39 | 0 |
| 14 | CK | 843 | 0 | 859 | 40 | 0 |
| 15 | AL | 957 | 0 | 1046 | 73 | 0 |
| 15 | CL | 957 | 0 | 1046 | 71 | 0 |
| 16 | AM | 934 | 0 | 992 | 50 | 0 |
| 16 | CM | 934 | 0 | 992 | 55 | 0 |
| 17 | AN | 492 | 0 | 530 | 47 | 0 |
| 17 | CN | 492 | 0 | 530 | 39 | 0 |
| 18 | AO | 734 | 0 | 771 | 34 | 0 |
| 18 | CO | 734 | 0 | 771 | 34 | 0 |
| 19 | AP | 701 | 0 | 720 | 51 | 0 |
| 19 | CP | 701 | 0 | 720 | 49 | 0 |
| 20 | AQ | 824 | 0 | 893 | 38 | 0 |
| 20 | CQ | 824 | 0 | 893 | 40 | 0 |
| 21 | AR | 574 | 0 | 644 | 37 | 0 |
| 21 | CR | 574 | 0 | 644 | 39 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 22 | AS | 630 | 0 | 652 | 55 | 0 |
| 22 | CS | 630 | 0 | 652 | 56 | 0 |
| 23 | AT | 762 | 0 | 859 | 38 | 0 |
| 23 | CT | 762 | 0 | 859 | 40 | 0 |
| 24 | AU | 209 | 0 | 221 | 16 | 0 |
| 24 | CU | 209 | 0 | 221 | 17 | 0 |
| 25 | BA | 60059 | 0 | 30274 | 1273 | 0 |
| 25 | DA | 60059 | 0 | 30274 | 1280 | 0 |
| 26 | BB | 2551 | 0 | 1295 | 81 | 0 |
| 26 | DB | 2551 | 0 | 1295 | 83 | 0 |
| 27 | BD | 2105 | 0 | 2182 | 176 | 0 |
| 27 | DD | 2105 | 0 | 2182 | 179 | 0 |
| 28 | BE | 1564 | 0 | 1629 | 122 | 0 |
| 28 | DE | 1564 | 0 | 1629 | 123 | 0 |
| 29 | BF | 1587 | 0 | 1632 | 100 | 0 |
| 29 | DF | 1587 | 0 | 1632 | 108 | 0 |
| 30 | BG | 1475 | 0 | 1537 | 110 | 0 |
| 30 | DG | 1475 | 0 | 1537 | 114 | 0 |
| 31 | BH | 1223 | 0 | 1282 | 76 | 0 |
| 31 | DH | 1223 | 0 | 1282 | 77 | 0 |
| 32 | BI | 1133 | 0 | 1220 | 100 | 0 |
| 32 | DI | 1133 | 0 | 1220 | 110 | 0 |
| 33 | BK | 1088 | 0 | 1138 | 58 | 0 |
| 33 | DK | 1088 | 0 | 1138 | 61 | 0 |
| 34 | BN | 1097 | 0 | 1168 | 80 | 0 |
| 34 | DN | 1097 | 0 | 1168 | 74 | 0 |
| 35 | BO | 932 | 0 | 994 | 45 | 0 |
| 35 | DO | 932 | 0 | 994 | 46 | 0 |
| 36 | BP | 1114 | 0 | 1187 | 184 | 0 |
| 36 | DP | 1114 | 0 | 1187 | 194 | 0 |
| 37 | BQ | 1065 | 0 | 1114 | 82 | 0 |
| 37 | DQ | 1065 | 0 | 1114 | 83 | 0 |
| 38 | BR | 960 | 0 | 1021 | 84 | 0 |
| 38 | DR | 960 | 0 | 1021 | 77 | 0 |
| 39 | BS | 771 | 0 | 832 | 60 | 0 |
| 39 | DS | 771 | 0 | 832 | 60 | 0 |
| 40 | BT | 1144 | 0 | 1211 | 76 | 0 |
| 40 | DT | 1144 | 0 | 1211 | 74 | 0 |
| 41 | BU | 964 | 0 | 1022 | 83 | 0 |
| 41 | DU | 964 | 0 | 1022 | 78 | 0 |
| 42 | BV | 779 | 0 | 852 | 83 | 0 |
| 42 | DV | 779 | 0 | 852 | 79 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 43 | BW | 891 | 0 | 951 | 58 | 0 |
| 43 | DW | 891 | 0 | 951 | 61 | 0 |
| 44 | BX | 726 | 0 | 778 | 64 | 0 |
| 44 | DX | 726 | 0 | 778 | 65 | 0 |
| 45 | BY | 776 | 0 | 870 | 80 | 0 |
| 45 | DY | 776 | 0 | 870 | 81 | 0 |
| 46 | BZ | 1483 | 0 | 1507 | 89 | 0 |
| 46 | DZ | 1483 | 0 | 1507 | 89 | 0 |
| 47 | B0 | 605 | 0 | 628 | 36 | 0 |
| 47 | D0 | 605 | 0 | 628 | 32 | 0 |
| 48 | B1 | 695 | 0 | 764 | 67 | 0 |
| 48 | D1 | 695 | 0 | 764 | 77 | 0 |
| 49 | B2 | 521 | 0 | 575 | 52 | 0 |
| 49 | D2 | 521 | 0 | 575 | 56 | 0 |
| 50 | B3 | 468 | 0 | 523 | 27 | 0 |
| 50 | D3 | 468 | 0 | 523 | 24 | 0 |
| 51 | B4 | 226 | 0 | 227 | 13 | 0 |
| 51 | D4 | 226 | 0 | 225 | 15 | 0 |
| 52 | B5 | 405 | 0 | 420 | 27 | 0 |
| 52 | D5 | 405 | 0 | 420 | 31 | 0 |
| 53 | B6 | 381 | 0 | 391 | 28 | 0 |
| 53 | D6 | 381 | 0 | 391 | 26 | 0 |
| 54 | B7 | 419 | 0 | 467 | 22 | 0 |
| 54 | D7 | 419 | 0 | 467 | 22 | 0 |
| 55 | B8 | 508 | 0 | 576 | 58 | 0 |
| 55 | D8 | 508 | 0 | 576 | 60 | 0 |
| 56 | AA | 393 | 0 | 0 | 0 | 0 |
| 56 | AC | 1 | 0 | 0 | 0 | 0 |
| 56 | AG | 1 | 0 | 0 | 0 | 0 |
| 56 | AO | 1 | 0 | 0 | 0 | 0 |
| 56 | AQ | 1 | 0 | 0 | 0 | 0 |
| 56 | AT | 3 | 0 | 0 | 0 | 0 |
| 56 | AV | 1 | 0 | 0 | 0 | 0 |
| 56 | AW | 18 | 0 | 0 | 0 | 0 |
| 56 | AY | 3 | 0 | 0 | 0 | 0 |
| 56 | B0 | 2 | 0 | 0 | 0 | 0 |
| 56 | B1 | 1 | 0 | 0 | 0 | 0 |
| 56 | B3 | 1 | 0 | 0 | 0 | 0 |
| 56 | B5 | 1 | 0 | 0 | 0 | 0 |
| 56 | B8 | 2 | 0 | 0 | 0 | 0 |
| 56 | BA | 824 | 0 | 0 | 0 | 0 |
| 56 | BB | 23 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 56 | BD | 1 | 0 | 0 | 0 | 0 |
| 56 | BE | 1 | 0 | 0 | 0 | 0 |
| 56 | BF | 1 | 0 | 0 | 0 | 0 |
| 56 | BP | 1 | 0 | 0 | 0 | 0 |
| 56 | BT | 1 | 0 | 0 | 0 | 0 |
| 56 | BX | 2 | 0 | 0 | 0 | 0 |
| 56 | BY | 1 | 0 | 0 | 0 | 0 |
| 56 | CA | 326 | 0 | 0 | 0 | 0 |
| 56 | CD | 1 | 0 | 0 | 0 | 0 |
| 56 | CM | 1 | 0 | 0 | 0 | 0 |
| 56 | CR | 1 | 0 | 0 | 0 | 0 |
| 56 | CV | 2 | 0 | 0 | 0 | 0 |
| 56 | CW | 16 | 0 | 0 | 0 | 0 |
| 56 | CY | 2 | 0 | 0 | 0 | 0 |
| 56 | D0 | 1 | 0 | 0 | 0 | 0 |
| 56 | D1 | 1 | 0 | 0 | 0 | 0 |
| 56 | D5 | 3 | 0 | 0 | 0 | 0 |
| 56 | D7 | 2 | 0 | 0 | 0 | 0 |
| 56 | DA | 732 | 0 | 0 | 0 | 0 |
| 56 | DB | 20 | 0 | 0 | 0 | 0 |
| 56 | DD | 1 | 0 | 0 | 0 | 0 |
| 56 | DE | 1 | 0 | 0 | 0 | 0 |
| 56 | DF | 2 | 0 | 0 | 0 | 0 |
| 56 | DH | 1 | 0 | 0 | 0 | 0 |
| 56 | DI | 2 | 0 | 0 | 0 | 0 |
| 56 | DN | 1 | 0 | 0 | 0 | 0 |
| 56 | DP | 2 | 0 | 0 | 0 | 0 |
| 56 | DQ | 4 | 0 | 0 | 0 | 0 |
| 56 | DV | 1 | 0 | 0 | 0 | 0 |
| 56 | DW | 2 | 0 | 0 | 0 | 0 |
| 56 | DX | 1 | 0 | 0 | 0 | 0 |
| 57 | AD | 1 | 0 | 0 | 0 | 0 |
| 57 | AN | 1 | 0 | 0 | 0 | 0 |
| 57 | CD | 1 | 0 | 0 | 0 | 0 |
| 57 | CN | 1 | 0 | 0 | 0 | 0 |
| All | All | 294074 | 0 | 200805 | 10187 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 10187 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CA:559:A:H4' | 1:CA:560:U:H3' | 1.26 | 1.16 |
| 25:BA:1899:G:N2 | 25:BA:1902:C:H41 | 1.43 | 1.15 |
| 45:DY:76:CYS:SG | 45:DY:77:PRO:HD2 | 1.91 | 1.11 |
| 25:DA:1899:G:N2 | 25:DA:1902:C:H41 | 1.48 | 1.10 |
| 1:AA:559:A:H4' | 1:AA:560:U:H3' | 1.26 | 1.09 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | AY | 360/362 (99%) | 301 (84%) | 41 (11%) | 18 (5%) | 2 | 14 |
| 4 | CY | 360/362 (99%) | 301 (84%) | 42 (12%) | 17 (5%) | 2 | 15 |
| 5 | AB | 232/234 (99%) | 185 (80%) | 37 (16%) | 10 (4%) | 2 | 17 |
| 5 | CB | 232/234 (99%) | 184 (79%) | 38 (16%) | 10 (4%) | 2 | 17 |
| 6 | AC | 204/206 (99%) | 144 (71%) | 40 (20%) | 20 (10%) | 0 | 4 |
| 6 | CC | 204/206 (99%) | 145 (71%) | 38 (19%) | 21 (10%) | 0 | 3 |
| 7 | AD | 206/208 (99%) | 165 (80%) | 32 (16%) | 9 (4%) | 2 | 16 |
| 7 | CD | 206/208 (99%) | 166 (81%) | 29 (14%) | 11 (5%) | 2 | 13 |
| 8 | AE | 149/151 (99%) | 113 (76%) | 32 (22%) | 4 (3%) | 5 | 26 |
| 8 | CE | 149/151 (99%) | 116 (78%) | 29 (20%) | 4 (3%) | 5 | 26 |
| 9 | AF | 99/101 (98%) | 82 (83%) | 16 (16%) | 1 (1%) | 15 | 46 |
| 9 | CF | 99/101 (98%) | 82 (83%) | 16 (16%) | 1 (1%) | 15 | 46 |
| 10 | AG | 153/155 (99%) | 136 (89%) | 13 (8%) | 4 (3%) | 5 | 26 |
| 10 | CG | 153/155 (99%) | 136 (89%) | 13 (8%) | 4 (3%) | 5 | 26 |
| 11 | AH | 136/138 (99%) | 111 (82%) | 23 (17%) | 2 (2%) | 10 | 36 |
| 11 | CH | 136/138 (99%) | 113 (83%) | 21 (15%) | 2 (2%) | 10 | 36 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 12 | AI | 125/127 (98%) | 90 (72%) | 27 (22%) | 8 (6%) | 1 | 9 |
| 12 | CI | 125/127 (98%) | 90 (72%) | 27 (22%) | 8 (6%) | 1 | 9 |
| 13 | AJ | 96/98 (98%) | 72 (75%) | 18 (19%) | 6 (6%) | 1 | 9 |
| 13 | CJ | 96/98 (98%) | 72 (75%) | 18 (19%) | 6 (6%) | 1 | 9 |
| 14 | AK | 112/114 (98%) | 93 (83%) | 14 (12%) | 5 (4%) | 2 | 16 |
| 14 | CK | 112/114 (98%) | 93 (83%) | 15 (13%) | 4 (4%) | 3 | 21 |
| 15 | AL | 120/122 (98%) | 94 (78%) | 21 (18%) | 5 (4%) | 3 | 18 |
| 15 | CL | 120/122 (98%) | 93 (78%) | 22 (18%) | 5 (4%) | 3 | 18 |
| 16 | AM | 115/117 (98%) | 97 (84%) | 15 (13%) | 3 (3%) | 5 | 26 |
| 16 | CM | 115/117 (98%) | 97 (84%) | 15 (13%) | 3 (3%) | 5 | 26 |
| 17 | AN | 58/60 (97%) | 47 (81%) | 9 (16%) | 2 (3%) | 3 | 21 |
| 17 | CN | 58/60 (97%) | 43 (74%) | 11 (19%) | 4 (7%) | 1 | 8 |
| 18 | AO | 86/88 (98%) | 75 (87%) | 8 (9%) | 3 (4%) | 3 | 21 |
| 18 | CO | 86/88 (98%) | 75 (87%) | 8 (9%) | 3 (4%) | 3 | 21 |
| 19 | AP | 81/83 (98%) | 62 (76%) | 16 (20%) | 3 (4%) | 3 | 20 |
| 19 | CP | 81/83 (98%) | 61 (75%) | 17 (21%) | 3 (4%) | 3 | 20 |
| 20 | AQ | 97/99 (98%) | 82 (84%) | 11 (11%) | 4 (4%) | 3 | 18 |
| 20 | CQ | 97/99 (98%) | 83 (86%) | 10 (10%) | 4 (4%) | 3 | 18 |
| 21 | AR | 68/70 (97%) | 49 (72%) | 17 (25%) | 2 (3%) | 4 | 24 |
| 21 | CR | 68/70 (97%) | 50 (74%) | 16 (24%) | 2 (3%) | 4 | 24 |
| 22 | AS | 76/78 (97%) | 53 (70%) | 15 (20%) | 8 (10%) | 0 | 3 |
| 22 | CS | 76/78 (97%) | 53 (70%) | 15 (20%) | 8 (10%) | 0 | 3 |
| 23 | AT | 97/99 (98%) | 75 (77%) | 14 (14%) | 8 (8%) | 1 | 5 |
| 23 | CT | 97/99 (98%) | 75 (77%) | 14 (14%) | 8 (8%) | 1 | 5 |
| 24 | AU | 22/24 (92%) | 13 (59%) | 7 (32%) | 2 (9%) | 1 | 4 |
| 24 | CU | 22/24 (92%) | 13 (59%) | 7 (32%) | 2 (9%) | 1 | 4 |
| 27 | BD | 269/271 (99%) | 227 (84%) | 29 (11%) | 13 (5%) | 2 | 15 |
| 27 | DD | 269/271 (99%) | 227 (84%) | 29 (11%) | 13 (5%) | 2 | 15 |
| 28 | BE | 202/204 (99%) | 167 (83%) | 26 (13%) | 9 (4%) | 2 | 16 |
| 28 | DE | 202/204 (99%) | 165 (82%) | 27 (13%) | 10 (5%) | 2 | 14 |
| 29 | BF | 200/202 (99%) | 172 (86%) | 21 (10%) | 7 (4%) | 3 | 21 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 29 | DF | 200/202 (99%) | 171 (86%) | 24 (12%) | 5 (2%) | 5 | 26 |
| 30 | BG | 179/181 (99%) | 141 (79%) | 28 (16%) | 10 (6%) | 2 | 12 |
| 30 | DG | 179/181 (99%) | 141 (79%) | 28 (16%) | 10 (6%) | 2 | 12 |
| 31 | BH | 157/159 (99%) | 130 (83%) | 19 (12%) | 8 (5%) | 2 | 14 |
| 31 | DH | 157/159 (99%) | 131 (83%) | 18 (12%) | 8 (5%) | 2 | 14 |
| 32 | BI | 143/145 (99%) | 113 (79%) | 25 (18%) | 5 (4%) | 3 | 21 |
| 32 | DI | 143/145 (99%) | 115 (80%) | 23 (16%) | 5 (4%) | 3 | 21 |
| 33 | BK | 145/147 (99%) | 99 (68%) | 41 (28%) | 5 (3%) | 3 | 21 |
| 33 | DK | 145/147 (99%) | 103 (71%) | 31 (21%) | 11 (8%) | 1 | 6 |
| 34 | BN | 135/137 (98%) | 96 (71%) | 29 (22%) | 10 (7%) | 1 | 7 |
| 34 | DN | 135/137 (98%) | 96 (71%) | 29 (22%) | 10 (7%) | 1 | 7 |
| 35 | BO | 120/122 (98%) | 103 (86%) | 14 (12%) | 3 (2%) | 5 | 26 |
| 35 | DO | 120/122 (98%) | 103 (86%) | 14 (12%) | 3 (2%) | 5 | 26 |
| 36 | BP | 144/146 (99%) | 91 (63%) | 32 (22%) | 21 (15%) | 0 | 1 |
| 36 | DP | 144/146 (99%) | 93 (65%) | 31 (22%) | 20 (14%) | 0 | 1 |
| 37 | BQ | 132/134 (98%) | 104 (79%) | 22 (17%) | 6 (4%) | 2 | 16 |
| 37 | DQ | 132/134 (98%) | 105 (80%) | 22 (17%) | 5 (4%) | 3 | 19 |
| 38 | BR | 115/117 (98%) | 96 (84%) | 17 (15%) | 2 (2%) | 9 | 34 |
| 38 | DR | 115/117 (98%) | 97 (84%) | 16 (14%) | 2 (2%) | 9 | 34 |
| 39 | BS | 96/98 (98%) | 62 (65%) | 20 (21%) | 14 (15%) | 0 | 1 |
| 39 | DS | 96/98 (98%) | 60 (62%) | 22 (23%) | 14 (15%) | 0 | 1 |
| 40 | BT | 135/137 (98%) | 100 (74%) | 24 (18%) | 11 (8%) | 1 | 5 |
| 40 | DT | 135/137 (98%) | 101 (75%) | 23 (17%) | 11 (8%) | 1 | 5 |
| 41 | BU | 115/117 (98%) | 99 (86%) | 13 (11%) | 3 (3%) | 5 | 26 |
| 41 | DU | 115/117 (98%) | 101 (88%) | 11 (10%) | 3 (3%) | 5 | 26 |
| 42 | BV | 99/101 (98%) | 75 (76%) | 18 (18%) | 6 (6%) | 1 | 10 |
| 42 | DV | 99/101 (98%) | 74 (75%) | 19 (19%) | 6 (6%) | 1 | 10 |
| 43 | BW | 110/112 (98%) | 98 (89%) | 12 (11%) | 0 | 100 | 100 |
| 43 | DW | 110/112 (98%) | 95 (86%) | 15 (14%) | 0 | 100 | 100 |
| 44 | BX | 90/92 (98%) | 82 (91%) | 7 (8%) | 1 (1%) | 14 | 44 |
| 44 | DX | 90/92 (98%) | 81 (90%) | 8 (9%) | 1 (1%) | 14 | 44 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 45 | BY | 98/100 (98%) | 68 (69%) | 14 (14%) | 16 (16%) | 0 | 0 |
| 45 | DY | 98/100 (98%) | 68 (69%) | 13 (13%) | 17 (17%) | 0 | 0 |
| 46 | BZ | 185/187 (99%) | 158 (85%) | 21 (11%) | 6 (3%) | 4 | 22 |
| 46 | DZ | 185/187 (99%) | 158 (85%) | 21 (11%) | 6 (3%) | 4 | 22 |
| 47 | B0 | 74/76 (97%) | 63 (85%) | 7 (10%) | 4 (5%) | 2 | 13 |
| 47 | D0 | 74/76 (97%) | 63 (85%) | 7 (10%) | 4 (5%) | 2 | 13 |
| 48 | B1 | 86/88 (98%) | 59 (69%) | 14 (16%) | 13 (15%) | 0 | 0 |
| 48 | D1 | 86/88 (98%) | 59 (69%) | 14 (16%) | 13 (15%) | 0 | 0 |
| 49 | B2 | 60/62 (97%) | 45 (75%) | 7 (12%) | 8 (13%) | 0 | 1 |
| 49 | D2 | 60/62 (97%) | 45 (75%) | 7 (12%) | 8 (13%) | 0 | 1 |
| 50 | B3 | 57/59 (97%) | 51 (90%) | 5 (9%) | 1 (2%) | 8 | 32 |
| 50 | D3 | 57/59 (97%) | 51 (90%) | 5 (9%) | 1 (2%) | 8 | 32 |
| 51 | B4 | 28/30 (93%) | 16 (57%) | 10 (36%) | 2 (7%) | 1 | 7 |
| 51 | D4 | 28/30 (93%) | 16 (57%) | 10 (36%) | 2 (7%) | 1 | 7 |
| 52 | B5 | 50/52 (96%) | 42 (84%) | 5 (10%) | 3 (6%) | 1 | 10 |
| 52 | D5 | 50/52 (96%) | 42 (84%) | 5 (10%) | 3 (6%) | 1 | 10 |
| 53 | B6 | 42/44 (96%) | 29 (69%) | 8 (19%) | 5 (12%) | 0 | 3 |
| 53 | D6 | 42/44 (96%) | 29 (69%) | 8 (19%) | 5 (12%) | 0 | 3 |
| 54 | B7 | 46/48 (96%) | 42 (91%) | 4 (9%) | 0 | 100 | 100 |
| 54 | D7 | 46/48 (96%) | 43 (94%) | 3 (6%) | 0 | 100 | 100 |
| 55 | B8 | 61/63 (97%) | 47 (77%) | 7 (12%) | 7 (12%) | 0 | 3 |
| 55 | D8 | 61/63 (97%) | 47 (77%) | 7 (12%) | 7 (12%) | 0 | 3 |
| All | All | 12130/12330 (98%) | 9635 (79%) | 1836 (15%) | 659 (5%) | 2 | 13 |

5 of 659 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | AY | 55 | PRO |
| 4 | AY | 95 | GLU |
| 4 | AY | 175 | ALA |
| 4 | AY | 225 | PRO |
| 4 | AY | 315 | VAL |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | AY | 305/305 (100%) | 278 (91%) | 27 (9%) | 9 | 33 |
| 4 | CY | 305/305 (100%) | 277 (91%) | 28 (9%) | 9 | 31 |
| 5 | AB | 202/202 (100%) | 189 (94%) | 13 (6%) | 17 | 47 |
| 5 | CB | 202/202 (100%) | 188 (93%) | 14 (7%) | 15 | 45 |
| 6 | AC | 160/160 (100%) | 147 (92%) | 13 (8%) | 11 | 38 |
| 6 | CC | 160/160 (100%) | 147 (92%) | 13 (8%) | 11 | 38 |
| 7 | AD | 180/180 (100%) | 149 (83%) | 31 (17%) | 2 | 8 |
| 7 | CD | 180/180 (100%) | 162 (90%) | 18 (10%) | 7 | 27 |
| 8 | AE | 116/116 (100%) | 108 (93%) | 8 (7%) | 15 | 45 |
| 8 | CE | 116/116 (100%) | 108 (93%) | 8 (7%) | 15 | 45 |
| 9 | AF | 90/90 (100%) | 85 (94%) | 5 (6%) | 21 | 51 |
| 9 | CF | 90/90 (100%) | 85 (94%) | 5 (6%) | 21 | 51 |
| 10 | AG | 126/126 (100%) | 123 (98%) | 3 (2%) | 49 | 74 |
| 10 | CG | 126/126 (100%) | 123 (98%) | 3 (2%) | 49 | 74 |
| 11 | AH | 119/119 (100%) | 111 (93%) | 8 (7%) | 16 | 46 |
| 11 | CH | 119/119 (100%) | 110 (92%) | 9 (8%) | 13 | 41 |
| 12 | AI | 98/98 (100%) | 88 (90%) | 10 (10%) | 7 | 26 |
| 12 | CI | 98/98 (100%) | 88 (90%) | 10 (10%) | 7 | 26 |
| 13 | AJ | 88/88 (100%) | 78 (89%) | 10 (11%) | 5 | 21 |
| 13 | CJ | 88/88 (100%) | 78 (89%) | 10 (11%) | 5 | 21 |
| 14 | AK | 86/86 (100%) | 82 (95%) | 4 (5%) | 26 | 57 |
| 14 | CK | 86/86 (100%) | 82 (95%) | 4 (5%) | 26 | 57 |
| 15 | AL | 103/103 (100%) | 95 (92%) | 8 (8%) | 12 | 39 |
| 15 | CL | 103/103 (100%) | 95 (92%) | 8 (8%) | 12 | 39 |
| 16 | AM | 94/94 (100%) | 86 (92%) | 8 (8%) | 10 | 35 |
| 16 | CM | 94/94 (100%) | 86 (92%) | 8 (8%) | 10 | 35 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 17 | AN | 49/49 (100%) | 44 (90%) | 5 (10%) | 7 | 26 |
| 17 | CN | 49/49 (100%) | 47 (96%) | 2 (4%) | 30 | 59 |
| 18 | AO | 79/79 (100%) | 71 (90%) | 8 (10%) | 7 | 27 |
| 18 | CO | 79/79 (100%) | 71 (90%) | 8 (10%) | 7 | 27 |
| 19 | AP | 72/72 (100%) | 65 (90%) | 7 (10%) | 8 | 28 |
| 19 | CP | 72/72 (100%) | 66 (92%) | 6 (8%) | 11 | 36 |
| 20 | AQ | 94/94 (100%) | 89 (95%) | 5 (5%) | 22 | 52 |
| 20 | CQ | 94/94 (100%) | 89 (95%) | 5 (5%) | 22 | 52 |
| 21 | AR | 61/61 (100%) | 60 (98%) | 1 (2%) | 62 | 81 |
| 21 | CR | 61/61 (100%) | 60 (98%) | 1 (2%) | 62 | 81 |
| 22 | AS | 69/69 (100%) | 57 (83%) | 12 (17%) | 2 | 7 |
| 22 | CS | 69/69 (100%) | 57 (83%) | 12 (17%) | 2 | 7 |
| 23 | AT | 76/76 (100%) | 72 (95%) | 4 (5%) | 22 | 52 |
| 23 | CT | 76/76 (100%) | 72 (95%) | 4 (5%) | 22 | 52 |
| 24 | AU | 19/19 (100%) | 18 (95%) | 1 (5%) | 22 | 52 |
| 24 | CU | 19/19 (100%) | 18 (95%) | 1 (5%) | 22 | 52 |
| 27 | BD | 213/213 (100%) | 188 (88%) | 25 (12%) | 5 | 20 |
| 27 | DD | 213/213 (100%) | 188 (88%) | 25 (12%) | 5 | 20 |
| 28 | BE | 165/165 (100%) | 149 (90%) | 16 (10%) | 8 | 28 |
| 28 | DE | 165/165 (100%) | 150 (91%) | 15 (9%) | 9 | 32 |
| 29 | BF | 161/161 (100%) | 145 (90%) | 16 (10%) | 8 | 27 |
| 29 | DF | 161/161 (100%) | 145 (90%) | 16 (10%) | 8 | 27 |
| 30 | BG | 155/155 (100%) | 140 (90%) | 15 (10%) | 8 | 28 |
| 30 | DG | 155/155 (100%) | 140 (90%) | 15 (10%) | 8 | 28 |
| 31 | BH | 132/132 (100%) | 123 (93%) | 9 (7%) | 16 | 45 |
| 31 | DH | 132/132 (100%) | 124 (94%) | 8 (6%) | 18 | 48 |
| 32 | BI | 122/122 (100%) | 111 (91%) | 11 (9%) | 9 | 32 |
| 32 | DI | 122/122 (100%) | 111 (91%) | 11 (9%) | 9 | 32 |
| 33 | BK | 111/111 (100%) | 98 (88%) | 13 (12%) | 5 | 20 |
| 33 | DK | 111/111 (100%) | 105 (95%) | 6 (5%) | 22 | 52 |
| 34 | BN | 116/116 (100%) | 99 (85%) | 17 (15%) | 3 | 12 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 34 | DN | 116/116 (100%) | 99 (85%) | 17 (15%) | 3 | 12 |
| 35 | BO | 100/100 (100%) | 95 (95%) | 5 (5%) | 24 | 54 |
| 35 | DO | 100/100 (100%) | 94 (94%) | 6 (6%) | 19 | 49 |
| 36 | BP | 112/112 (100%) | 87 (78%) | 25 (22%) | 1 | 2 |
| 36 | DP | 112/112 (100%) | 87 (78%) | 25 (22%) | 1 | 2 |
| 37 | BQ | 105/105 (100%) | 94 (90%) | 11 (10%) | 7 | 25 |
| 37 | DQ | 105/105 (100%) | 95 (90%) | 10 (10%) | 8 | 29 |
| 38 | BR | 100/100 (100%) | 86 (86%) | 14 (14%) | 3 | 13 |
| 38 | DR | 100/100 (100%) | 85 (85%) | 15 (15%) | 3 | 12 |
| 39 | BS | 77/77 (100%) | 66 (86%) | 11 (14%) | 3 | 13 |
| 39 | DS | 77/77 (100%) | 66 (86%) | 11 (14%) | 3 | 13 |
| 40 | BT | 121/121 (100%) | 101 (84%) | 20 (16%) | 2 | 9 |
| 40 | DT | 121/121 (100%) | 99 (82%) | 22 (18%) | 1 | 6 |
| 41 | BU | 93/93 (100%) | 85 (91%) | 8 (9%) | 10 | 35 |
| 41 | DU | 93/93 (100%) | 85 (91%) | 8 (9%) | 10 | 35 |
| 42 | BV | 82/82 (100%) | 67 (82%) | 15 (18%) | 1 | 5 |
| 42 | DV | 82/82 (100%) | 67 (82%) | 15 (18%) | 1 | 5 |
| 43 | BW | 91/91 (100%) | 81 (89%) | 10 (11%) | 6 | 23 |
| 43 | DW | 91/91 (100%) | 81 (89%) | 10 (11%) | 6 | 23 |
| 44 | BX | 74/74 (100%) | 69 (93%) | 5 (7%) | 16 | 45 |
| 44 | DX | 74/74 (100%) | 69 (93%) | 5 (7%) | 16 | 45 |
| 45 | BY | 84/84 (100%) | 78 (93%) | 6 (7%) | 14 | 44 |
| 45 | DY | 84/84 (100%) | 78 (93%) | 6 (7%) | 14 | 44 |
| 46 | BZ | 162/162 (100%) | 153 (94%) | 9 (6%) | 21 | 51 |
| 46 | DZ | 162/162 (100%) | 153 (94%) | 9 (6%) | 21 | 51 |
| 47 | B0 | 61/61 (100%) | 52 (85%) | 9 (15%) | 3 | 12 |
| 47 | D0 | 61/61 (100%) | 52 (85%) | 9 (15%) | 3 | 12 |
| 48 | B1 | 73/73 (100%) | 58 (80%) | 15 (20%) | 1 | 3 |
| 48 | D1 | 73/73 (100%) | 58 (80%) | 15 (20%) | 1 | 3 |
| 49 | B2 | 58/58 (100%) | 52 (90%) | 6 (10%) | 7 | 26 |
| 49 | D2 | 58/58 (100%) | 51 (88%) | 7 (12%) | 5 | 18 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 50 | B3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 8 28 |
| 50 | D3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 8 28 |
| 51 | B4 | 27/27 (100%) | 26 (96%) | 1 (4%) | 34 62 |
| 51 | D4 | 27/27 (100%) | 26 (96%) | 1 (4%) | 34 62 |
| 52 | B5 | 45/45 (100%) | 42 (93%) | 3 (7%) | 16 46 |
| 52 | D5 | 45/45 (100%) | 42 (93%) | 3 (7%) | 16 46 |
| 53 | B6 | 43/43 (100%) | 37 (86%) | 6 (14%) | 3 13 |
| 53 | D6 | 43/43 (100%) | 37 (86%) | 6 (14%) | 3 13 |
| 54 | B7 | 41/41 (100%) | 34 (83%) | 7 (17%) | 2 8 |
| 54 | D7 | 41/41 (100%) | 34 (83%) | 7 (17%) | 2 8 |
| 55 | B8 | 53/53 (100%) | 45 (85%) | 8 (15%) | 3 12 |
| 55 | D8 | 53/53 (100%) | 45 (85%) | 8 (15%) | 3 12 |
| All | All | 10228/10228 (100%) | 9223 (90%) | 1005 (10%) | 8 28 |

5 of 1005 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | B1 | 18 | ILE |
| 40 | DT | 111 | ARG |
| 7 | CD | 68 | TYR |
| 40 | DT | 62 | THR |
| 47 | D0 | 20 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | DR | 53 | HIS |
| 41 | DU | 72 | HIS |
| 50 | D3 | 52 | HIS |
| 41 | BU | 44 | ASN |
| 38 | BR | 91 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | AA | 1503/1504 (99%) | 216 (14%) | 20 (1%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | CA | 1503/1504 (99%) | 217 (14%) | 20 (1%) |
| 2 | AV | 9/10 (90%) | 2 (22%) | 0 |
| 2 | CV | 9/10 (90%) | 2 (22%) | 0 |
| 25 | BA | 2787/2879 (96%) | 431 (15%) | 19 (0%) |
| 25 | DA | 2787/2879 (96%) | 432 (15%) | 19 (0%) |
| 26 | BB | 118/119 (99%) | 15 (12%) | 0 |
| 26 | DB | 118/119 (99%) | 15 (12%) | 0 |
| 3 | AW | 76/77 (98%) | 7 (9%) | 0 |
| 3 | CW | 76/77 (98%) | 7 (9%) | 0 |
| All | All | 8986/9178 (97%) | 1344 (14%) | 78 (0%) |

5 of 1344 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 41 | G |

5 of 78 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CA | 1362(A) | C |
| 25 | DA | 1786 | A |
| 25 | DA | 352 | G |
| 25 | DA | 1022 | G |
| 25 | DA | 2447 | G |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2414 ligands modelled in this entry, 2414 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | AA | 1504/1504 (100%) | 0.20 | 37 (2%) | 57 | 55 | 46, 108, 215, 381 | 0 |
| 1 | CA | 1504/1504 (100%) | 0.36 | 40 (2%) | 54 | 53 | 48, 122, 235, 451 | 0 |
| 2 | AV | 10/10 (100%) | 1.06 | 1 (10%) | 7 | 8 | 76, 120, 198, 250 | 0 |
| 2 | CV | 10/10 (100%) | 0.97 | 3 (30%) | 0 | 0 | 74, 123, 204, 230 | 0 |
| 3 | AW | 77/77 (100%) | 0.28 | 1 (1%) | 77 | 76 | 73, 106, 160, 212 | 0 |
| 3 | CW | 77/77 (100%) | 0.14 | 1 (1%) | 77 | 76 | 65, 104, 140, 219 | 0 |
| 4 | AY | 362/362 (100%) | 1.93 | 128 (35%) | 0 | 0 | 72, 164, 304, 366 | 0 |
| 4 | CY | 362/362 (100%) | 2.14 | 131 (36%) | 0 | 0 | 69, 180, 326, 473 | 0 |
| 5 | AB | 234/234 (100%) | 1.25 | 53 (22%) | 0 | 1 | 84, 152, 249, 335 | 0 |
| 5 | CB | 234/234 (100%) | 1.23 | 63 (26%) | 0 | 0 | 84, 173, 267, 348 | 0 |
| 6 | AC | 206/206 (100%) | 0.57 | 25 (12%) | 4 | 5 | 69, 141, 224, 325 | 0 |
| 6 | CC | 206/206 (100%) | 0.53 | 22 (10%) | 6 | 7 | 88, 154, 252, 385 | 0 |
| 7 | AD | 208/208 (100%) | 0.25 | 4 (1%) | 66 | 65 | 46, 104, 158, 201 | 0 |
| 7 | CD | 208/208 (100%) | 0.59 | 19 (9%) | 9 | 10 | 78, 146, 224, 346 | 0 |
| 8 | AE | 151/151 (100%) | 0.29 | 13 (8%) | 10 | 12 | 61, 102, 156, 274 | 0 |
| 8 | CE | 151/151 (100%) | 0.62 | 15 (9%) | 7 | 8 | 84, 125, 202, 274 | 0 |
| 9 | AF | 101/101 (100%) | 0.72 | 17 (16%) | 1 | 2 | 92, 150, 222, 283 | 0 |
| 9 | CF | 101/101 (100%) | 0.28 | 10 (9%) | 7 | 8 | 60, 104, 157, 216 | 0 |
| 10 | AG | 155/155 (100%) | 0.60 | 17 (10%) | 5 | 6 | 81, 147, 220, 290 | 0 |
| 10 | CG | 155/155 (100%) | 0.56 | 19 (12%) | 4 | 5 | 91, 147, 209, 352 | 0 |
| 11 | AH | 138/138 (100%) | 0.27 | 7 (5%) | 28 | 28 | 58, 110, 163, 235 | 0 |
| 11 | CH | 138/138 (100%) | 0.54 | 9 (6%) | 18 | 20 | 74, 130, 191, 271 | 0 |
| 12 | AI | 127/127 (100%) | 1.61 | 41 (32%) | 0 | 0 | 94, 172, 247, 329 | 0 |
| 12 | CI | 127/127 (100%) | 1.65 | 40 (31%) | 0 | 0 | 85, 174, 242, 307 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 13 | AJ | 98/98 (100%) | 1.79 | 34 (34%) | 0 | 0 | 85, 172, 278, 357 | 0 |
| 13 | CJ | 98/98 (100%) | 2.15 | 37 (37%) | 0 | 0 | 86, 197, 311, 435 | 0 |
| 14 | AK | 114/114 (100%) | 0.84 | 19 (16%) | 1 | 2 | 59, 110, 172, 233 | 0 |
| 14 | CK | 114/114 (100%) | 0.47 | 7 (6%) | 21 | 22 | 55, 99, 165, 372 | 0 |
| 15 | AL | 122/122 (100%) | 0.23 | 3 (2%) | 57 | 55 | 44, 85, 148, 192 | 0 |
| 15 | CL | 122/122 (100%) | 0.25 | 3 (2%) | 57 | 55 | 48, 99, 149, 268 | 0 |
| 16 | AM | 117/117 (100%) | 0.64 | 15 (12%) | 3 | 4 | 81, 166, 258, 377 | 0 |
| 16 | CM | 117/117 (100%) | 1.12 | 20 (17%) | 1 | 2 | 109, 159, 244, 340 | 0 |
| 17 | AN | 60/60 (100%) | 0.82 | 10 (16%) | 1 | 2 | 72, 128, 174, 224 | 0 |
| 17 | CN | 60/60 (100%) | 1.05 | 11 (18%) | 1 | 1 | 80, 151, 191, 265 | 0 |
| 18 | AO | 88/88 (100%) | 0.46 | 2 (2%) | 60 | 59 | 67, 109, 157, 188 | 0 |
| 18 | CO | 88/88 (100%) | 0.12 | 1 (1%) | 80 | 79 | 58, 106, 146, 168 | 0 |
| 19 | AP | 83/83 (100%) | 0.62 | 4 (4%) | 30 | 31 | 65, 99, 135, 245 | 0 |
| 19 | CP | 83/83 (100%) | 1.39 | 26 (31%) | 0 | 0 | 78, 139, 192, 243 | 0 |
| 20 | AQ | 99/99 (100%) | 0.33 | 4 (4%) | 38 | 37 | 63, 102, 157, 211 | 0 |
| 20 | CQ | 99/99 (100%) | 0.67 | 6 (6%) | 21 | 22 | 76, 116, 167, 283 | 0 |
| 21 | AR | 70/70 (100%) | 2.07 | 28 (40%) | 0 | 0 | 76, 134, 215, 266 | 0 |
| 21 | CR | 70/70 (100%) | 0.90 | 10 (14%) | 2 | 3 | 70, 112, 182, 225 | 0 |
| 22 | AS | 78/78 (100%) | 1.44 | 25 (32%) | 0 | 0 | 113, 164, 229, 318 | 0 |
| 22 | CS | 78/78 (100%) | 1.62 | 28 (35%) | 0 | 0 | 112, 174, 250, 339 | 0 |
| 23 | AT | 99/99 (100%) | 0.84 | 14 (14%) | 2 | 3 | 68, 115, 202, 272 | 0 |
| 23 | CT | 99/99 (100%) | 0.80 | 17 (17%) | 1 | 1 | 84, 134, 222, 336 | 0 |
| 24 | AU | 24/24 (100%) | 3.89 | 23 (95%) | 0 | 0 | 102, 150, 217, 233 | 0 |
| 24 | CU | 24/24 (100%) | 3.60 | 19 (79%) | 0 | 0 | 126, 169, 229, 236 | 0 |
| 25 | BA | 2789/2879 (96%) | 0.12 | 72 (2%) | 56 | 54 | 36, 76, 211, 411 | 0 |
| 25 | DA | 2789/2879 (96%) | 0.06 | 84 (3%) | 50 | 49 | 27, 65, 189, 401 | 0 |
| 26 | BB | 119/119 (100%) | 0.27 | 0 | 100 | 100 | 63, 129, 186, 245 | 0 |
| 26 | DB | 119/119 (100%) | 0.30 | 2 (1%) | 70 | 68 | 73, 119, 167, 276 | 0 |
| 27 | BD | 271/271 (100%) | 0.30 | 13 (4%) | 30 | 31 | 31, 66, 114, 224 | 0 |
| 27 | DD | 271/271 (100%) | -0.01 | 5 (1%) | 68 | 67 | 14, 56, 107, 221 | 0 |
| 28 | BE | 204/204 (100%) | 0.40 | 10 (4%) | 29 | 29 | 35, 82, 148, 377 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | DE | 204/204 (100%) | 0.09 | 5 (2%) 57 55 | 29, 74, 138, 256 | 0 |
| 29 | BF | 202/202 (100%) | 0.01 | 1 (0%) 91 90 | 28, 81, 163, 345 | 0 |
| 29 | DF | 202/202 (100%) | 0.10 | 2 (0%) 82 81 | 13, 69, 145, 300 | 0 |
| 30 | BG | 181/181 (100%) | 1.06 | 40 (22%) 0 1 | 78, 147, 221, 323 | 0 |
| 30 | DG | 181/181 (100%) | 0.75 | 29 (16%) 1 2 | 73, 136, 220, 288 | 0 |
| 31 | BH | 159/159 (100%) | 1.37 | 49 (30%) 0 0 | 86, 172, 263, 376 | 0 |
| 31 | DH | 159/159 (100%) | 0.07 | 7 (4%) 34 34 | 48, 100, 157, 286 | 0 |
| 32 | BI | 145/145 (100%) | 2.16 | 60 (41%) 0 0 | 74, 188, 473, 558 | 0 |
| 32 | DI | 145/145 (100%) | 0.76 | 15 (10%) 6 8 | 47, 118, 209, 462 | 0 |
| 33 | BK | 147/147 (100%) | 5.37 | 122 (82%) 0 0 | 155, 266, 359, 430 | 0 |
| 33 | DK | 147/147 (100%) | 4.51 | 120 (81%) 0 0 | 115, 275, 372, 435 | 0 |
| 34 | BN | 137/137 (100%) | 0.44 | 6 (4%) 34 34 | 51, 89, 139, 220 | 0 |
| 34 | DN | 137/137 (100%) | 0.02 | 0 100 100 | 37, 84, 149, 192 | 0 |
| 35 | BO | 122/122 (100%) | -0.15 | 0 100 100 | 44, 77, 121, 158 | 0 |
| 35 | DO | 122/122 (100%) | -0.15 | 0 100 100 | 31, 67, 117, 149 | 0 |
| 36 | BP | 146/146 (100%) | 0.75 | 13 (8%) 9 11 | 27, 100, 201, 293 | 0 |
| 36 | DP | 146/146 (100%) | 0.55 | 15 (10%) 6 8 | 23, 85, 172, 304 | 0 |
| 37 | BQ | 134/134 (100%) | 0.39 | 7 (5%) 27 27 | 45, 86, 159, 419 | 0 |
| 37 | DQ | 134/134 (100%) | 0.25 | 7 (5%) 27 27 | 41, 83, 175, 469 | 0 |
| 38 | BR | 117/117 (100%) | 0.21 | 1 (0%) 84 83 | 37, 83, 141, 190 | 0 |
| 38 | DR | 117/117 (100%) | 0.13 | 4 (3%) 45 44 | 32, 74, 137, 174 | 0 |
| 39 | BS | 98/98 (100%) | 1.15 | 25 (25%) 0 0 | 61, 135, 212, 245 | 0 |
| 39 | DS | 98/98 (100%) | 0.70 | 14 (14%) 2 3 | 72, 116, 180, 203 | 0 |
| 40 | BT | 137/137 (100%) | 0.51 | 7 (5%) 28 28 | 54, 95, 195, 362 | 0 |
| 40 | DT | 137/137 (100%) | 0.44 | 14 (10%) 6 8 | 34, 90, 194, 343 | 0 |
| 41 | BU | 117/117 (100%) | 0.47 | 6 (5%) 28 28 | 36, 73, 137, 173 | 0 |
| 41 | DU | 117/117 (100%) | 0.57 | 4 (3%) 45 44 | 35, 74, 125, 363 | 0 |
| 42 | BV | 101/101 (100%) | 0.16 | 2 (1%) 65 64 | 49, 93, 159, 283 | 0 |
| 42 | DV | 101/101 (100%) | 0.44 | 9 (8%) 9 11 | 34, 96, 153, 283 | 0 |
| 43 | BW | 112/112 (100%) | -0.09 | 1 (0%) 84 83 | 28, 66, 124, 378 | 0 |
| 43 | DW | 112/112 (100%) | -0.11 | 0 100 100 | 38, 66, 125, 210 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | BX | 92/92 (100%) | 0.08 | 2 (2%) 62 60 | 61, 87, 139, 179 | 0 |
| 44 | DX | 92/92 (100%) | 0.09 | 1 (1%) 80 79 | 34, 66, 106, 168 | 0 |
| 45 | BY | 100/100 (100%) | 1.41 | 23 (23%) 0 1 | 46, 112, 248, 418 | 0 |
| 45 | DY | 100/100 (100%) | 1.11 | 15 (15%) 2 2 | 50, 92, 223, 452 | 0 |
| 46 | BZ | 187/187 (100%) | 0.67 | 17 (9%) 9 10 | 75, 130, 200, 267 | 0 |
| 46 | DZ | 187/187 (100%) | 0.46 | 11 (5%) 22 23 | 56, 123, 182, 260 | 0 |
| 47 | B0 | 76/76 (100%) | 0.30 | 2 (2%) 56 54 | 54, 84, 150, 259 | 0 |
| 47 | D0 | 76/76 (100%) | 0.33 | 3 (3%) 39 38 | 37, 80, 115, 238 | 0 |
| 48 | B1 | 88/88 (100%) | 0.44 | 5 (5%) 23 24 | 46, 90, 156, 264 | 0 |
| 48 | D1 | 88/88 (100%) | 0.36 | 4 (4%) 33 33 | 23, 69, 147, 267 | 0 |
| 49 | B2 | 62/62 (100%) | 0.50 | 6 (9%) 7 9 | 67, 119, 210, 257 | 0 |
| 49 | D2 | 62/62 (100%) | 0.61 | 7 (11%) 5 6 | 33, 75, 176, 304 | 0 |
| 50 | B3 | 59/59 (100%) | 0.86 | 6 (10%) 6 8 | 52, 80, 144, 224 | 0 |
| 50 | D3 | 59/59 (100%) | 0.42 | 3 (5%) 28 28 | 42, 81, 143, 236 | 0 |
| 51 | B4 | 30/30 (100%) | 0.75 | 5 (16%) 1 2 | 107, 184, 297, 335 | 0 |
| 51 | D4 | 30/30 (100%) | 1.43 | 11 (36%) 0 0 | 125, 215, 272, 361 | 0 |
| 52 | B5 | 52/52 (100%) | 0.33 | 3 (5%) 23 24 | 32, 75, 181, 213 | 0 |
| 52 | D5 | 52/52 (100%) | -0.14 | 1 (1%) 66 65 | 20, 77, 172, 269 | 0 |
| 53 | B6 | 44/44 (100%) | 8.21 | 44 (100%) 0 0 | 118, 225, 304, 330 | 0 |
| 53 | D6 | 44/44 (100%) | 7.05 | 42 (95%) 0 0 | 136, 208, 276, 330 | 0 |
| 54 | B7 | 48/48 (100%) | 0.89 | 6 (12%) 3 4 | 35, 60, 131, 156 | 0 |
| 54 | D7 | 48/48 (100%) | 0.27 | 3 (6%) 20 21 | 19, 36, 94, 156 | 0 |
| 55 | B8 | 63/63 (100%) | 0.39 | 2 (3%) 47 46 | 38, 78, 155, 190 | 0 |
| 55 | D8 | 63/63 (100%) | 0.24 | 3 (4%) 30 31 | 33, 62, 142, 213 | 0 |
| All | All | 21328/21508 (99%) | 0.56 | 2078 (9%) 7 9 | 13, 103, 238, 558 | 0 |

The worst 5 of 2078 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 33 | DK | 6 | ALA | 23.8 |
| 53 | B6 | 40 | CYS | 20.9 |
| 33 | DK | 1 | MET | 20.5 |
| 33 | BK | 135 | GLY | 18.7 |
| 53 | D6 | 13 | CYS | 18.6 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3022 | 1/1 | -0.48 | 0.79 | 168,168,168,168 | 0 |
| 56 | MG | AA | 1831 | 1/1 | -0.15 | 1.10 | 203,203,203,203 | 0 |
| 56 | MG | BA | 2918 | 1/1 | -0.08 | 1.68 | 191,191,191,191 | 0 |
| 56 | MG | CA | 1792 | 1/1 | -0.04 | 1.12 | 122,122,122,122 | 0 |
| 56 | MG | AA | 1854 | 1/1 | -0.03 | 0.48 | 187,187,187,187 | 0 |
| 56 | MG | CA | 1746 | 1/1 | 0.01 | 0.15 | 255,255,255,255 | 0 |
| 56 | MG | BA | 3197 | 1/1 | 0.01 | 0.14 | 215,215,215,215 | 0 |
| 56 | MG | CA | 1626 | 1/1 | 0.04 | 0.43 | 109,109,109,109 | 0 |
| 56 | MG | DA | 2921 | 1/1 | 0.04 | 0.21 | 113,113,113,113 | 0 |
| 56 | MG | AA | 1764 | 1/1 | 0.06 | 0.91 | 103,103,103,103 | 0 |
| 56 | MG | CA | 1898 | 1/1 | 0.07 | 0.36 | 126,126,126,126 | 0 |
| 56 | MG | AA | 1780 | 1/1 | 0.07 | 1.15 | 105,105,105,105 | 0 |
| 56 | MG | AT | 201 | 1/1 | 0.09 | 0.32 | 117,117,117,117 | 0 |
| 56 | MG | CA | 1736 | 1/1 | 0.10 | 0.39 | 193,193,193,193 | 0 |
| 56 | MG | CA | 1677 | 1/1 | 0.11 | 1.25 | 138,138,138,138 | 0 |
| 56 | MG | BA | 3078 | 1/1 | 0.14 | 0.76 | 117,117,117,117 | 0 |
| 56 | MG | DA | 3348 | 1/1 | 0.14 | 0.71 | 165,165,165,165 | 0 |
| 56 | MG | AC | 301 | 1/1 | 0.17 | 1.50 | 98,98,98,98 | 0 |
| 56 | MG | BA | 3435 | 1/1 | 0.22 | 1.05 | 112,112,112,112 | 0 |
| 56 | MG | DA | 3484 | 1/1 | 0.26 | 0.59 | 98,98,98,98 | 0 |
| 56 | MG | BA | 3717 | 1/1 | 0.27 | 0.16 | 100,100,100,100 | 0 |
| 56 | MG | BB | 223 | 1/1 | 0.28 | 0.41 | 242,242,242,242 | 0 |
| 56 | MG | CA | 1633 | 1/1 | 0.28 | 0.33 | 143,143,143,143 | 0 |
| 56 | MG | DB | 218 | 1/1 | 0.28 | 0.51 | 111,111,111,111 | 0 |
| 56 | MG | BA | 3713 | 1/1 | 0.29 | 0.98 | 123,123,123,123 | 0 |
| 56 | MG | DA | 3072 | 1/1 | 0.30 | 0.63 | 94,94,94,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1979 | 1/1 | 0.31 | 0.77 | 118,118,118,118 | 0 |
| 56 | MG | CA | 1631 | 1/1 | 0.32 | 1.38 | 119,119,119,119 | 0 |
| 56 | MG | BA | 3153 | 1/1 | 0.32 | 0.33 | 81,81,81,81 | 0 |
| 56 | MG | BA | 3369 | 1/1 | 0.35 | 1.02 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1765 | 1/1 | 0.35 | 0.61 | 74,74,74,74 | 0 |
| 56 | MG | CA | 1809 | 1/1 | 0.35 | 1.24 | 117,117,117,117 | 0 |
| 56 | MG | CA | 1613 | 1/1 | 0.36 | 0.87 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3004 | 1/1 | 0.37 | 0.41 | 100,100,100,100 | 0 |
| 56 | MG | AA | 1612 | 1/1 | 0.38 | 0.67 | 87,87,87,87 | 0 |
| 56 | MG | CA | 1748 | 1/1 | 0.38 | 0.52 | 78,78,78,78 | 0 |
| 56 | MG | CA | 1605 | 1/1 | 0.38 | 0.31 | 159,159,159,159 | 0 |
| 56 | MG | BA | 3672 | 1/1 | 0.38 | 0.47 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3718 | 1/1 | 0.38 | 0.25 | 163,163,163,163 | 0 |
| 56 | MG | CA | 1912 | 1/1 | 0.38 | 0.43 | 152,152,152,152 | 0 |
| 56 | MG | DB | 209 | 1/1 | 0.39 | 0.73 | 143,143,143,143 | 0 |
| 56 | MG | DA | 3541 | 1/1 | 0.39 | 0.79 | 70,70,70,70 | 0 |
| 56 | MG | CA | 1806 | 1/1 | 0.40 | 0.32 | 95,95,95,95 | 0 |
| 56 | MG | AA | 1629 | 1/1 | 0.40 | 0.90 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1717 | 1/1 | 0.40 | 0.31 | 99,99,99,99 | 0 |
| 56 | MG | AA | 1950 | 1/1 | 0.41 | 0.41 | 102,102,102,102 | 0 |
| 56 | MG | CA | 1833 | 1/1 | 0.41 | 0.82 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1741 | 1/1 | 0.41 | 0.30 | 104,104,104,104 | 0 |
| 56 | MG | CA | 1606 | 1/1 | 0.42 | 0.37 | 115,115,115,115 | 0 |
| 56 | MG | BA | 3186 | 1/1 | 0.42 | 0.47 | 98,98,98,98 | 0 |
| 56 | MG | BA | 2922 | 1/1 | 0.42 | 0.75 | 108,108,108,108 | 0 |
| 56 | MG | BA | 3592 | 1/1 | 0.42 | 0.24 | 132,132,132,132 | 0 |
| 56 | MG | BA | 3607 | 1/1 | 0.43 | 0.18 | 105,105,105,105 | 0 |
| 56 | MG | BA | 3450 | 1/1 | 0.43 | 0.97 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3092 | 1/1 | 0.43 | 1.39 | 200,200,200,200 | 0 |
| 56 | MG | CA | 1800 | 1/1 | 0.43 | 0.63 | 124,124,124,124 | 0 |
| 56 | MG | AA | 1723 | 1/1 | 0.44 | 0.31 | 106,106,106,106 | 0 |
| 56 | MG | AA | 1642 | 1/1 | 0.44 | 0.30 | 120,120,120,120 | 0 |
| 56 | MG | AA | 1945 | 1/1 | 0.44 | 0.41 | 115,115,115,115 | 0 |
| 56 | MG | DA | 3401 | 1/1 | 0.46 | 0.39 | 81,81,81,81 | 0 |
| 56 | MG | AA | 1697 | 1/1 | 0.46 | 0.20 | 148,148,148,148 | 0 |
| 56 | MG | BA | 3588 | 1/1 | 0.46 | 0.80 | 120,120,120,120 | 0 |
| 56 | MG | CY | 401 | 1/1 | 0.46 | 0.53 | 103,103,103,103 | 0 |
| 56 | MG | CA | 1699 | 1/1 | 0.46 | 0.44 | 152,152,152,152 | 0 |
| 56 | MG | CA | 1860 | 1/1 | 0.47 | 0.27 | 133,133,133,133 | 0 |
| 56 | MG | AA | 1639 | 1/1 | 0.47 | 0.79 | 114,114,114,114 | 0 |
| 56 | MG | DA | 2948 | 1/1 | 0.47 | 0.64 | 94,94,94,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3591 | 1/1 | 0.47 | 1.28 | 102,102,102,102 | 0 |
| 56 | MG | CA | 1772 | 1/1 | 0.48 | 0.64 | 66,66,66,66 | 0 |
| 56 | MG | CA | 1681 | 1/1 | 0.48 | 0.56 | 136,136,136,136 | 0 |
| 56 | MG | BA | 3618 | 1/1 | 0.48 | 0.58 | 79,79,79,79 | 0 |
| 56 | MG | CA | 1643 | 1/1 | 0.49 | 0.10 | 126,126,126,126 | 0 |
| 56 | MG | DA | 3054 | 1/1 | 0.49 | 0.64 | 93,93,93,93 | 0 |
| 56 | MG | CA | 1794 | 1/1 | 0.50 | 0.34 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3542 | 1/1 | 0.50 | 0.40 | 116,116,116,116 | 0 |
| 56 | MG | AA | 1770 | 1/1 | 0.50 | 0.36 | 86,86,86,86 | 0 |
| 56 | MG | BB | 206 | 1/1 | 0.50 | 0.23 | 188,188,188,188 | 0 |
| 56 | MG | CA | 1750 | 1/1 | 0.50 | 0.25 | 222,222,222,222 | 0 |
| 56 | MG | AA | 1957 | 1/1 | 0.50 | 0.79 | 109,109,109,109 | 0 |
| 56 | MG | BA | 3247 | 1/1 | 0.50 | 0.55 | 105,105,105,105 | 0 |
| 56 | MG | DA | 3044 | 1/1 | 0.51 | 0.42 | 87,87,87,87 | 0 |
| 56 | MG | CA | 1712 | 1/1 | 0.51 | 0.21 | 106,106,106,106 | 0 |
| 56 | MG | CA | 1856 | 1/1 | 0.52 | 0.40 | 136,136,136,136 | 0 |
| 56 | MG | CA | 1732 | 1/1 | 0.52 | 0.77 | 131,131,131,131 | 0 |
| 56 | MG | CA | 1777 | 1/1 | 0.52 | 0.29 | 98,98,98,98 | 0 |
| 56 | MG | AA | 1653 | 1/1 | 0.52 | 0.26 | 105,105,105,105 | 0 |
| 56 | MG | BA | 3261 | 1/1 | 0.52 | 0.72 | 89,89,89,89 | 0 |
| 56 | MG | CA | 1842 | 1/1 | 0.52 | 0.79 | 137,137,137,137 | 0 |
| 56 | MG | DV | 201 | 1/1 | 0.52 | 0.43 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3213 | 1/1 | 0.53 | 0.48 | 125,125,125,125 | 0 |
| 56 | MG | BA | 3606 | 1/1 | 0.53 | 0.38 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3569 | 1/1 | 0.53 | 0.48 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3003 | 1/1 | 0.53 | 0.59 | 113,113,113,113 | 0 |
| 56 | MG | AA | 1687 | 1/1 | 0.53 | 0.13 | 85,85,85,85 | 0 |
| 56 | MG | CA | 1725 | 1/1 | 0.54 | 0.90 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1796 | 1/1 | 0.54 | 0.68 | 129,129,129,129 | 0 |
| 56 | MG | DB | 204 | 1/1 | 0.54 | 0.28 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1846 | 1/1 | 0.54 | 0.42 | 118,118,118,118 | 0 |
| 56 | MG | BA | 3548 | 1/1 | 0.54 | 0.64 | 88,88,88,88 | 0 |
| 56 | MG | CA | 1914 | 1/1 | 0.54 | 0.27 | 96,96,96,96 | 0 |
| 56 | MG | AA | 1804 | 1/1 | 0.55 | 1.32 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3405 | 1/1 | 0.55 | 0.21 | 91,91,91,91 | 0 |
| 56 | MG | CA | 1817 | 1/1 | 0.55 | 0.32 | 111,111,111,111 | 0 |
| 56 | MG | BA | 3119 | 1/1 | 0.55 | 1.15 | 133,133,133,133 | 0 |
| 56 | MG | CA | 1907 | 1/1 | 0.55 | 0.54 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3665 | 1/1 | 0.55 | 0.24 | 117,117,117,117 | 0 |
| 56 | MG | DA | 3350 | 1/1 | 0.55 | 0.19 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3351 | 1/1 | 0.55 | 0.45 | 116,116,116,116 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3583 | 1/1 | 0.56 | 0.69 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3582 | 1/1 | 0.56 | 0.38 | 95,95,95,95 | 0 |
| 56 | MG | DA | 3060 | 1/1 | 0.56 | 0.20 | 77,77,77,77 | 0 |
| 56 | MG | BA | 2950 | 1/1 | 0.56 | 0.85 | 87,87,87,87 | 0 |
| 56 | MG | CA | 1706 | 1/1 | 0.56 | 0.18 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3600 | 1/1 | 0.56 | 0.59 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3064 | 1/1 | 0.57 | 0.44 | 63,63,63,63 | 0 |
| 56 | MG | BA | 2974 | 1/1 | 0.57 | 0.29 | 85,85,85,85 | 0 |
| 56 | MG | BA | 2997 | 1/1 | 0.57 | 0.21 | 104,104,104,104 | 0 |
| 56 | MG | BA | 2935 | 1/1 | 0.57 | 0.53 | 89,89,89,89 | 0 |
| 56 | MG | CA | 1820 | 1/1 | 0.57 | 0.85 | 193,193,193,193 | 0 |
| 56 | MG | BA | 3263 | 1/1 | 0.57 | 0.40 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3173 | 1/1 | 0.57 | 0.81 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1790 | 1/1 | 0.57 | 0.40 | 53,53,53,53 | 0 |
| 56 | MG | DA | 2949 | 1/1 | 0.57 | 1.12 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3236 | 1/1 | 0.58 | 0.34 | 132,132,132,132 | 0 |
| 56 | MG | DA | 3548 | 1/1 | 0.58 | 0.43 | 85,85,85,85 | 0 |
| 56 | MG | AA | 1728 | 1/1 | 0.58 | 0.21 | 130,130,130,130 | 0 |
| 56 | MG | BA | 3599 | 1/1 | 0.58 | 0.59 | 93,93,93,93 | 0 |
| 56 | MG | AA | 1783 | 1/1 | 0.58 | 0.41 | 127,127,127,127 | 0 |
| 56 | MG | DA | 3244 | 1/1 | 0.58 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3248 | 1/1 | 0.58 | 1.19 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1699 | 1/1 | 0.59 | 0.42 | 85,85,85,85 | 0 |
| 56 | MG | CA | 1724 | 1/1 | 0.59 | 0.30 | 108,108,108,108 | 0 |
| 56 | MG | BA | 2915 | 1/1 | 0.59 | 0.27 | 102,102,102,102 | 0 |
| 56 | MG | BA | 2939 | 1/1 | 0.59 | 0.45 | 79,79,79,79 | 0 |
| 56 | MG | BB | 211 | 1/1 | 0.59 | 1.35 | 132,132,132,132 | 0 |
| 56 | MG | BA | 3012 | 1/1 | 0.59 | 0.99 | 91,91,91,91 | 0 |
| 56 | MG | AA | 1631 | 1/1 | 0.59 | 0.81 | 76,76,76,76 | 0 |
| 56 | MG | BA | 2958 | 1/1 | 0.59 | 0.15 | 103,103,103,103 | 0 |
| 56 | MG | DA | 3339 | 1/1 | 0.59 | 0.32 | 63,63,63,63 | 0 |
| 56 | MG | BA | 2959 | 1/1 | 0.59 | 0.71 | 81,81,81,81 | 0 |
| 56 | MG | CA | 1710 | 1/1 | 0.59 | 1.27 | 97,97,97,97 | 0 |
| 56 | MG | AW | 109 | 1/1 | 0.60 | 0.69 | 91,91,91,91 | 0 |
| 56 | MG | AA | 1767 | 1/1 | 0.60 | 0.56 | 102,102,102,102 | 0 |
| 56 | MG | CA | 1753 | 1/1 | 0.60 | 0.28 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3531 | 1/1 | 0.60 | 0.42 | 92,92,92,92 | 0 |
| 56 | MG | CA | 1682 | 1/1 | 0.60 | 0.14 | 152,152,152,152 | 0 |
| 56 | MG | CA | 1687 | 1/1 | 0.60 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | CA | 1836 | 1/1 | 0.60 | 0.33 | 94,94,94,94 | 0 |
| 56 | MG | CA | 1837 | 1/1 | 0.60 | 0.24 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1689 | 1/1 | 0.60 | 0.14 | 169,169,169,169 | 0 |
| 56 | MG | AW | 107 | 1/1 | 0.60 | 0.46 | 102,102,102,102 | 0 |
| 56 | MG | BA | 2943 | 1/1 | 0.60 | 1.09 | 98,98,98,98 | 0 |
| 56 | MG | AT | 203 | 1/1 | 0.61 | 1.74 | 99,99,99,99 | 0 |
| 56 | MG | BA | 3697 | 1/1 | 0.61 | 0.12 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3011 | 1/1 | 0.61 | 0.58 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3158 | 1/1 | 0.61 | 0.28 | 150,150,150,150 | 0 |
| 56 | MG | BA | 2926 | 1/1 | 0.61 | 0.56 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3584 | 1/1 | 0.61 | 0.49 | 96,96,96,96 | 0 |
| 56 | MG | BA | 3175 | 1/1 | 0.61 | 0.54 | 109,109,109,109 | 0 |
| 56 | MG | CA | 1752 | 1/1 | 0.61 | 0.44 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3381 | 1/1 | 0.61 | 0.44 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3465 | 1/1 | 0.61 | 0.60 | 114,114,114,114 | 0 |
| 56 | MG | BA | 3589 | 1/1 | 0.62 | 0.20 | 135,135,135,135 | 0 |
| 56 | MG | CA | 1640 | 1/1 | 0.62 | 0.33 | 78,78,78,78 | 0 |
| 56 | MG | CA | 1816 | 1/1 | 0.62 | 0.64 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3168 | 1/1 | 0.62 | 1.18 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3577 | 1/1 | 0.62 | 0.64 | 80,80,80,80 | 0 |
| 56 | MG | CA | 1647 | 1/1 | 0.62 | 0.43 | 98,98,98,98 | 0 |
| 56 | MG | DA | 3626 | 1/1 | 0.62 | 0.29 | 117,117,117,117 | 0 |
| 56 | MG | DA | 3632 | 1/1 | 0.62 | 0.19 | 135,135,135,135 | 0 |
| 56 | MG | CA | 1669 | 1/1 | 0.62 | 1.73 | 118,118,118,118 | 0 |
| 56 | MG | DB | 205 | 1/1 | 0.62 | 0.33 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3602 | 1/1 | 0.62 | 0.46 | 117,117,117,117 | 0 |
| 56 | MG | AA | 1726 | 1/1 | 0.62 | 0.51 | 141,141,141,141 | 0 |
| 56 | MG | DA | 2914 | 1/1 | 0.62 | 0.46 | 97,97,97,97 | 0 |
| 56 | MG | AA | 1947 | 1/1 | 0.63 | 0.49 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3722 | 1/1 | 0.63 | 0.26 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3081 | 1/1 | 0.63 | 0.18 | 79,79,79,79 | 0 |
| 56 | MG | CA | 1920 | 1/1 | 0.63 | 0.13 | 138,138,138,138 | 0 |
| 56 | MG | CA | 1735 | 1/1 | 0.63 | 0.84 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3398 | 1/1 | 0.63 | 0.79 | 107,107,107,107 | 0 |
| 56 | MG | DA | 2903 | 1/1 | 0.63 | 0.45 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3085 | 1/1 | 0.63 | 0.49 | 116,116,116,116 | 0 |
| 56 | MG | DB | 208 | 1/1 | 0.63 | 0.31 | 83,83,83,83 | 0 |
| 56 | MG | AY | 403 | 1/1 | 0.63 | 0.87 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3497 | 1/1 | 0.63 | 0.28 | 61,61,61,61 | 0 |
| 56 | MG | CA | 1603 | 1/1 | 0.63 | 0.23 | 255,255,255,255 | 0 |
| 56 | MG | BA | 3482 | 1/1 | 0.64 | 1.30 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1727 | 1/1 | 0.64 | 0.48 | 93,93,93,93 | 0 |
| 56 | MG | AA | 1742 | 1/1 | 0.64 | 1.36 | 197,197,197,197 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | CA | 1926 | 1/1 | 0.64 | 0.73 | 101,101,101,101 | 0 |
| 56 | MG | DA | 3097 | 1/1 | 0.64 | 0.51 | 68,68,68,68 | 0 |
| 56 | MG | DA | 2953 | 1/1 | 0.64 | 0.17 | 151,151,151,151 | 0 |
| 56 | MG | AA | 1855 | 1/1 | 0.64 | 0.15 | 103,103,103,103 | 0 |
| 56 | MG | DA | 3428 | 1/1 | 0.64 | 0.65 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3308 | 1/1 | 0.64 | 0.90 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3489 | 1/1 | 0.64 | 0.33 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3573 | 1/1 | 0.64 | 0.24 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3516 | 1/1 | 0.64 | 0.42 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3527 | 1/1 | 0.64 | 0.27 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3052 | 1/1 | 0.65 | 0.52 | 76,76,76,76 | 0 |
| 56 | MG | CA | 1796 | 1/1 | 0.65 | 0.16 | 41,41,41,41 | 0 |
| 56 | MG | AA | 1645 | 1/1 | 0.65 | 0.32 | 82,82,82,82 | 0 |
| 56 | MG | CA | 1645 | 1/1 | 0.65 | 1.03 | 113,113,113,113 | 0 |
| 56 | MG | CA | 1828 | 1/1 | 0.65 | 0.28 | 135,135,135,135 | 0 |
| 56 | MG | AA | 1702 | 1/1 | 0.65 | 0.65 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3105 | 1/1 | 0.66 | 0.24 | 122,122,122,122 | 0 |
| 56 | MG | CA | 1740 | 1/1 | 0.66 | 0.21 | 101,101,101,101 | 0 |
| 56 | MG | CA | 1884 | 1/1 | 0.66 | 0.53 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1890 | 1/1 | 0.66 | 0.15 | 124,124,124,124 | 0 |
| 56 | MG | DA | 3088 | 1/1 | 0.66 | 0.38 | 86,86,86,86 | 0 |
| 56 | MG | AA | 1782 | 1/1 | 0.66 | 0.56 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3577 | 1/1 | 0.66 | 0.91 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3118 | 1/1 | 0.66 | 0.18 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3122 | 1/1 | 0.66 | 0.35 | 67,67,67,67 | 0 |
| 56 | MG | BA | 2949 | 1/1 | 0.66 | 0.43 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3001 | 1/1 | 0.66 | 0.53 | 79,79,79,79 | 0 |
| 56 | MG | AY | 401 | 1/1 | 0.66 | 0.54 | 119,119,119,119 | 0 |
| 56 | MG | CA | 1646 | 1/1 | 0.66 | 0.12 | 113,113,113,113 | 0 |
| 56 | MG | BA | 3255 | 1/1 | 0.67 | 0.38 | 66,66,66,66 | 0 |
| 56 | MG | CA | 1874 | 1/1 | 0.67 | 1.45 | 89,89,89,89 | 0 |
| 56 | MG | CA | 1877 | 1/1 | 0.67 | 0.84 | 154,154,154,154 | 0 |
| 56 | MG | CA | 1882 | 1/1 | 0.67 | 0.52 | 81,81,81,81 | 0 |
| 56 | MG | BB | 216 | 1/1 | 0.67 | 0.54 | 109,109,109,109 | 0 |
| 56 | MG | BA | 2976 | 1/1 | 0.67 | 0.44 | 112,112,112,112 | 0 |
| 56 | MG | CA | 1658 | 1/1 | 0.67 | 0.49 | 93,93,93,93 | 0 |
| 56 | MG | AW | 102 | 1/1 | 0.67 | 0.48 | 94,94,94,94 | 0 |
| 56 | MG | CA | 1671 | 1/1 | 0.67 | 0.31 | 92,92,92,92 | 0 |
| 56 | MG | AW | 104 | 1/1 | 0.67 | 1.33 | 95,95,95,95 | 0 |
| 56 | MG | AA | 1688 | 1/1 | 0.67 | 0.24 | 80,80,80,80 | 0 |
| 56 | MG | AA | 1952 | 1/1 | 0.67 | 0.09 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3111 | 1/1 | 0.67 | 0.12 | 96,96,96,96 | 0 |
| 56 | MG | BA | 3212 | 1/1 | 0.67 | 0.36 | 109,109,109,109 | 0 |
| 56 | MG | BA | 2946 | 1/1 | 0.67 | 0.46 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3123 | 1/1 | 0.67 | 0.25 | 156,156,156,156 | 0 |
| 56 | MG | BA | 3062 | 1/1 | 0.67 | 0.21 | 110,110,110,110 | 0 |
| 56 | MG | CA | 1843 | 1/1 | 0.67 | 0.32 | 103,103,103,103 | 0 |
| 56 | MG | CA | 1854 | 1/1 | 0.67 | 0.41 | 98,98,98,98 | 0 |
| 56 | MG | CA | 1790 | 1/1 | 0.67 | 0.84 | 86,86,86,86 | 0 |
| 56 | MG | CW | 113 | 1/1 | 0.68 | 0.20 | 89,89,89,89 | 0 |
| 56 | MG | CA | 1698 | 1/1 | 0.68 | 0.27 | 100,100,100,100 | 0 |
| 56 | MG | CA | 1801 | 1/1 | 0.68 | 0.31 | 76,76,76,76 | 0 |
| 56 | MG | AW | 113 | 1/1 | 0.68 | 0.31 | 96,96,96,96 | 0 |
| 56 | MG | CA | 1703 | 1/1 | 0.68 | 0.19 | 89,89,89,89 | 0 |
| 56 | MG | DA | 2940 | 1/1 | 0.68 | 0.18 | 94,94,94,94 | 0 |
| 56 | MG | AW | 115 | 1/1 | 0.68 | 0.35 | 111,111,111,111 | 0 |
| 56 | MG | DA | 3532 | 1/1 | 0.68 | 0.25 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1619 | 1/1 | 0.68 | 0.74 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3544 | 1/1 | 0.68 | 0.41 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3284 | 1/1 | 0.68 | 0.46 | 82,82,82,82 | 0 |
| 56 | MG | DA | 2964 | 1/1 | 0.68 | 0.41 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3343 | 1/1 | 0.68 | 0.49 | 76,76,76,76 | 0 |
| 56 | MG | DA | 2975 | 1/1 | 0.68 | 0.91 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3290 | 1/1 | 0.68 | 0.25 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1917 | 1/1 | 0.68 | 0.15 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3373 | 1/1 | 0.68 | 0.19 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3218 | 1/1 | 0.68 | 0.60 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3065 | 1/1 | 0.68 | 0.23 | 90,90,90,90 | 0 |
| 56 | MG | BA | 3073 | 1/1 | 0.68 | 0.51 | 124,124,124,124 | 0 |
| 56 | MG | BA | 3639 | 1/1 | 0.68 | 0.41 | 79,79,79,79 | 0 |
| 56 | MG | CA | 1783 | 1/1 | 0.69 | 0.10 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3073 | 1/1 | 0.69 | 0.46 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3075 | 1/1 | 0.69 | 0.38 | 75,75,75,75 | 0 |
| 56 | MG | AA | 1824 | 1/1 | 0.69 | 0.68 | 108,108,108,108 | 0 |
| 56 | MG | DA | 2911 | 1/1 | 0.69 | 1.04 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1731 | 1/1 | 0.69 | 0.11 | 139,139,139,139 | 0 |
| 56 | MG | DA | 3511 | 1/1 | 0.69 | 0.36 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3663 | 1/1 | 0.69 | 0.28 | 105,105,105,105 | 0 |
| 56 | MG | DA | 3119 | 1/1 | 0.69 | 0.50 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1829 | 1/1 | 0.69 | 1.54 | 232,232,232,232 | 0 |
| 56 | MG | DA | 3128 | 1/1 | 0.69 | 0.27 | 101,101,101,101 | 0 |
| 56 | MG | AA | 1879 | 1/1 | 0.69 | 0.48 | 99,99,99,99 | 0 |
| 56 | MG | BA | 2932 | 1/1 | 0.69 | 0.16 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3536 | 1/1 | 0.69 | 0.64 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3338 | 1/1 | 0.69 | 0.79 | 76,76,76,76 | 0 |
| 56 | MG | CA | 1743 | 1/1 | 0.69 | 0.34 | 169,169,169,169 | 0 |
| 56 | MG | BA | 3596 | 1/1 | 0.69 | 0.38 | 140,140,140,140 | 0 |
| 56 | MG | AA | 1772 | 1/1 | 0.69 | 0.41 | 94,94,94,94 | 0 |
| 56 | MG | AA | 1794 | 1/1 | 0.69 | 0.15 | 151,151,151,151 | 0 |
| 56 | MG | BA | 3202 | 1/1 | 0.69 | 0.20 | 205,205,205,205 | 0 |
| 56 | MG | DA | 3353 | 1/1 | 0.69 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | BA | 2941 | 1/1 | 0.69 | 0.37 | 87,87,87,87 | 0 |
| 56 | MG | AA | 1934 | 1/1 | 0.69 | 0.40 | 96,96,96,96 | 0 |
| 56 | MG | BA | 3393 | 1/1 | 0.69 | 0.17 | 99,99,99,99 | 0 |
| 56 | MG | DA | 3326 | 1/1 | 0.70 | 0.42 | 47,47,47,47 | 0 |
| 56 | MG | AA | 1981 | 1/1 | 0.70 | 0.18 | 90,90,90,90 | 0 |
| 56 | MG | CA | 1719 | 1/1 | 0.70 | 0.50 | 106,106,106,106 | 0 |
| 56 | MG | BB | 208 | 1/1 | 0.70 | 0.70 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1615 | 1/1 | 0.70 | 0.17 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3239 | 1/1 | 0.70 | 0.45 | 99,99,99,99 | 0 |
| 56 | MG | DA | 3086 | 1/1 | 0.70 | 0.77 | 120,120,120,120 | 0 |
| 56 | MG | BA | 3533 | 1/1 | 0.70 | 0.17 | 97,97,97,97 | 0 |
| 56 | MG | CA | 1822 | 1/1 | 0.70 | 0.27 | 112,112,112,112 | 0 |
| 56 | MG | CA | 1734 | 1/1 | 0.70 | 0.22 | 196,196,196,196 | 0 |
| 56 | MG | BA | 3332 | 1/1 | 0.70 | 0.83 | 58,58,58,58 | 0 |
| 56 | MG | AW | 110 | 1/1 | 0.70 | 0.27 | 145,145,145,145 | 0 |
| 56 | MG | DA | 2983 | 1/1 | 0.70 | 0.33 | 77,77,77,77 | 0 |
| 56 | MG | CA | 1739 | 1/1 | 0.70 | 0.16 | 122,122,122,122 | 0 |
| 56 | MG | DA | 3439 | 1/1 | 0.70 | 0.34 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1672 | 1/1 | 0.70 | 0.66 | 73,73,73,73 | 0 |
| 56 | MG | CA | 1607 | 1/1 | 0.70 | 0.43 | 138,138,138,138 | 0 |
| 56 | MG | BA | 2920 | 1/1 | 0.70 | 0.41 | 70,70,70,70 | 0 |
| 56 | MG | DA | 2917 | 1/1 | 0.71 | 0.45 | 83,83,83,83 | 0 |
| 56 | MG | CA | 1614 | 1/1 | 0.71 | 0.42 | 122,122,122,122 | 0 |
| 56 | MG | AA | 1990 | 1/1 | 0.71 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3346 | 1/1 | 0.71 | 0.26 | 90,90,90,90 | 0 |
| 56 | MG | BA | 3080 | 1/1 | 0.71 | 0.31 | 112,112,112,112 | 0 |
| 56 | MG | AA | 1621 | 1/1 | 0.71 | 0.17 | 74,74,74,74 | 0 |
| 56 | MG | BA | 2993 | 1/1 | 0.71 | 0.30 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3540 | 1/1 | 0.71 | 0.59 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3224 | 1/1 | 0.71 | 0.64 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3230 | 1/1 | 0.71 | 0.58 | 103,103,103,103 | 0 |
| 56 | MG | DA | 3385 | 1/1 | 0.71 | 0.40 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3676 | 1/1 | 0.71 | 0.43 | 181,181,181,181 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3553 | 1/1 | 0.71 | 0.46 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3016 | 1/1 | 0.71 | 0.41 | 99,99,99,99 | 0 |
| 56 | MG | DA | 3023 | 1/1 | 0.71 | 0.40 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3709 | 1/1 | 0.71 | 0.34 | 97,97,97,97 | 0 |
| 56 | MG | BA | 2996 | 1/1 | 0.71 | 0.19 | 209,209,209,209 | 0 |
| 56 | MG | CA | 1675 | 1/1 | 0.71 | 0.45 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3059 | 1/1 | 0.71 | 0.30 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1786 | 1/1 | 0.71 | 0.46 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1632 | 1/1 | 0.71 | 0.45 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3004 | 1/1 | 0.71 | 0.46 | 99,99,99,99 | 0 |
| 56 | MG | BA | 3131 | 1/1 | 0.71 | 0.36 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1902 | 1/1 | 0.71 | 0.63 | 128,128,128,128 | 0 |
| 56 | MG | AA | 1951 | 1/1 | 0.71 | 0.50 | 73,73,73,73 | 0 |
| 56 | MG | BA | 2917 | 1/1 | 0.71 | 0.59 | 188,188,188,188 | 0 |
| 56 | MG | AA | 1605 | 1/1 | 0.71 | 0.19 | 142,142,142,142 | 0 |
| 56 | MG | BA | 3170 | 1/1 | 0.71 | 0.37 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1892 | 1/1 | 0.71 | 0.24 | 108,108,108,108 | 0 |
| 56 | MG | AA | 1839 | 1/1 | 0.71 | 0.52 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1660 | 1/1 | 0.71 | 0.27 | 105,105,105,105 | 0 |
| 56 | MG | DA | 3243 | 1/1 | 0.71 | 0.55 | 77,77,77,77 | 0 |
| 56 | MG | CA | 1807 | 1/1 | 0.71 | 0.70 | 195,195,195,195 | 0 |
| 56 | MG | DA | 2910 | 1/1 | 0.71 | 0.10 | 90,90,90,90 | 0 |
| 56 | MG | DA | 3284 | 1/1 | 0.71 | 0.36 | 53,53,53,53 | 0 |
| 56 | MG | BA | 2973 | 1/1 | 0.71 | 0.53 | 160,160,160,160 | 0 |
| 56 | MG | BA | 3605 | 1/1 | 0.71 | 0.09 | 72,72,72,72 | 0 |
| 56 | MG | CA | 1904 | 1/1 | 0.72 | 0.26 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3093 | 1/1 | 0.72 | 0.43 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1802 | 1/1 | 0.72 | 0.31 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3098 | 1/1 | 0.72 | 0.59 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3189 | 1/1 | 0.72 | 0.45 | 105,105,105,105 | 0 |
| 56 | MG | BA | 3307 | 1/1 | 0.72 | 0.20 | 83,83,83,83 | 0 |
| 56 | MG | BA | 3711 | 1/1 | 0.72 | 0.16 | 104,104,104,104 | 0 |
| 56 | MG | DA | 3430 | 1/1 | 0.72 | 0.16 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3194 | 1/1 | 0.72 | 0.34 | 91,91,91,91 | 0 |
| 56 | MG | DA | 3449 | 1/1 | 0.72 | 0.25 | 53,53,53,53 | 0 |
| 56 | MG | CD | 302 | 1/1 | 0.72 | 0.43 | 111,111,111,111 | 0 |
| 56 | MG | BA | 3055 | 1/1 | 0.72 | 0.28 | 71,71,71,71 | 0 |
| 56 | MG | BA | 2951 | 1/1 | 0.72 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | AG | 201 | 1/1 | 0.72 | 0.88 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3448 | 1/1 | 0.72 | 0.35 | 72,72,72,72 | 0 |
| 56 | MG | CA | 1676 | 1/1 | 0.72 | 0.21 | 88,88,88,88 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3597 | 1/1 | 0.72 | 0.54 | 91,91,91,91 | 0 |
| 56 | MG | CA | 1840 | 1/1 | 0.72 | 0.56 | 101,101,101,101 | 0 |
| 56 | MG | DA | 2944 | 1/1 | 0.72 | 0.18 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3002 | 1/1 | 0.72 | 0.40 | 91,91,91,91 | 0 |
| 56 | MG | AA | 1942 | 1/1 | 0.72 | 0.16 | 92,92,92,92 | 0 |
| 56 | MG | BA | 3147 | 1/1 | 0.72 | 0.42 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3148 | 1/1 | 0.72 | 0.19 | 111,111,111,111 | 0 |
| 56 | MG | AA | 1860 | 1/1 | 0.72 | 0.41 | 62,62,62,62 | 0 |
| 56 | MG | BA | 2907 | 1/1 | 0.72 | 0.38 | 129,129,129,129 | 0 |
| 56 | MG | BA | 3612 | 1/1 | 0.72 | 0.40 | 96,96,96,96 | 0 |
| 56 | MG | AA | 1714 | 1/1 | 0.72 | 0.58 | 114,114,114,114 | 0 |
| 56 | MG | DA | 3009 | 1/1 | 0.72 | 0.62 | 130,130,130,130 | 0 |
| 56 | MG | BA | 3252 | 1/1 | 0.72 | 0.48 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1725 | 1/1 | 0.72 | 0.66 | 121,121,121,121 | 0 |
| 56 | MG | BA | 3092 | 1/1 | 0.72 | 0.46 | 99,99,99,99 | 0 |
| 56 | MG | CW | 102 | 1/1 | 0.73 | 0.57 | 105,105,105,105 | 0 |
| 56 | MG | BA | 2927 | 1/1 | 0.73 | 0.25 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3070 | 1/1 | 0.73 | 0.60 | 69,69,69,69 | 0 |
| 56 | MG | BA | 2930 | 1/1 | 0.73 | 0.60 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3529 | 1/1 | 0.73 | 0.31 | 79,79,79,79 | 0 |
| 56 | MG | CA | 1670 | 1/1 | 0.73 | 0.29 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3416 | 1/1 | 0.73 | 0.18 | 60,60,60,60 | 0 |
| 56 | MG | DA | 2905 | 1/1 | 0.73 | 0.14 | 87,87,87,87 | 0 |
| 56 | MG | AA | 1778 | 1/1 | 0.73 | 0.19 | 159,159,159,159 | 0 |
| 56 | MG | CA | 1674 | 1/1 | 0.73 | 0.20 | 107,107,107,107 | 0 |
| 56 | MG | AA | 1750 | 1/1 | 0.73 | 0.31 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3117 | 1/1 | 0.73 | 0.24 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3273 | 1/1 | 0.73 | 0.30 | 110,110,110,110 | 0 |
| 56 | MG | BA | 3278 | 1/1 | 0.73 | 0.51 | 115,115,115,115 | 0 |
| 56 | MG | DA | 3510 | 1/1 | 0.73 | 0.76 | 69,69,69,69 | 0 |
| 56 | MG | AA | 1622 | 1/1 | 0.73 | 0.66 | 70,70,70,70 | 0 |
| 56 | MG | BE | 301 | 1/1 | 0.73 | 0.56 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3522 | 1/1 | 0.73 | 0.19 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1811 | 1/1 | 0.73 | 0.38 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3300 | 1/1 | 0.73 | 0.39 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3629 | 1/1 | 0.73 | 0.88 | 129,129,129,129 | 0 |
| 56 | MG | BA | 2925 | 1/1 | 0.73 | 0.59 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3287 | 1/1 | 0.73 | 0.84 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3574 | 1/1 | 0.73 | 0.40 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3325 | 1/1 | 0.73 | 0.48 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3309 | 1/1 | 0.73 | 0.35 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3668 | 1/1 | 0.73 | 0.20 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1874 | 1/1 | 0.73 | 0.41 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1720 | 1/1 | 0.73 | 0.45 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3084 | 1/1 | 0.73 | 0.50 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3020 | 1/1 | 0.73 | 0.55 | 107,107,107,107 | 0 |
| 56 | MG | BA | 2981 | 1/1 | 0.73 | 0.36 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3035 | 1/1 | 0.73 | 0.13 | 158,158,158,158 | 0 |
| 56 | MG | BA | 3053 | 1/1 | 0.73 | 0.45 | 95,95,95,95 | 0 |
| 56 | MG | D0 | 101 | 1/1 | 0.73 | 0.33 | 42,42,42,42 | 0 |
| 56 | MG | DA | 2936 | 1/1 | 0.74 | 0.50 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3329 | 1/1 | 0.74 | 0.34 | 46,46,46,46 | 0 |
| 56 | MG | CA | 1667 | 1/1 | 0.74 | 0.28 | 118,118,118,118 | 0 |
| 56 | MG | BA | 3389 | 1/1 | 0.74 | 0.31 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3054 | 1/1 | 0.74 | 0.30 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3229 | 1/1 | 0.74 | 0.53 | 92,92,92,92 | 0 |
| 56 | MG | AA | 1975 | 1/1 | 0.74 | 0.26 | 121,121,121,121 | 0 |
| 56 | MG | CA | 1717 | 1/1 | 0.74 | 0.25 | 121,121,121,121 | 0 |
| 56 | MG | CW | 112 | 1/1 | 0.74 | 0.27 | 103,103,103,103 | 0 |
| 56 | MG | AA | 1850 | 1/1 | 0.74 | 0.23 | 98,98,98,98 | 0 |
| 56 | MG | BA | 3267 | 1/1 | 0.74 | 0.41 | 123,123,123,123 | 0 |
| 56 | MG | DA | 3375 | 1/1 | 0.74 | 0.49 | 78,78,78,78 | 0 |
| 56 | MG | CA | 1644 | 1/1 | 0.74 | 1.32 | 120,120,120,120 | 0 |
| 56 | MG | CA | 1678 | 1/1 | 0.74 | 1.80 | 128,128,128,128 | 0 |
| 56 | MG | DA | 3586 | 1/1 | 0.74 | 0.77 | 133,133,133,133 | 0 |
| 56 | MG | BA | 3139 | 1/1 | 0.74 | 0.41 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3630 | 1/1 | 0.74 | 0.15 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3517 | 1/1 | 0.74 | 0.53 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1780 | 1/1 | 0.74 | 0.53 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3359 | 1/1 | 0.74 | 0.10 | 106,106,106,106 | 0 |
| 56 | MG | AA | 1858 | 1/1 | 0.74 | 0.28 | 132,132,132,132 | 0 |
| 56 | MG | CA | 1905 | 1/1 | 0.74 | 0.39 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3292 | 1/1 | 0.74 | 0.31 | 34,34,34,34 | 0 |
| 56 | MG | DA | 2930 | 1/1 | 0.74 | 0.45 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3066 | 1/1 | 0.74 | 1.50 | 90,90,90,90 | 0 |
| 56 | MG | D7 | 101 | 1/1 | 0.74 | 0.48 | 62,62,62,62 | 0 |
| 56 | MG | CW | 101 | 1/1 | 0.75 | 0.35 | 96,96,96,96 | 0 |
| 56 | MG | DA | 3441 | 1/1 | 0.75 | 0.38 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3256 | 1/1 | 0.75 | 0.57 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3455 | 1/1 | 0.75 | 0.26 | 64,64,64,64 | 0 |
| 56 | MG | AW | 112 | 1/1 | 0.75 | 0.57 | 82,82,82,82 | 0 |
| 56 | MG | CW | 116 | 1/1 | 0.75 | 0.14 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3479 | 1/1 | 0.75 | 0.47 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1850 | 1/1 | 0.75 | 0.40 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3082 | 1/1 | 0.75 | 0.34 | 119,119,119,119 | 0 |
| 56 | MG | DA | 3521 | 1/1 | 0.75 | 0.30 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3494 | 1/1 | 0.75 | 0.18 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3496 | 1/1 | 0.75 | 0.43 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3501 | 1/1 | 0.75 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3264 | 1/1 | 0.75 | 0.48 | 89,89,89,89 | 0 |
| 56 | MG | CA | 1738 | 1/1 | 0.75 | 0.38 | 123,123,123,123 | 0 |
| 56 | MG | BA | 3130 | 1/1 | 0.75 | 0.50 | 82,82,82,82 | 0 |
| 56 | MG | CA | 1887 | 1/1 | 0.75 | 0.43 | 116,116,116,116 | 0 |
| 56 | MG | BA | 3156 | 1/1 | 0.75 | 0.50 | 74,74,74,74 | 0 |
| 56 | MG | DA | 2937 | 1/1 | 0.75 | 0.67 | 104,104,104,104 | 0 |
| 56 | MG | AA | 1681 | 1/1 | 0.75 | 0.22 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3117 | 1/1 | 0.75 | 0.21 | 92,92,92,92 | 0 |
| 56 | MG | BA | 3433 | 1/1 | 0.75 | 0.37 | 97,97,97,97 | 0 |
| 56 | MG | DA | 3386 | 1/1 | 0.75 | 0.22 | 102,102,102,102 | 0 |
| 56 | MG | BA | 3225 | 1/1 | 0.75 | 0.28 | 96,96,96,96 | 0 |
| 56 | MG | BB | 202 | 1/1 | 0.75 | 0.19 | 98,98,98,98 | 0 |
| 56 | MG | DA | 3403 | 1/1 | 0.75 | 0.81 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3442 | 1/1 | 0.75 | 0.39 | 79,79,79,79 | 0 |
| 56 | MG | DA | 2972 | 1/1 | 0.75 | 0.62 | 187,187,187,187 | 0 |
| 56 | MG | DF | 301 | 1/1 | 0.75 | 0.45 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3427 | 1/1 | 0.75 | 1.15 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3557 | 1/1 | 0.75 | 0.15 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3299 | 1/1 | 0.75 | 0.65 | 102,102,102,102 | 0 |
| 56 | MG | BA | 3297 | 1/1 | 0.76 | 0.63 | 122,122,122,122 | 0 |
| 56 | MG | BA | 3298 | 1/1 | 0.76 | 0.38 | 101,101,101,101 | 0 |
| 56 | MG | CA | 1918 | 1/1 | 0.76 | 0.15 | 107,107,107,107 | 0 |
| 56 | MG | DA | 3453 | 1/1 | 0.76 | 0.19 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3137 | 1/1 | 0.76 | 0.28 | 83,83,83,83 | 0 |
| 56 | MG | BA | 2929 | 1/1 | 0.76 | 0.53 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3491 | 1/1 | 0.76 | 0.35 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3196 | 1/1 | 0.76 | 0.09 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1747 | 1/1 | 0.76 | 1.26 | 122,122,122,122 | 0 |
| 56 | MG | AA | 1722 | 1/1 | 0.76 | 0.24 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3016 | 1/1 | 0.76 | 0.28 | 168,168,168,168 | 0 |
| 56 | MG | DA | 3033 | 1/1 | 0.76 | 0.41 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3257 | 1/1 | 0.76 | 0.51 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3342 | 1/1 | 0.76 | 0.09 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1835 | 1/1 | 0.76 | 0.99 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 2934 | 1/1 | 0.76 | 0.72 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3114 | 1/1 | 0.76 | 0.20 | 119,119,119,119 | 0 |
| 56 | MG | BA | 3403 | 1/1 | 0.76 | 0.50 | 79,79,79,79 | 0 |
| 56 | MG | CA | 1718 | 1/1 | 0.76 | 0.12 | 136,136,136,136 | 0 |
| 56 | MG | BA | 3407 | 1/1 | 0.76 | 0.61 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3364 | 1/1 | 0.76 | 0.10 | 80,80,80,80 | 0 |
| 56 | MG | CA | 1863 | 1/1 | 0.76 | 0.30 | 69,69,69,69 | 0 |
| 56 | MG | DA | 2915 | 1/1 | 0.76 | 0.42 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3546 | 1/1 | 0.76 | 0.63 | 200,200,200,200 | 0 |
| 56 | MG | CA | 1663 | 1/1 | 0.76 | 0.63 | 210,210,210,210 | 0 |
| 56 | MG | DB | 201 | 1/1 | 0.76 | 0.34 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1748 | 1/1 | 0.76 | 0.24 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3550 | 1/1 | 0.76 | 0.12 | 68,68,68,68 | 0 |
| 56 | MG | DB | 206 | 1/1 | 0.76 | 0.41 | 121,121,121,121 | 0 |
| 56 | MG | BA | 3049 | 1/1 | 0.76 | 0.30 | 90,90,90,90 | 0 |
| 56 | MG | DA | 2938 | 1/1 | 0.76 | 0.38 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1977 | 1/1 | 0.76 | 0.37 | 126,126,126,126 | 0 |
| 56 | MG | AA | 1607 | 1/1 | 0.76 | 0.47 | 97,97,97,97 | 0 |
| 56 | MG | AA | 1652 | 1/1 | 0.76 | 0.19 | 98,98,98,98 | 0 |
| 56 | MG | DW | 201 | 1/1 | 0.76 | 0.53 | 76,76,76,76 | 0 |
| 56 | MG | CA | 1808 | 1/1 | 0.76 | 0.56 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3655 | 1/1 | 0.76 | 0.41 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3436 | 1/1 | 0.77 | 0.19 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3211 | 1/1 | 0.77 | 0.49 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1967 | 1/1 | 0.77 | 0.27 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3720 | 1/1 | 0.77 | 0.22 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3601 | 1/1 | 0.77 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3456 | 1/1 | 0.77 | 0.20 | 116,116,116,116 | 0 |
| 56 | MG | BA | 2913 | 1/1 | 0.77 | 0.35 | 77,77,77,77 | 0 |
| 56 | MG | CA | 1911 | 1/1 | 0.77 | 1.07 | 107,107,107,107 | 0 |
| 56 | MG | BB | 203 | 1/1 | 0.77 | 0.37 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3303 | 1/1 | 0.77 | 0.27 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3501 | 1/1 | 0.77 | 0.09 | 96,96,96,96 | 0 |
| 56 | MG | DA | 2989 | 1/1 | 0.77 | 0.47 | 53,53,53,53 | 0 |
| 56 | MG | DA | 2999 | 1/1 | 0.77 | 0.19 | 102,102,102,102 | 0 |
| 56 | MG | CA | 1810 | 1/1 | 0.77 | 0.71 | 121,121,121,121 | 0 |
| 56 | MG | DA | 3003 | 1/1 | 0.77 | 0.43 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3306 | 1/1 | 0.77 | 0.39 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1891 | 1/1 | 0.77 | 0.19 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3528 | 1/1 | 0.77 | 0.33 | 54,54,54,54 | 0 |
| 56 | MG | BB | 215 | 1/1 | 0.77 | 0.34 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3110 | 1/1 | 0.77 | 0.37 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BB | 222 | 1/1 | 0.77 | 0.19 | 206,206,206,206 | 0 |
| 56 | MG | BA | 3570 | 1/1 | 0.77 | 0.15 | 83,83,83,83 | 0 |
| 56 | MG | BA | 3141 | 1/1 | 0.77 | 0.71 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3568 | 1/1 | 0.77 | 0.41 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1825 | 1/1 | 0.77 | 0.43 | 138,138,138,138 | 0 |
| 56 | MG | BA | 3270 | 1/1 | 0.77 | 0.40 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3193 | 1/1 | 0.77 | 0.31 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3514 | 1/1 | 0.77 | 1.15 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3627 | 1/1 | 0.77 | 0.28 | 81,81,81,81 | 0 |
| 56 | MG | AA | 1909 | 1/1 | 0.77 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3380 | 1/1 | 0.77 | 0.28 | 85,85,85,85 | 0 |
| 56 | MG | CA | 1756 | 1/1 | 0.77 | 0.37 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1721 | 1/1 | 0.77 | 0.40 | 128,128,128,128 | 0 |
| 56 | MG | CA | 1704 | 1/1 | 0.77 | 0.71 | 88,88,88,88 | 0 |
| 56 | MG | BA | 2972 | 1/1 | 0.77 | 0.53 | 122,122,122,122 | 0 |
| 56 | MG | BA | 3696 | 1/1 | 0.77 | 0.17 | 96,96,96,96 | 0 |
| 56 | MG | BA | 3414 | 1/1 | 0.77 | 0.67 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3593 | 1/1 | 0.77 | 0.32 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3107 | 1/1 | 0.77 | 0.60 | 139,139,139,139 | 0 |
| 56 | MG | BA | 3538 | 1/1 | 0.77 | 0.37 | 82,82,82,82 | 0 |
| 56 | MG | CA | 1885 | 1/1 | 0.77 | 0.27 | 270,270,270,270 | 0 |
| 56 | MG | BA | 2999 | 1/1 | 0.77 | 0.09 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3432 | 1/1 | 0.77 | 0.30 | 104,104,104,104 | 0 |
| 56 | MG | BA | 3115 | 1/1 | 0.78 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3320 | 1/1 | 0.78 | 0.11 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3007 | 1/1 | 0.78 | 0.13 | 70,70,70,70 | 0 |
| 56 | MG | CA | 1691 | 1/1 | 0.78 | 0.32 | 161,161,161,161 | 0 |
| 56 | MG | CA | 1693 | 1/1 | 0.78 | 0.42 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3502 | 1/1 | 0.78 | 1.32 | 73,73,73,73 | 0 |
| 56 | MG | CA | 1617 | 1/1 | 0.78 | 0.38 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3030 | 1/1 | 0.78 | 1.40 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1686 | 1/1 | 0.78 | 0.42 | 85,85,85,85 | 0 |
| 56 | MG | DA | 3517 | 1/1 | 0.78 | 0.42 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3519 | 1/1 | 0.78 | 1.54 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1777 | 1/1 | 0.78 | 0.17 | 101,101,101,101 | 0 |
| 56 | MG | AA | 1826 | 1/1 | 0.78 | 0.36 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1900 | 1/1 | 0.78 | 0.30 | 213,213,213,213 | 0 |
| 56 | MG | BA | 3182 | 1/1 | 0.78 | 0.60 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3185 | 1/1 | 0.78 | 0.65 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1866 | 1/1 | 0.78 | 0.18 | 118,118,118,118 | 0 |
| 56 | MG | CA | 1869 | 1/1 | 0.78 | 0.38 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3462 | 1/1 | 0.78 | 0.41 | 95,95,95,95 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | CA | 1793 | 1/1 | 0.78 | 0.26 | 114,114,114,114 | 0 |
| 56 | MG | BA | 3610 | 1/1 | 0.78 | 0.40 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3248 | 1/1 | 0.78 | 0.49 | 102,102,102,102 | 0 |
| 56 | MG | AA | 1757 | 1/1 | 0.78 | 0.32 | 74,74,74,74 | 0 |
| 56 | MG | BA | 2983 | 1/1 | 0.78 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3611 | 1/1 | 0.78 | 0.88 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3395 | 1/1 | 0.78 | 0.13 | 95,95,95,95 | 0 |
| 56 | MG | DA | 3095 | 1/1 | 0.78 | 0.13 | 100,100,100,100 | 0 |
| 56 | MG | BA | 3140 | 1/1 | 0.78 | 0.34 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1900 | 1/1 | 0.78 | 0.49 | 112,112,112,112 | 0 |
| 56 | MG | BA | 3650 | 1/1 | 0.78 | 0.48 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3067 | 1/1 | 0.78 | 0.17 | 142,142,142,142 | 0 |
| 56 | MG | BA | 3661 | 1/1 | 0.78 | 0.69 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3143 | 1/1 | 0.78 | 0.43 | 81,81,81,81 | 0 |
| 56 | MG | AW | 116 | 1/1 | 0.78 | 0.19 | 86,86,86,86 | 0 |
| 56 | MG | CA | 1812 | 1/1 | 0.78 | 0.58 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3377 | 1/1 | 0.78 | 0.46 | 56,56,56,56 | 0 |
| 56 | MG | AA | 1953 | 1/1 | 0.78 | 0.38 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3270 | 1/1 | 0.78 | 0.64 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3112 | 1/1 | 0.78 | 0.18 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1625 | 1/1 | 0.78 | 0.48 | 85,85,85,85 | 0 |
| 56 | MG | CA | 1686 | 1/1 | 0.78 | 0.27 | 286,286,286,286 | 0 |
| 56 | MG | BA | 3237 | 1/1 | 0.79 | 0.59 | 90,90,90,90 | 0 |
| 56 | MG | DA | 3257 | 1/1 | 0.79 | 0.28 | 90,90,90,90 | 0 |
| 56 | MG | DA | 3463 | 1/1 | 0.79 | 0.36 | 60,60,60,60 | 0 |
| 56 | MG | B0 | 102 | 1/1 | 0.79 | 0.45 | 68,68,68,68 | 0 |
| 56 | MG | DA | 2988 | 1/1 | 0.79 | 0.22 | 85,85,85,85 | 0 |
| 56 | MG | CA | 1602 | 1/1 | 0.79 | 0.25 | 112,112,112,112 | 0 |
| 56 | MG | CA | 1819 | 1/1 | 0.79 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3498 | 1/1 | 0.79 | 0.43 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3188 | 1/1 | 0.79 | 0.40 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3244 | 1/1 | 0.79 | 1.33 | 67,67,67,67 | 0 |
| 56 | MG | CA | 1683 | 1/1 | 0.79 | 0.58 | 62,62,62,62 | 0 |
| 56 | MG | BA | 2910 | 1/1 | 0.79 | 0.11 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3008 | 1/1 | 0.79 | 0.52 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1941 | 1/1 | 0.79 | 0.75 | 100,100,100,100 | 0 |
| 56 | MG | CW | 110 | 1/1 | 0.79 | 0.11 | 90,90,90,90 | 0 |
| 56 | MG | AA | 1815 | 1/1 | 0.79 | 0.35 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3507 | 1/1 | 0.79 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | BA | 2992 | 1/1 | 0.79 | 0.51 | 73,73,73,73 | 0 |
| 56 | MG | AA | 1823 | 1/1 | 0.79 | 0.29 | 96,96,96,96 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 2994 | 1/1 | 0.79 | 0.51 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3205 | 1/1 | 0.79 | 0.45 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3032 | 1/1 | 0.79 | 0.67 | 97,97,97,97 | 0 |
| 56 | MG | AA | 1946 | 1/1 | 0.79 | 0.30 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3367 | 1/1 | 0.79 | 0.21 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3371 | 1/1 | 0.79 | 0.39 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3062 | 1/1 | 0.79 | 0.47 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3265 | 1/1 | 0.79 | 0.21 | 114,114,114,114 | 0 |
| 56 | MG | BA | 3048 | 1/1 | 0.79 | 0.33 | 54,54,54,54 | 0 |
| 56 | MG | CA | 1872 | 1/1 | 0.79 | 0.31 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3618 | 1/1 | 0.79 | 0.27 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3621 | 1/1 | 0.79 | 0.40 | 77,77,77,77 | 0 |
| 56 | MG | DA | 2916 | 1/1 | 0.79 | 0.49 | 57,57,57,57 | 0 |
| 56 | MG | AA | 1797 | 1/1 | 0.79 | 0.36 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3128 | 1/1 | 0.79 | 0.99 | 111,111,111,111 | 0 |
| 56 | MG | CA | 1879 | 1/1 | 0.79 | 0.35 | 53,53,53,53 | 0 |
| 56 | MG | DA | 2931 | 1/1 | 0.79 | 0.22 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3275 | 1/1 | 0.79 | 0.44 | 102,102,102,102 | 0 |
| 56 | MG | AA | 1752 | 1/1 | 0.79 | 0.37 | 183,183,183,183 | 0 |
| 56 | MG | AA | 1646 | 1/1 | 0.79 | 0.10 | 73,73,73,73 | 0 |
| 56 | MG | CA | 1728 | 1/1 | 0.79 | 0.20 | 195,195,195,195 | 0 |
| 56 | MG | CA | 1892 | 1/1 | 0.79 | 0.14 | 150,150,150,150 | 0 |
| 56 | MG | BA | 3568 | 1/1 | 0.79 | 0.17 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3628 | 1/1 | 0.79 | 0.67 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1937 | 1/1 | 0.79 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3161 | 1/1 | 0.79 | 0.21 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3234 | 1/1 | 0.79 | 0.12 | 83,83,83,83 | 0 |
| 56 | MG | BA | 3097 | 1/1 | 0.79 | 0.73 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3109 | 1/1 | 0.80 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3616 | 1/1 | 0.80 | 0.61 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3043 | 1/1 | 0.80 | 0.46 | 155,155,155,155 | 0 |
| 56 | MG | BA | 3622 | 1/1 | 0.80 | 0.97 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3120 | 1/1 | 0.80 | 0.37 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3404 | 1/1 | 0.80 | 1.16 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3215 | 1/1 | 0.80 | 0.18 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3121 | 1/1 | 0.80 | 0.81 | 137,137,137,137 | 0 |
| 56 | MG | DA | 3188 | 1/1 | 0.80 | 0.47 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3471 | 1/1 | 0.80 | 0.33 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3238 | 1/1 | 0.80 | 0.30 | 89,89,89,89 | 0 |
| 56 | MG | CA | 1896 | 1/1 | 0.80 | 0.38 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3641 | 1/1 | 0.80 | 0.61 | 60,60,60,60 | 0 |
| 56 | MG | CA | 1709 | 1/1 | 0.80 | 0.26 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3422 | 1/1 | 0.80 | 0.55 | 42,42,42,42 | 0 |
| 56 | MG | DA | 2980 | 1/1 | 0.80 | 0.38 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3563 | 1/1 | 0.80 | 0.69 | 83,83,83,83 | 0 |
| 56 | MG | BA | 2940 | 1/1 | 0.80 | 0.15 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1912 | 1/1 | 0.80 | 0.23 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3180 | 1/1 | 0.80 | 0.72 | 113,113,113,113 | 0 |
| 56 | MG | AA | 1635 | 1/1 | 0.80 | 0.36 | 106,106,106,106 | 0 |
| 56 | MG | AA | 1929 | 1/1 | 0.80 | 0.36 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3287 | 1/1 | 0.80 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3095 | 1/1 | 0.80 | 0.41 | 90,90,90,90 | 0 |
| 56 | MG | BA | 3292 | 1/1 | 0.80 | 0.64 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1644 | 1/1 | 0.80 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3010 | 1/1 | 0.80 | 0.79 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3008 | 1/1 | 0.80 | 0.47 | 66,66,66,66 | 0 |
| 56 | MG | CW | 105 | 1/1 | 0.80 | 0.64 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3026 | 1/1 | 0.80 | 0.24 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3349 | 1/1 | 0.80 | 0.58 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3027 | 1/1 | 0.80 | 0.15 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3576 | 1/1 | 0.80 | 0.28 | 102,102,102,102 | 0 |
| 56 | MG | BA | 3488 | 1/1 | 0.80 | 0.33 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3352 | 1/1 | 0.80 | 0.13 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3583 | 1/1 | 0.80 | 0.16 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3585 | 1/1 | 0.80 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | CA | 1665 | 1/1 | 0.80 | 0.58 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3362 | 1/1 | 0.80 | 0.99 | 83,83,83,83 | 0 |
| 56 | MG | CA | 1737 | 1/1 | 0.80 | 0.93 | 98,98,98,98 | 0 |
| 56 | MG | BA | 3241 | 1/1 | 0.80 | 0.62 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1897 | 1/1 | 0.80 | 1.14 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3245 | 1/1 | 0.80 | 0.58 | 185,185,185,185 | 0 |
| 56 | MG | CM | 201 | 1/1 | 0.80 | 1.20 | 84,84,84,84 | 0 |
| 56 | MG | BA | 2985 | 1/1 | 0.80 | 0.34 | 61,61,61,61 | 0 |
| 56 | MG | BA | 2988 | 1/1 | 0.80 | 0.37 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1675 | 1/1 | 0.80 | 0.89 | 96,96,96,96 | 0 |
| 56 | MG | BA | 2954 | 1/1 | 0.80 | 0.46 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3532 | 1/1 | 0.80 | 0.29 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1744 | 1/1 | 0.80 | 0.48 | 103,103,103,103 | 0 |
| 56 | MG | BA | 3206 | 1/1 | 0.80 | 0.24 | 176,176,176,176 | 0 |
| 56 | MG | DB | 214 | 1/1 | 0.80 | 0.13 | 110,110,110,110 | 0 |
| 56 | MG | BA | 3259 | 1/1 | 0.80 | 0.27 | 77,77,77,77 | 0 |
| 56 | MG | CA | 1871 | 1/1 | 0.80 | 0.13 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3157 | 1/1 | 0.80 | 0.72 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3426 | 1/1 | 0.80 | 0.50 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AV | 101 | 1/1 | 0.80 | 0.75 | 109,109,109,109 | 0 |
| 56 | MG | BA | 3613 | 1/1 | 0.80 | 0.60 | 76,76,76,76 | 0 |
| 56 | MG | CA | 1630 | 1/1 | 0.81 | 0.22 | 177,177,177,177 | 0 |
| 56 | MG | DA | 3043 | 1/1 | 0.81 | 1.55 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3327 | 1/1 | 0.81 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | CA | 1708 | 1/1 | 0.81 | 0.37 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1738 | 1/1 | 0.81 | 0.65 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1872 | 1/1 | 0.81 | 0.69 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1873 | 1/1 | 0.81 | 0.23 | 110,110,110,110 | 0 |
| 56 | MG | BA | 3712 | 1/1 | 0.81 | 0.50 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3419 | 1/1 | 0.81 | 0.35 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3064 | 1/1 | 0.81 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | BA | 2964 | 1/1 | 0.81 | 0.25 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1700 | 1/1 | 0.81 | 0.51 | 158,158,158,158 | 0 |
| 56 | MG | CA | 1895 | 1/1 | 0.81 | 0.31 | 126,126,126,126 | 0 |
| 56 | MG | BA | 3543 | 1/1 | 0.81 | 0.29 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3074 | 1/1 | 0.81 | 1.36 | 99,99,99,99 | 0 |
| 56 | MG | BA | 3086 | 1/1 | 0.81 | 0.55 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3436 | 1/1 | 0.81 | 0.30 | 86,86,86,86 | 0 |
| 56 | MG | AA | 1989 | 1/1 | 0.81 | 0.21 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1828 | 1/1 | 0.81 | 0.10 | 97,97,97,97 | 0 |
| 56 | MG | AA | 1716 | 1/1 | 0.81 | 0.46 | 103,103,103,103 | 0 |
| 56 | MG | DA | 2956 | 1/1 | 0.81 | 0.32 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3106 | 1/1 | 0.81 | 0.32 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3096 | 1/1 | 0.81 | 0.79 | 173,173,173,173 | 0 |
| 56 | MG | BB | 213 | 1/1 | 0.81 | 0.35 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3060 | 1/1 | 0.81 | 0.53 | 80,80,80,80 | 0 |
| 56 | MG | DA | 2979 | 1/1 | 0.81 | 0.39 | 81,81,81,81 | 0 |
| 56 | MG | BA | 3331 | 1/1 | 0.81 | 0.69 | 121,121,121,121 | 0 |
| 56 | MG | DA | 3595 | 1/1 | 0.81 | 0.42 | 106,106,106,106 | 0 |
| 56 | MG | AA | 1830 | 1/1 | 0.81 | 0.73 | 179,179,179,179 | 0 |
| 56 | MG | BA | 3571 | 1/1 | 0.81 | 0.49 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3346 | 1/1 | 0.81 | 0.12 | 111,111,111,111 | 0 |
| 56 | MG | AA | 1733 | 1/1 | 0.81 | 1.05 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3421 | 1/1 | 0.81 | 0.35 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3364 | 1/1 | 0.81 | 0.14 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1774 | 1/1 | 0.81 | 0.41 | 68,68,68,68 | 0 |
| 56 | MG | AT | 202 | 1/1 | 0.81 | 0.40 | 100,100,100,100 | 0 |
| 56 | MG | BA | 3585 | 1/1 | 0.81 | 0.48 | 87,87,87,87 | 0 |
| 56 | MG | BA | 2991 | 1/1 | 0.81 | 0.36 | 80,80,80,80 | 0 |
| 56 | MG | CA | 1610 | 1/1 | 0.81 | 0.27 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3391 | 1/1 | 0.81 | 0.64 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | CA | 1766 | 1/1 | 0.81 | 0.39 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3447 | 1/1 | 0.81 | 0.64 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3242 | 1/1 | 0.81 | 0.52 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3290 | 1/1 | 0.81 | 0.29 | 38,38,38,38 | 0 |
| 56 | MG | CA | 1866 | 1/1 | 0.81 | 0.71 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3520 | 1/1 | 0.81 | 0.46 | 51,51,51,51 | 0 |
| 56 | MG | DX | 101 | 1/1 | 0.81 | 0.41 | 99,99,99,99 | 0 |
| 56 | MG | DA | 3317 | 1/1 | 0.81 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | AA | 1971 | 1/1 | 0.81 | 0.18 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3266 | 1/1 | 0.82 | 0.55 | 64,64,64,64 | 0 |
| 56 | MG | CA | 1689 | 1/1 | 0.82 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3459 | 1/1 | 0.82 | 0.26 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3087 | 1/1 | 0.82 | 0.49 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3258 | 1/1 | 0.82 | 0.56 | 67,67,67,67 | 0 |
| 56 | MG | CA | 1696 | 1/1 | 0.82 | 0.30 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3151 | 1/1 | 0.82 | 0.30 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3307 | 1/1 | 0.82 | 0.18 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1931 | 1/1 | 0.82 | 0.24 | 102,102,102,102 | 0 |
| 56 | MG | BA | 2923 | 1/1 | 0.82 | 1.32 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3068 | 1/1 | 0.82 | 0.44 | 115,115,115,115 | 0 |
| 56 | MG | AA | 1973 | 1/1 | 0.82 | 0.64 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3035 | 1/1 | 0.82 | 0.36 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3038 | 1/1 | 0.82 | 0.37 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3523 | 1/1 | 0.82 | 0.59 | 47,47,47,47 | 0 |
| 56 | MG | BA | 2960 | 1/1 | 0.82 | 0.50 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1679 | 1/1 | 0.82 | 0.13 | 112,112,112,112 | 0 |
| 56 | MG | CA | 1649 | 1/1 | 0.82 | 0.15 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1650 | 1/1 | 0.82 | 0.18 | 170,170,170,170 | 0 |
| 56 | MG | BA | 3135 | 1/1 | 0.82 | 0.45 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1795 | 1/1 | 0.82 | 0.62 | 84,84,84,84 | 0 |
| 56 | MG | DA | 2926 | 1/1 | 0.82 | 0.54 | 91,91,91,91 | 0 |
| 56 | MG | CA | 1662 | 1/1 | 0.82 | 0.55 | 90,90,90,90 | 0 |
| 56 | MG | DA | 3535 | 1/1 | 0.82 | 0.31 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3539 | 1/1 | 0.82 | 0.31 | 98,98,98,98 | 0 |
| 56 | MG | CA | 1798 | 1/1 | 0.82 | 0.32 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3587 | 1/1 | 0.82 | 0.93 | 104,104,104,104 | 0 |
| 56 | MG | CA | 1722 | 1/1 | 0.82 | 0.72 | 168,168,168,168 | 0 |
| 56 | MG | AA | 1751 | 1/1 | 0.82 | 0.58 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3571 | 1/1 | 0.82 | 0.94 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3276 | 1/1 | 0.82 | 0.56 | 107,107,107,107 | 0 |
| 56 | MG | AA | 1616 | 1/1 | 0.82 | 0.46 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3578 | 1/1 | 0.82 | 0.55 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3369 | 1/1 | 0.82 | 0.59 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3279 | 1/1 | 0.82 | 0.34 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3089 | 1/1 | 0.82 | 0.10 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3664 | 1/1 | 0.82 | 0.21 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3589 | 1/1 | 0.82 | 0.18 | 74,74,74,74 | 0 |
| 56 | MG | DA | 2950 | 1/1 | 0.82 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3601 | 1/1 | 0.82 | 0.33 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3083 | 1/1 | 0.82 | 0.22 | 69,69,69,69 | 0 |
| 56 | MG | CA | 1811 | 1/1 | 0.82 | 0.27 | 54,54,54,54 | 0 |
| 56 | MG | DA | 2963 | 1/1 | 0.82 | 0.34 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3477 | 1/1 | 0.82 | 0.32 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3112 | 1/1 | 0.82 | 0.21 | 141,141,141,141 | 0 |
| 56 | MG | AA | 1753 | 1/1 | 0.82 | 0.52 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3674 | 1/1 | 0.82 | 0.32 | 55,55,55,55 | 0 |
| 56 | MG | AA | 1746 | 1/1 | 0.82 | 0.38 | 93,93,93,93 | 0 |
| 56 | MG | AA | 1713 | 1/1 | 0.82 | 0.14 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3121 | 1/1 | 0.82 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3424 | 1/1 | 0.82 | 0.40 | 52,52,52,52 | 0 |
| 56 | MG | CA | 1916 | 1/1 | 0.82 | 0.62 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3491 | 1/1 | 0.82 | 0.25 | 85,85,85,85 | 0 |
| 56 | MG | DB | 213 | 1/1 | 0.82 | 0.21 | 76,76,76,76 | 0 |
| 56 | MG | CA | 1823 | 1/1 | 0.82 | 0.30 | 166,166,166,166 | 0 |
| 56 | MG | DA | 3178 | 1/1 | 0.82 | 0.31 | 40,40,40,40 | 0 |
| 56 | MG | DA | 2991 | 1/1 | 0.82 | 0.68 | 80,80,80,80 | 0 |
| 56 | MG | DQ | 201 | 1/1 | 0.82 | 0.22 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1921 | 1/1 | 0.82 | 0.26 | 108,108,108,108 | 0 |
| 56 | MG | BA | 3701 | 1/1 | 0.82 | 0.34 | 74,74,74,74 | 0 |
| 56 | MG | CA | 1831 | 1/1 | 0.82 | 0.48 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3560 | 1/1 | 0.82 | 0.37 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3561 | 1/1 | 0.82 | 0.33 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3454 | 1/1 | 0.83 | 0.34 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3304 | 1/1 | 0.83 | 0.45 | 167,167,167,167 | 0 |
| 56 | MG | BX | 102 | 1/1 | 0.83 | 0.35 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1864 | 1/1 | 0.83 | 0.20 | 116,116,116,116 | 0 |
| 56 | MG | DA | 3470 | 1/1 | 0.83 | 0.22 | 81,81,81,81 | 0 |
| 56 | MG | BA | 2975 | 1/1 | 0.83 | 0.23 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3478 | 1/1 | 0.83 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3460 | 1/1 | 0.83 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | AA | 1650 | 1/1 | 0.83 | 0.16 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3318 | 1/1 | 0.83 | 0.18 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3473 | 1/1 | 0.83 | 0.81 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3326 | 1/1 | 0.83 | 0.63 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1992 | 1/1 | 0.83 | 0.27 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3480 | 1/1 | 0.83 | 0.29 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3222 | 1/1 | 0.83 | 0.46 | 70,70,70,70 | 0 |
| 56 | MG | CA | 1622 | 1/1 | 0.83 | 0.40 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3487 | 1/1 | 0.83 | 0.40 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3223 | 1/1 | 0.83 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3581 | 1/1 | 0.83 | 0.45 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3176 | 1/1 | 0.83 | 0.29 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3179 | 1/1 | 0.83 | 0.88 | 98,98,98,98 | 0 |
| 56 | MG | CW | 111 | 1/1 | 0.83 | 0.30 | 82,82,82,82 | 0 |
| 56 | MG | CA | 1642 | 1/1 | 0.83 | 0.73 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3693 | 1/1 | 0.83 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1727 | 1/1 | 0.83 | 0.14 | 112,112,112,112 | 0 |
| 56 | MG | BA | 3367 | 1/1 | 0.83 | 0.36 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3500 | 1/1 | 0.83 | 0.38 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3698 | 1/1 | 0.83 | 0.32 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3542 | 1/1 | 0.83 | 0.51 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3010 | 1/1 | 0.83 | 0.48 | 93,93,93,93 | 0 |
| 56 | MG | AA | 1640 | 1/1 | 0.83 | 0.12 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3063 | 1/1 | 0.83 | 0.18 | 99,99,99,99 | 0 |
| 56 | MG | DA | 2907 | 1/1 | 0.83 | 0.10 | 75,75,75,75 | 0 |
| 56 | MG | AA | 1641 | 1/1 | 0.83 | 0.12 | 121,121,121,121 | 0 |
| 56 | MG | CA | 1653 | 1/1 | 0.83 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | AA | 1938 | 1/1 | 0.83 | 0.13 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3579 | 1/1 | 0.83 | 0.36 | 36,36,36,36 | 0 |
| 56 | MG | CA | 1844 | 1/1 | 0.83 | 0.82 | 104,104,104,104 | 0 |
| 56 | MG | CA | 1660 | 1/1 | 0.83 | 0.41 | 94,94,94,94 | 0 |
| 56 | MG | AA | 1903 | 1/1 | 0.83 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3077 | 1/1 | 0.83 | 0.35 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3081 | 1/1 | 0.83 | 0.40 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3594 | 1/1 | 0.83 | 0.30 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3082 | 1/1 | 0.83 | 0.09 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3522 | 1/1 | 0.83 | 1.09 | 96,96,96,96 | 0 |
| 56 | MG | BA | 3069 | 1/1 | 0.83 | 0.23 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3616 | 1/1 | 0.83 | 0.23 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1740 | 1/1 | 0.83 | 0.40 | 105,105,105,105 | 0 |
| 56 | MG | DA | 3390 | 1/1 | 0.83 | 0.74 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3405 | 1/1 | 0.83 | 0.70 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3074 | 1/1 | 0.83 | 0.09 | 108,108,108,108 | 0 |
| 56 | MG | CA | 1870 | 1/1 | 0.83 | 0.11 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3075 | 1/1 | 0.83 | 0.69 | 73,73,73,73 | 0 |
| 56 | MG | BB | 205 | 1/1 | 0.83 | 0.30 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1609 | 1/1 | 0.83 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | AA | 1705 | 1/1 | 0.83 | 0.28 | 101,101,101,101 | 0 |
| 56 | MG | BB | 209 | 1/1 | 0.83 | 0.27 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3541 | 1/1 | 0.83 | 0.21 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3608 | 1/1 | 0.83 | 0.95 | 54,54,54,54 | 0 |
| 56 | MG | AA | 1921 | 1/1 | 0.83 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3429 | 1/1 | 0.83 | 0.78 | 59,59,59,59 | 0 |
| 56 | MG | AA | 1925 | 1/1 | 0.83 | 0.52 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1890 | 1/1 | 0.83 | 0.26 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1789 | 1/1 | 0.83 | 0.93 | 184,184,184,184 | 0 |
| 56 | MG | DA | 3130 | 1/1 | 0.83 | 0.61 | 69,69,69,69 | 0 |
| 56 | MG | CA | 1893 | 1/1 | 0.83 | 0.46 | 125,125,125,125 | 0 |
| 56 | MG | DA | 3162 | 1/1 | 0.83 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3209 | 1/1 | 0.83 | 0.33 | 96,96,96,96 | 0 |
| 56 | MG | AA | 1986 | 1/1 | 0.83 | 0.79 | 69,69,69,69 | 0 |
| 56 | MG | AA | 1775 | 1/1 | 0.84 | 0.95 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3409 | 1/1 | 0.84 | 0.19 | 115,115,115,115 | 0 |
| 56 | MG | CA | 1604 | 1/1 | 0.84 | 0.47 | 99,99,99,99 | 0 |
| 56 | MG | BA | 3138 | 1/1 | 0.84 | 0.28 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3554 | 1/1 | 0.84 | 0.39 | 62,62,62,62 | 0 |
| 56 | MG | DA | 2934 | 1/1 | 0.84 | 0.29 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3067 | 1/1 | 0.84 | 0.58 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3068 | 1/1 | 0.84 | 0.28 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3050 | 1/1 | 0.84 | 0.34 | 60,60,60,60 | 0 |
| 56 | MG | CA | 1897 | 1/1 | 0.84 | 0.24 | 227,227,227,227 | 0 |
| 56 | MG | BA | 3208 | 1/1 | 0.84 | 0.40 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3071 | 1/1 | 0.84 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | CA | 1901 | 1/1 | 0.84 | 0.24 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3702 | 1/1 | 0.84 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3503 | 1/1 | 0.84 | 0.69 | 195,195,195,195 | 0 |
| 56 | MG | BA | 2987 | 1/1 | 0.84 | 0.40 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3083 | 1/1 | 0.84 | 0.76 | 125,125,125,125 | 0 |
| 56 | MG | AA | 1966 | 1/1 | 0.84 | 0.29 | 51,51,51,51 | 0 |
| 56 | MG | CA | 1908 | 1/1 | 0.84 | 0.27 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1690 | 1/1 | 0.84 | 0.16 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3090 | 1/1 | 0.84 | 0.25 | 47,47,47,47 | 0 |
| 56 | MG | AA | 1787 | 1/1 | 0.84 | 0.31 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3560 | 1/1 | 0.84 | 0.42 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3564 | 1/1 | 0.84 | 0.54 | 25,25,25,25 | 0 |
| 56 | MG | DA | 2967 | 1/1 | 0.84 | 0.90 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3376 | 1/1 | 0.84 | 0.42 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3574 | 1/1 | 0.84 | 0.44 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3715 | 1/1 | 0.84 | 0.44 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3098 | 1/1 | 0.84 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3077 | 1/1 | 0.84 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | DA | 2976 | 1/1 | 0.84 | 0.39 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3122 | 1/1 | 0.84 | 0.14 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3451 | 1/1 | 0.84 | 0.60 | 83,83,83,83 | 0 |
| 56 | MG | CA | 1761 | 1/1 | 0.84 | 0.48 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3524 | 1/1 | 0.84 | 0.26 | 95,95,95,95 | 0 |
| 56 | MG | DA | 3402 | 1/1 | 0.84 | 0.65 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3591 | 1/1 | 0.84 | 0.15 | 129,129,129,129 | 0 |
| 56 | MG | CV | 102 | 1/1 | 0.84 | 0.70 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1993 | 1/1 | 0.84 | 0.36 | 73,73,73,73 | 0 |
| 56 | MG | DA | 2993 | 1/1 | 0.84 | 0.41 | 85,85,85,85 | 0 |
| 56 | MG | DA | 3609 | 1/1 | 0.84 | 0.24 | 27,27,27,27 | 0 |
| 56 | MG | DA | 2997 | 1/1 | 0.84 | 0.89 | 132,132,132,132 | 0 |
| 56 | MG | CA | 1776 | 1/1 | 0.84 | 0.68 | 125,125,125,125 | 0 |
| 56 | MG | CW | 104 | 1/1 | 0.84 | 0.28 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3158 | 1/1 | 0.84 | 0.46 | 18,18,18,18 | 0 |
| 56 | MG | CA | 1851 | 1/1 | 0.84 | 0.36 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3582 | 1/1 | 0.84 | 0.57 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3638 | 1/1 | 0.84 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | BA | 2921 | 1/1 | 0.84 | 0.66 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3191 | 1/1 | 0.84 | 0.32 | 64,64,64,64 | 0 |
| 56 | MG | CW | 115 | 1/1 | 0.84 | 0.30 | 81,81,81,81 | 0 |
| 56 | MG | CA | 1865 | 1/1 | 0.84 | 0.48 | 108,108,108,108 | 0 |
| 56 | MG | BA | 3390 | 1/1 | 0.84 | 0.41 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1714 | 1/1 | 0.84 | 0.18 | 104,104,104,104 | 0 |
| 56 | MG | BA | 3653 | 1/1 | 0.84 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3654 | 1/1 | 0.84 | 0.24 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3455 | 1/1 | 0.84 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3537 | 1/1 | 0.84 | 0.32 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3039 | 1/1 | 0.84 | 0.78 | 176,176,176,176 | 0 |
| 56 | MG | AA | 1680 | 1/1 | 0.84 | 0.17 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3397 | 1/1 | 0.84 | 0.89 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3297 | 1/1 | 0.84 | 0.42 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3162 | 1/1 | 0.84 | 0.51 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1676 | 1/1 | 0.84 | 0.32 | 152,152,152,152 | 0 |
| 56 | MG | D1 | 101 | 1/1 | 0.84 | 0.17 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3199 | 1/1 | 0.84 | 0.29 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3468 | 1/1 | 0.85 | 0.26 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3494 | 1/1 | 0.85 | 0.28 | 112,112,112,112 | 0 |
| 56 | MG | CA | 1857 | 1/1 | 0.85 | 0.59 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3472 | 1/1 | 0.85 | 0.48 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3499 | 1/1 | 0.85 | 0.17 | 98,98,98,98 | 0 |
| 56 | MG | DA | 3057 | 1/1 | 0.85 | 0.11 | 107,107,107,107 | 0 |
| 56 | MG | CA | 1861 | 1/1 | 0.85 | 0.50 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3623 | 1/1 | 0.85 | 0.28 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3336 | 1/1 | 0.85 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3204 | 1/1 | 0.85 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1755 | 1/1 | 0.85 | 0.91 | 120,120,120,120 | 0 |
| 56 | MG | BA | 3343 | 1/1 | 0.85 | 0.24 | 73,73,73,73 | 0 |
| 56 | MG | BA | 2971 | 1/1 | 0.85 | 1.04 | 89,89,89,89 | 0 |
| 56 | MG | AA | 1817 | 1/1 | 0.85 | 0.55 | 175,175,175,175 | 0 |
| 56 | MG | BA | 3154 | 1/1 | 0.85 | 0.84 | 169,169,169,169 | 0 |
| 56 | MG | CA | 1688 | 1/1 | 0.85 | 0.26 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3530 | 1/1 | 0.85 | 0.29 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3567 | 1/1 | 0.85 | 0.40 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3485 | 1/1 | 0.85 | 0.49 | 53,53,53,53 | 0 |
| 56 | MG | CA | 1782 | 1/1 | 0.85 | 0.54 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3486 | 1/1 | 0.85 | 0.27 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3356 | 1/1 | 0.85 | 0.13 | 107,107,107,107 | 0 |
| 56 | MG | CA | 1788 | 1/1 | 0.85 | 0.19 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1819 | 1/1 | 0.85 | 0.96 | 84,84,84,84 | 0 |
| 56 | MG | BA | 2904 | 1/1 | 0.85 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | AA | 1822 | 1/1 | 0.85 | 0.17 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3492 | 1/1 | 0.85 | 0.60 | 102,102,102,102 | 0 |
| 56 | MG | AW | 105 | 1/1 | 0.85 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3167 | 1/1 | 0.85 | 0.38 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1882 | 1/1 | 0.85 | 0.48 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3031 | 1/1 | 0.85 | 0.50 | 255,255,255,255 | 0 |
| 56 | MG | AA | 1848 | 1/1 | 0.85 | 0.26 | 125,125,125,125 | 0 |
| 56 | MG | AA | 1678 | 1/1 | 0.85 | 0.16 | 101,101,101,101 | 0 |
| 56 | MG | CA | 1711 | 1/1 | 0.85 | 0.66 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3508 | 1/1 | 0.85 | 0.30 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1939 | 1/1 | 0.85 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3124 | 1/1 | 0.85 | 0.54 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3519 | 1/1 | 0.85 | 0.64 | 93,93,93,93 | 0 |
| 56 | MG | CA | 1909 | 1/1 | 0.85 | 0.16 | 133,133,133,133 | 0 |
| 56 | MG | AA | 1668 | 1/1 | 0.85 | 0.35 | 90,90,90,90 | 0 |
| 56 | MG | AA | 1724 | 1/1 | 0.85 | 0.46 | 133,133,133,133 | 0 |
| 56 | MG | AA | 1729 | 1/1 | 0.85 | 0.49 | 99,99,99,99 | 0 |
| 56 | MG | BA | 3132 | 1/1 | 0.85 | 0.40 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3604 | 1/1 | 0.85 | 0.42 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1745 | 1/1 | 0.85 | 0.21 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3425 | 1/1 | 0.85 | 0.55 | 52,52,52,52 | 0 |
| 56 | MG | DA | 2995 | 1/1 | 0.85 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3240 | 1/1 | 0.85 | 0.22 | 75,75,75,75 | 0 |
| 56 | MG | AA | 1809 | 1/1 | 0.85 | 0.18 | 106,106,106,106 | 0 |
| 56 | MG | CA | 1922 | 1/1 | 0.85 | 0.32 | 67,67,67,67 | 0 |
| 56 | MG | CA | 1730 | 1/1 | 0.85 | 0.16 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3629 | 1/1 | 0.85 | 0.23 | 67,67,67,67 | 0 |
| 56 | MG | CA | 1657 | 1/1 | 0.85 | 0.24 | 95,95,95,95 | 0 |
| 56 | MG | DA | 3434 | 1/1 | 0.85 | 0.45 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3190 | 1/1 | 0.85 | 0.27 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1659 | 1/1 | 0.85 | 0.38 | 57,57,57,57 | 0 |
| 56 | MG | AA | 1604 | 1/1 | 0.85 | 0.21 | 91,91,91,91 | 0 |
| 56 | MG | AA | 1867 | 1/1 | 0.85 | 1.19 | 96,96,96,96 | 0 |
| 56 | MG | DA | 3014 | 1/1 | 0.85 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | CW | 107 | 1/1 | 0.85 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | DB | 210 | 1/1 | 0.85 | 0.25 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3261 | 1/1 | 0.85 | 0.26 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3059 | 1/1 | 0.85 | 0.36 | 43,43,43,43 | 0 |
| 56 | MG | AA | 1758 | 1/1 | 0.85 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | DD | 301 | 1/1 | 0.85 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3310 | 1/1 | 0.85 | 0.50 | 117,117,117,117 | 0 |
| 56 | MG | DF | 302 | 1/1 | 0.85 | 0.25 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3029 | 1/1 | 0.85 | 0.29 | 73,73,73,73 | 0 |
| 56 | MG | DQ | 202 | 1/1 | 0.85 | 0.28 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3611 | 1/1 | 0.85 | 0.23 | 67,67,67,67 | 0 |
| 56 | MG | BA | 2965 | 1/1 | 0.85 | 0.47 | 167,167,167,167 | 0 |
| 56 | MG | BA | 2966 | 1/1 | 0.85 | 0.36 | 49,49,49,49 | 0 |
| 56 | MG | BA | 2967 | 1/1 | 0.85 | 0.59 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3486 | 1/1 | 0.85 | 0.37 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3617 | 1/1 | 0.85 | 0.16 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1763 | 1/1 | 0.86 | 0.27 | 88,88,88,88 | 0 |
| 56 | MG | DA | 2996 | 1/1 | 0.86 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3070 | 1/1 | 0.86 | 0.55 | 159,159,159,159 | 0 |
| 56 | MG | CA | 1919 | 1/1 | 0.86 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3708 | 1/1 | 0.86 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3196 | 1/1 | 0.86 | 0.35 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3002 | 1/1 | 0.86 | 0.33 | 139,139,139,139 | 0 |
| 56 | MG | BA | 2952 | 1/1 | 0.86 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3024 | 1/1 | 0.86 | 0.31 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1729 | 1/1 | 0.86 | 0.21 | 139,139,139,139 | 0 |
| 56 | MG | DA | 3250 | 1/1 | 0.86 | 0.61 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3604 | 1/1 | 0.86 | 0.37 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3260 | 1/1 | 0.86 | 0.27 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1732 | 1/1 | 0.86 | 0.23 | 60,60,60,60 | 0 |
| 56 | MG | BA | 2957 | 1/1 | 0.86 | 0.46 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3013 | 1/1 | 0.86 | 0.39 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3271 | 1/1 | 0.86 | 0.27 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1835 | 1/1 | 0.86 | 0.57 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3166 | 1/1 | 0.86 | 0.29 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3504 | 1/1 | 0.86 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3289 | 1/1 | 0.86 | 0.26 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3017 | 1/1 | 0.86 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1913 | 1/1 | 0.86 | 0.39 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3294 | 1/1 | 0.86 | 0.53 | 64,64,64,64 | 0 |
| 56 | MG | CA | 1839 | 1/1 | 0.86 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3300 | 1/1 | 0.86 | 0.27 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3478 | 1/1 | 0.86 | 0.12 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3028 | 1/1 | 0.86 | 0.35 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1841 | 1/1 | 0.86 | 0.77 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3721 | 1/1 | 0.86 | 0.19 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3361 | 1/1 | 0.86 | 0.19 | 106,106,106,106 | 0 |
| 56 | MG | BA | 3723 | 1/1 | 0.86 | 0.20 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1643 | 1/1 | 0.86 | 0.25 | 114,114,114,114 | 0 |
| 56 | MG | BA | 3040 | 1/1 | 0.86 | 0.27 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3614 | 1/1 | 0.86 | 0.16 | 107,107,107,107 | 0 |
| 56 | MG | DA | 3046 | 1/1 | 0.86 | 0.35 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3047 | 1/1 | 0.86 | 0.71 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3049 | 1/1 | 0.86 | 0.61 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3559 | 1/1 | 0.86 | 0.61 | 51,51,51,51 | 0 |
| 56 | MG | CR | 101 | 1/1 | 0.86 | 1.59 | 182,182,182,182 | 0 |
| 56 | MG | BA | 3559 | 1/1 | 0.86 | 0.31 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3055 | 1/1 | 0.86 | 0.12 | 75,75,75,75 | 0 |
| 56 | MG | AA | 1734 | 1/1 | 0.86 | 0.24 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3058 | 1/1 | 0.86 | 0.10 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3370 | 1/1 | 0.86 | 0.36 | 50,50,50,50 | 0 |
| 56 | MG | BA | 2962 | 1/1 | 0.86 | 0.70 | 78,78,78,78 | 0 |
| 56 | MG | BA | 2995 | 1/1 | 0.86 | 0.22 | 92,92,92,92 | 0 |
| 56 | MG | BB | 214 | 1/1 | 0.86 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | CA | 1754 | 1/1 | 0.86 | 1.40 | 162,162,162,162 | 0 |
| 56 | MG | AA | 1923 | 1/1 | 0.86 | 0.11 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3365 | 1/1 | 0.86 | 0.37 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3227 | 1/1 | 0.86 | 0.22 | 90,90,90,90 | 0 |
| 56 | MG | AA | 1684 | 1/1 | 0.86 | 0.86 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1881 | 1/1 | 0.86 | 0.46 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3592 | 1/1 | 0.86 | 0.19 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3640 | 1/1 | 0.86 | 0.51 | 60,60,60,60 | 0 |
| 56 | MG | BF | 1901 | 1/1 | 0.86 | 0.28 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1658 | 1/1 | 0.86 | 0.16 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3088 | 1/1 | 0.86 | 0.18 | 167,167,167,167 | 0 |
| 56 | MG | BA | 3089 | 1/1 | 0.86 | 0.58 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3610 | 1/1 | 0.86 | 0.52 | 56,56,56,56 | 0 |
| 56 | MG | AA | 1606 | 1/1 | 0.86 | 0.13 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3612 | 1/1 | 0.86 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | CA | 1886 | 1/1 | 0.86 | 0.18 | 100,100,100,100 | 0 |
| 56 | MG | AA | 1651 | 1/1 | 0.86 | 0.30 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3392 | 1/1 | 0.86 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | AA | 1827 | 1/1 | 0.86 | 0.41 | 98,98,98,98 | 0 |
| 56 | MG | CA | 1695 | 1/1 | 0.86 | 0.41 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3400 | 1/1 | 0.86 | 0.35 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1637 | 1/1 | 0.86 | 0.12 | 67,67,67,67 | 0 |
| 56 | MG | DA | 2951 | 1/1 | 0.86 | 0.20 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3091 | 1/1 | 0.86 | 0.57 | 96,96,96,96 | 0 |
| 56 | MG | DA | 2952 | 1/1 | 0.86 | 0.69 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3407 | 1/1 | 0.86 | 0.11 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3411 | 1/1 | 0.86 | 0.56 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3302 | 1/1 | 0.86 | 0.69 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3423 | 1/1 | 0.86 | 0.28 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3423 | 1/1 | 0.86 | 0.20 | 35,35,35,35 | 0 |
| 56 | MG | DB | 212 | 1/1 | 0.86 | 0.09 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1611 | 1/1 | 0.86 | 0.32 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1898 | 1/1 | 0.86 | 0.23 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1759 | 1/1 | 0.86 | 0.88 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3590 | 1/1 | 0.86 | 0.26 | 90,90,90,90 | 0 |
| 56 | MG | CA | 1618 | 1/1 | 0.86 | 0.48 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1619 | 1/1 | 0.86 | 0.11 | 128,128,128,128 | 0 |
| 56 | MG | BA | 3305 | 1/1 | 0.86 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3149 | 1/1 | 0.86 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | AA | 1762 | 1/1 | 0.86 | 0.25 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3308 | 1/1 | 0.86 | 0.16 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3152 | 1/1 | 0.86 | 0.13 | 72,72,72,72 | 0 |
| 56 | MG | CA | 1637 | 1/1 | 0.86 | 0.29 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3700 | 1/1 | 0.86 | 0.37 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3145 | 1/1 | 0.86 | 0.26 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3322 | 1/1 | 0.87 | 0.28 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3662 | 1/1 | 0.87 | 0.42 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3221 | 1/1 | 0.87 | 0.22 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3079 | 1/1 | 0.87 | 0.38 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3080 | 1/1 | 0.87 | 0.38 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3181 | 1/1 | 0.87 | 0.51 | 56,56,56,56 | 0 |
| 56 | MG | CA | 1917 | 1/1 | 0.87 | 0.33 | 123,123,123,123 | 0 |
| 56 | MG | CA | 1672 | 1/1 | 0.87 | 0.25 | 78,78,78,78 | 0 |
| 56 | MG | B0 | 101 | 1/1 | 0.87 | 0.27 | 33,33,33,33 | 0 |
| 56 | MG | DA | 2986 | 1/1 | 0.87 | 0.36 | 110,110,110,110 | 0 |
| 56 | MG | BA | 3146 | 1/1 | 0.87 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3666 | 1/1 | 0.87 | 0.28 | 67,67,67,67 | 0 |
| 56 | MG | BA | 2903 | 1/1 | 0.87 | 0.41 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1894 | 1/1 | 0.87 | 0.27 | 124,124,124,124 | 0 |
| 56 | MG | DA | 3094 | 1/1 | 0.87 | 0.26 | 30,30,30,30 | 0 |
| 56 | MG | AA | 1666 | 1/1 | 0.87 | 0.43 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3013 | 1/1 | 0.87 | 0.81 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3368 | 1/1 | 0.87 | 0.14 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1667 | 1/1 | 0.87 | 0.30 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3104 | 1/1 | 0.87 | 0.33 | 70,70,70,70 | 0 |
| 56 | MG | CA | 1684 | 1/1 | 0.87 | 0.48 | 87,87,87,87 | 0 |
| 56 | MG | CA | 1847 | 1/1 | 0.87 | 0.28 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1849 | 1/1 | 0.87 | 0.23 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3469 | 1/1 | 0.87 | 0.16 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3366 | 1/1 | 0.87 | 0.45 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3569 | 1/1 | 0.87 | 0.34 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3384 | 1/1 | 0.87 | 0.31 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3017 | 1/1 | 0.87 | 0.36 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3281 | 1/1 | 0.87 | 0.23 | 73,73,73,73 | 0 |
| 56 | MG | CA | 1615 | 1/1 | 0.87 | 0.50 | 110,110,110,110 | 0 |
| 56 | MG | BA | 3192 | 1/1 | 0.87 | 0.26 | 90,90,90,90 | 0 |
| 56 | MG | CA | 1770 | 1/1 | 0.87 | 0.31 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1634 | 1/1 | 0.87 | 0.28 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3380 | 1/1 | 0.87 | 0.69 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1621 | 1/1 | 0.87 | 0.36 | 48,48,48,48 | 0 |
| 56 | MG | CA | 1779 | 1/1 | 0.87 | 0.36 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3160 | 1/1 | 0.87 | 0.57 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3387 | 1/1 | 0.87 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | BA | 2936 | 1/1 | 0.87 | 0.10 | 65,65,65,65 | 0 |
| 56 | MG | DA | 2909 | 1/1 | 0.87 | 0.60 | 85,85,85,85 | 0 |
| 56 | MG | CA | 1700 | 1/1 | 0.87 | 0.81 | 180,180,180,180 | 0 |
| 56 | MG | DA | 3189 | 1/1 | 0.87 | 0.52 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3291 | 1/1 | 0.87 | 0.48 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3216 | 1/1 | 0.87 | 0.30 | 23,23,23,23 | 0 |
| 56 | MG | AA | 1638 | 1/1 | 0.87 | 0.81 | 132,132,132,132 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | CA | 1705 | 1/1 | 0.87 | 0.24 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3037 | 1/1 | 0.87 | 0.42 | 77,77,77,77 | 0 |
| 56 | MG | CA | 1881 | 1/1 | 0.87 | 0.19 | 111,111,111,111 | 0 |
| 56 | MG | DA | 3042 | 1/1 | 0.87 | 0.62 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1988 | 1/1 | 0.87 | 0.40 | 53,53,53,53 | 0 |
| 56 | MG | CA | 1636 | 1/1 | 0.87 | 0.97 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3045 | 1/1 | 0.87 | 0.40 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1801 | 1/1 | 0.87 | 0.16 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3564 | 1/1 | 0.87 | 0.42 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3200 | 1/1 | 0.87 | 0.95 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3163 | 1/1 | 0.87 | 0.53 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3164 | 1/1 | 0.87 | 0.29 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3288 | 1/1 | 0.87 | 0.37 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3497 | 1/1 | 0.87 | 0.17 | 78,78,78,78 | 0 |
| 56 | MG | DB | 207 | 1/1 | 0.87 | 0.14 | 87,87,87,87 | 0 |
| 56 | MG | BA | 3626 | 1/1 | 0.87 | 0.57 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1935 | 1/1 | 0.87 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1956 | 1/1 | 0.87 | 0.32 | 110,110,110,110 | 0 |
| 56 | MG | DA | 2945 | 1/1 | 0.87 | 0.50 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1698 | 1/1 | 0.87 | 0.70 | 97,97,97,97 | 0 |
| 56 | MG | DA | 3304 | 1/1 | 0.87 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3472 | 1/1 | 0.87 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3415 | 1/1 | 0.87 | 0.24 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3482 | 1/1 | 0.87 | 0.54 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1868 | 1/1 | 0.87 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | DH | 201 | 1/1 | 0.87 | 0.26 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3309 | 1/1 | 0.87 | 0.27 | 81,81,81,81 | 0 |
| 56 | MG | AA | 1914 | 1/1 | 0.87 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3644 | 1/1 | 0.87 | 0.32 | 106,106,106,106 | 0 |
| 56 | MG | AA | 1806 | 1/1 | 0.87 | 0.47 | 111,111,111,111 | 0 |
| 56 | MG | BA | 3107 | 1/1 | 0.87 | 0.56 | 87,87,87,87 | 0 |
| 56 | MG | AA | 1920 | 1/1 | 0.87 | 0.11 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3079 | 1/1 | 0.87 | 0.41 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3500 | 1/1 | 0.87 | 0.76 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3217 | 1/1 | 0.88 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1867 | 1/1 | 0.88 | 0.23 | 82,82,82,82 | 0 |
| 56 | MG | CA | 1868 | 1/1 | 0.88 | 0.25 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3473 | 1/1 | 0.88 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3474 | 1/1 | 0.88 | 0.26 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1767 | 1/1 | 0.88 | 0.49 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3481 | 1/1 | 0.88 | 0.17 | 73,73,73,73 | 0 |
| 56 | MG | CA | 1768 | 1/1 | 0.88 | 0.24 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1617 | 1/1 | 0.88 | 0.24 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3296 | 1/1 | 0.88 | 0.14 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3682 | 1/1 | 0.88 | 0.27 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3490 | 1/1 | 0.88 | 0.26 | 96,96,96,96 | 0 |
| 56 | MG | BA | 3685 | 1/1 | 0.88 | 1.06 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3302 | 1/1 | 0.88 | 0.40 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3496 | 1/1 | 0.88 | 0.33 | 40,40,40,40 | 0 |
| 56 | MG | CA | 1876 | 1/1 | 0.88 | 0.31 | 127,127,127,127 | 0 |
| 56 | MG | BA | 3598 | 1/1 | 0.88 | 0.29 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3178 | 1/1 | 0.88 | 0.42 | 52,52,52,52 | 0 |
| 56 | MG | CA | 1616 | 1/1 | 0.88 | 0.41 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3358 | 1/1 | 0.88 | 0.50 | 150,150,150,150 | 0 |
| 56 | MG | DA | 3318 | 1/1 | 0.88 | 0.46 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3319 | 1/1 | 0.88 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3508 | 1/1 | 0.88 | 0.36 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1852 | 1/1 | 0.88 | 0.13 | 89,89,89,89 | 0 |
| 56 | MG | DA | 3321 | 1/1 | 0.88 | 0.36 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3322 | 1/1 | 0.88 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3539 | 1/1 | 0.88 | 0.53 | 71,71,71,71 | 0 |
| 56 | MG | CA | 1620 | 1/1 | 0.88 | 0.23 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3603 | 1/1 | 0.88 | 0.12 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1779 | 1/1 | 0.88 | 0.52 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3523 | 1/1 | 0.88 | 0.96 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3331 | 1/1 | 0.88 | 0.24 | 93,93,93,93 | 0 |
| 56 | MG | DA | 3335 | 1/1 | 0.88 | 0.29 | 38,38,38,38 | 0 |
| 56 | MG | CA | 1702 | 1/1 | 0.88 | 0.43 | 75,75,75,75 | 0 |
| 56 | MG | BA | 2968 | 1/1 | 0.88 | 0.22 | 46,46,46,46 | 0 |
| 56 | MG | AA | 1739 | 1/1 | 0.88 | 0.10 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3076 | 1/1 | 0.88 | 0.26 | 88,88,88,88 | 0 |
| 56 | MG | DA | 2955 | 1/1 | 0.88 | 0.26 | 30,30,30,30 | 0 |
| 56 | MG | AA | 1624 | 1/1 | 0.88 | 0.42 | 45,45,45,45 | 0 |
| 56 | MG | AA | 1808 | 1/1 | 0.88 | 0.20 | 70,70,70,70 | 0 |
| 56 | MG | CA | 1634 | 1/1 | 0.88 | 0.26 | 74,74,74,74 | 0 |
| 56 | MG | DA | 2966 | 1/1 | 0.88 | 0.31 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3282 | 1/1 | 0.88 | 0.52 | 78,78,78,78 | 0 |
| 56 | MG | DA | 2970 | 1/1 | 0.88 | 0.66 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3371 | 1/1 | 0.88 | 0.74 | 55,55,55,55 | 0 |
| 56 | MG | BA | 2908 | 1/1 | 0.88 | 0.37 | 235,235,235,235 | 0 |
| 56 | MG | AA | 1613 | 1/1 | 0.88 | 0.11 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1620 | 1/1 | 0.88 | 0.31 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3150 | 1/1 | 0.88 | 0.32 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1970 | 1/1 | 0.88 | 0.29 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1690 | 1/1 | 0.88 | 0.57 | 174,174,174,174 | 0 |
| 56 | MG | AA | 1695 | 1/1 | 0.88 | 0.11 | 71,71,71,71 | 0 |
| 56 | MG | CA | 1813 | 1/1 | 0.88 | 0.38 | 99,99,99,99 | 0 |
| 56 | MG | CA | 1815 | 1/1 | 0.88 | 0.18 | 80,80,80,80 | 0 |
| 56 | MG | CA | 1648 | 1/1 | 0.88 | 0.47 | 155,155,155,155 | 0 |
| 56 | MG | BA | 2986 | 1/1 | 0.88 | 0.40 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3379 | 1/1 | 0.88 | 0.26 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3076 | 1/1 | 0.88 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3590 | 1/1 | 0.88 | 0.45 | 74,74,74,74 | 0 |
| 56 | MG | BA | 2919 | 1/1 | 0.88 | 0.09 | 127,127,127,127 | 0 |
| 56 | MG | DA | 3116 | 1/1 | 0.88 | 0.17 | 124,124,124,124 | 0 |
| 56 | MG | CA | 1655 | 1/1 | 0.88 | 0.23 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3246 | 1/1 | 0.88 | 0.42 | 47,47,47,47 | 0 |
| 56 | MG | CA | 1825 | 1/1 | 0.88 | 0.21 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3406 | 1/1 | 0.88 | 0.44 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3393 | 1/1 | 0.88 | 0.74 | 95,95,95,95 | 0 |
| 56 | MG | AA | 1907 | 1/1 | 0.88 | 0.49 | 45,45,45,45 | 0 |
| 56 | MG | AA | 1908 | 1/1 | 0.88 | 0.47 | 56,56,56,56 | 0 |
| 56 | MG | AA | 1836 | 1/1 | 0.88 | 0.39 | 139,139,139,139 | 0 |
| 56 | MG | AA | 1792 | 1/1 | 0.88 | 0.32 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3139 | 1/1 | 0.88 | 0.20 | 33,33,33,33 | 0 |
| 56 | MG | CA | 1664 | 1/1 | 0.88 | 0.25 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3165 | 1/1 | 0.88 | 0.26 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3651 | 1/1 | 0.88 | 0.30 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3015 | 1/1 | 0.88 | 0.53 | 91,91,91,91 | 0 |
| 56 | MG | CA | 1668 | 1/1 | 0.88 | 0.37 | 118,118,118,118 | 0 |
| 56 | MG | BA | 2924 | 1/1 | 0.88 | 1.07 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3019 | 1/1 | 0.88 | 0.29 | 67,67,67,67 | 0 |
| 56 | MG | DB | 202 | 1/1 | 0.88 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3511 | 1/1 | 0.88 | 0.34 | 91,91,91,91 | 0 |
| 56 | MG | AA | 1760 | 1/1 | 0.88 | 0.16 | 172,172,172,172 | 0 |
| 56 | MG | DA | 3201 | 1/1 | 0.88 | 0.34 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3431 | 1/1 | 0.88 | 0.28 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3223 | 1/1 | 0.88 | 0.18 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3432 | 1/1 | 0.88 | 0.43 | 69,69,69,69 | 0 |
| 56 | MG | AA | 1614 | 1/1 | 0.88 | 0.33 | 51,51,51,51 | 0 |
| 56 | MG | B8 | 101 | 1/1 | 0.88 | 0.28 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3032 | 1/1 | 0.88 | 0.18 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3052 | 1/1 | 0.88 | 0.41 | 118,118,118,118 | 0 |
| 56 | MG | AA | 1916 | 1/1 | 0.88 | 0.48 | 49,49,49,49 | 0 |
| 56 | MG | DB | 219 | 1/1 | 0.88 | 0.80 | 66,66,66,66 | 0 |
| 56 | MG | CA | 1680 | 1/1 | 0.88 | 0.88 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 2928 | 1/1 | 0.88 | 0.24 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3262 | 1/1 | 0.88 | 0.42 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3444 | 1/1 | 0.88 | 0.52 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3531 | 1/1 | 0.88 | 0.30 | 71,71,71,71 | 0 |
| 56 | MG | CA | 1764 | 1/1 | 0.88 | 0.38 | 50,50,50,50 | 0 |
| 56 | MG | DQ | 204 | 1/1 | 0.88 | 0.40 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3275 | 1/1 | 0.88 | 0.83 | 52,52,52,52 | 0 |
| 56 | MG | DA | 2912 | 1/1 | 0.88 | 0.30 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3460 | 1/1 | 0.88 | 0.16 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3461 | 1/1 | 0.88 | 0.13 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3285 | 1/1 | 0.88 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3467 | 1/1 | 0.88 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1837 | 1/1 | 0.89 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | CA | 1742 | 1/1 | 0.89 | 0.56 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3620 | 1/1 | 0.89 | 0.23 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3039 | 1/1 | 0.89 | 0.81 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3041 | 1/1 | 0.89 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3621 | 1/1 | 0.89 | 0.38 | 106,106,106,106 | 0 |
| 56 | MG | AA | 1803 | 1/1 | 0.89 | 0.37 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1932 | 1/1 | 0.89 | 0.47 | 159,159,159,159 | 0 |
| 56 | MG | BB | 212 | 1/1 | 0.89 | 0.35 | 99,99,99,99 | 0 |
| 56 | MG | BA | 3476 | 1/1 | 0.89 | 0.69 | 52,52,52,52 | 0 |
| 56 | MG | AA | 1933 | 1/1 | 0.89 | 0.54 | 63,63,63,63 | 0 |
| 56 | MG | DA | 2918 | 1/1 | 0.89 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | AA | 1627 | 1/1 | 0.89 | 0.52 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3286 | 1/1 | 0.89 | 0.55 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3382 | 1/1 | 0.89 | 0.67 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3301 | 1/1 | 0.89 | 0.33 | 52,52,52,52 | 0 |
| 56 | MG | CA | 1673 | 1/1 | 0.89 | 0.33 | 73,73,73,73 | 0 |
| 56 | MG | AA | 1682 | 1/1 | 0.89 | 0.81 | 124,124,124,124 | 0 |
| 56 | MG | CA | 1765 | 1/1 | 0.89 | 0.25 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3289 | 1/1 | 0.89 | 0.23 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3061 | 1/1 | 0.89 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3315 | 1/1 | 0.89 | 0.65 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1972 | 1/1 | 0.89 | 0.41 | 56,56,56,56 | 0 |
| 56 | MG | BP | 201 | 1/1 | 0.89 | 0.31 | 54,54,54,54 | 0 |
| 56 | MG | BT | 201 | 1/1 | 0.89 | 0.27 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3505 | 1/1 | 0.89 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3645 | 1/1 | 0.89 | 0.33 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3647 | 1/1 | 0.89 | 0.30 | 88,88,88,88 | 0 |
| 56 | MG | AA | 1807 | 1/1 | 0.89 | 0.27 | 45,45,45,45 | 0 |
| 56 | MG | B1 | 101 | 1/1 | 0.89 | 0.44 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3392 | 1/1 | 0.89 | 0.47 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3099 | 1/1 | 0.89 | 0.54 | 141,141,141,141 | 0 |
| 56 | MG | BA | 2979 | 1/1 | 0.89 | 1.08 | 77,77,77,77 | 0 |
| 56 | MG | DA | 2954 | 1/1 | 0.89 | 0.50 | 90,90,90,90 | 0 |
| 56 | MG | DA | 3333 | 1/1 | 0.89 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | CA | 1785 | 1/1 | 0.89 | 0.37 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1786 | 1/1 | 0.89 | 0.41 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3337 | 1/1 | 0.89 | 0.28 | 51,51,51,51 | 0 |
| 56 | MG | DA | 2960 | 1/1 | 0.89 | 0.50 | 68,68,68,68 | 0 |
| 56 | MG | BA | 2947 | 1/1 | 0.89 | 0.44 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3533 | 1/1 | 0.89 | 0.26 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3340 | 1/1 | 0.89 | 0.37 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1718 | 1/1 | 0.89 | 0.16 | 75,75,75,75 | 0 |
| 56 | MG | DA | 2965 | 1/1 | 0.89 | 0.33 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1630 | 1/1 | 0.89 | 0.58 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3499 | 1/1 | 0.89 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3026 | 1/1 | 0.89 | 0.60 | 114,114,114,114 | 0 |
| 56 | MG | AA | 1691 | 1/1 | 0.89 | 0.11 | 84,84,84,84 | 0 |
| 56 | MG | AA | 1857 | 1/1 | 0.89 | 0.59 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3412 | 1/1 | 0.89 | 0.82 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3198 | 1/1 | 0.89 | 0.41 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3355 | 1/1 | 0.89 | 0.19 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3570 | 1/1 | 0.89 | 0.37 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3093 | 1/1 | 0.89 | 0.53 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3358 | 1/1 | 0.89 | 0.18 | 141,141,141,141 | 0 |
| 56 | MG | BA | 3034 | 1/1 | 0.89 | 0.23 | 36,36,36,36 | 0 |
| 56 | MG | DA | 2982 | 1/1 | 0.89 | 0.25 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3251 | 1/1 | 0.89 | 0.26 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3366 | 1/1 | 0.89 | 0.29 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3515 | 1/1 | 0.89 | 0.42 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3103 | 1/1 | 0.89 | 0.15 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3683 | 1/1 | 0.89 | 0.72 | 55,55,55,55 | 0 |
| 56 | MG | BA | 2953 | 1/1 | 0.89 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | DA | 2990 | 1/1 | 0.89 | 0.29 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3688 | 1/1 | 0.89 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3594 | 1/1 | 0.89 | 0.34 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3113 | 1/1 | 0.89 | 0.22 | 110,110,110,110 | 0 |
| 56 | MG | DA | 2994 | 1/1 | 0.89 | 0.33 | 62,62,62,62 | 0 |
| 56 | MG | CA | 1624 | 1/1 | 0.89 | 0.36 | 98,98,98,98 | 0 |
| 56 | MG | DA | 3600 | 1/1 | 0.89 | 0.22 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3383 | 1/1 | 0.89 | 0.38 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3602 | 1/1 | 0.89 | 0.25 | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1692 | 1/1 | 0.89 | 0.55 | 134,134,134,134 | 0 |
| 56 | MG | CA | 1629 | 1/1 | 0.89 | 0.24 | 93,93,93,93 | 0 |
| 56 | MG | DA | 2998 | 1/1 | 0.89 | 0.62 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1710 | 1/1 | 0.89 | 0.22 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3000 | 1/1 | 0.89 | 0.22 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3125 | 1/1 | 0.89 | 0.72 | 161,161,161,161 | 0 |
| 56 | MG | DA | 3127 | 1/1 | 0.89 | 0.52 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3313 | 1/1 | 0.89 | 0.31 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3623 | 1/1 | 0.89 | 0.29 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3625 | 1/1 | 0.89 | 0.14 | 82,82,82,82 | 0 |
| 56 | MG | AQ | 201 | 1/1 | 0.89 | 0.17 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3434 | 1/1 | 0.89 | 0.55 | 55,55,55,55 | 0 |
| 56 | MG | AA | 1661 | 1/1 | 0.89 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3006 | 1/1 | 0.89 | 0.43 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3704 | 1/1 | 0.89 | 0.22 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3323 | 1/1 | 0.89 | 0.25 | 47,47,47,47 | 0 |
| 56 | MG | CA | 1723 | 1/1 | 0.89 | 0.15 | 76,76,76,76 | 0 |
| 56 | MG | DB | 203 | 1/1 | 0.89 | 0.14 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3174 | 1/1 | 0.89 | 0.29 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3438 | 1/1 | 0.89 | 0.66 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3710 | 1/1 | 0.89 | 0.27 | 81,81,81,81 | 0 |
| 56 | MG | BA | 3126 | 1/1 | 0.89 | 0.80 | 235,235,235,235 | 0 |
| 56 | MG | AA | 1895 | 1/1 | 0.89 | 0.24 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3198 | 1/1 | 0.89 | 0.44 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3129 | 1/1 | 0.89 | 0.31 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3449 | 1/1 | 0.89 | 0.33 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3219 | 1/1 | 0.89 | 0.30 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3169 | 1/1 | 0.89 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3224 | 1/1 | 0.89 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3233 | 1/1 | 0.89 | 0.33 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1922 | 1/1 | 0.89 | 0.33 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3241 | 1/1 | 0.89 | 0.19 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3171 | 1/1 | 0.89 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1651 | 1/1 | 0.89 | 0.38 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3456 | 1/1 | 0.89 | 0.11 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3451 | 1/1 | 0.89 | 0.52 | 56,56,56,56 | 0 |
| 56 | MG | DQ | 203 | 1/1 | 0.89 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1896 | 1/1 | 0.89 | 0.77 | 77,77,77,77 | 0 |
| 56 | MG | BA | 2931 | 1/1 | 0.89 | 0.47 | 98,98,98,98 | 0 |
| 56 | MG | DA | 3258 | 1/1 | 0.89 | 0.49 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3031 | 1/1 | 0.89 | 0.25 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3458 | 1/1 | 0.89 | 0.17 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1656 | 1/1 | 0.89 | 0.26 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3177 | 1/1 | 0.89 | 0.15 | 78,78,78,78 | 0 |
| 56 | MG | D7 | 102 | 1/1 | 0.89 | 0.21 | 32,32,32,32 | 0 |
| 56 | MG | DA | 2987 | 1/1 | 0.90 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3038 | 1/1 | 0.90 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1648 | 1/1 | 0.90 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3493 | 1/1 | 0.90 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | CA | 1827 | 1/1 | 0.90 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | AA | 1669 | 1/1 | 0.90 | 0.60 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3332 | 1/1 | 0.90 | 0.33 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3041 | 1/1 | 0.90 | 0.25 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3127 | 1/1 | 0.90 | 0.47 | 102,102,102,102 | 0 |
| 56 | MG | BA | 3504 | 1/1 | 0.90 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1820 | 1/1 | 0.90 | 0.32 | 166,166,166,166 | 0 |
| 56 | MG | BA | 3430 | 1/1 | 0.90 | 0.26 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3509 | 1/1 | 0.90 | 0.30 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3321 | 1/1 | 0.90 | 0.21 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3341 | 1/1 | 0.90 | 0.52 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3262 | 1/1 | 0.90 | 0.16 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3671 | 1/1 | 0.90 | 0.24 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3512 | 1/1 | 0.90 | 0.48 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3114 | 1/1 | 0.90 | 0.19 | 81,81,81,81 | 0 |
| 56 | MG | BA | 2969 | 1/1 | 0.90 | 0.27 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3000 | 1/1 | 0.90 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | AA | 1841 | 1/1 | 0.90 | 0.31 | 113,113,113,113 | 0 |
| 56 | MG | BA | 3679 | 1/1 | 0.90 | 0.26 | 27,27,27,27 | 0 |
| 56 | MG | CA | 1608 | 1/1 | 0.90 | 0.05 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3526 | 1/1 | 0.90 | 0.29 | 61,61,61,61 | 0 |
| 56 | MG | AA | 1701 | 1/1 | 0.90 | 0.12 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3133 | 1/1 | 0.90 | 0.26 | 48,48,48,48 | 0 |
| 56 | MG | AW | 118 | 1/1 | 0.90 | 0.61 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3357 | 1/1 | 0.90 | 0.51 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3011 | 1/1 | 0.90 | 0.40 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3687 | 1/1 | 0.90 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3353 | 1/1 | 0.90 | 0.35 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3689 | 1/1 | 0.90 | 0.32 | 67,67,67,67 | 0 |
| 56 | MG | DA | 2906 | 1/1 | 0.90 | 0.26 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3527 | 1/1 | 0.90 | 0.42 | 31,31,31,31 | 0 |
| 56 | MG | CA | 1864 | 1/1 | 0.90 | 0.39 | 157,157,157,157 | 0 |
| 56 | MG | CA | 1773 | 1/1 | 0.90 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1802 | 1/1 | 0.90 | 0.40 | 55,55,55,55 | 0 |
| 56 | MG | AA | 1955 | 1/1 | 0.90 | 0.33 | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1654 | 1/1 | 0.90 | 0.41 | 61,61,61,61 | 0 |
| 56 | MG | BA | 2977 | 1/1 | 0.90 | 0.41 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1899 | 1/1 | 0.90 | 0.15 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3142 | 1/1 | 0.90 | 0.48 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3459 | 1/1 | 0.90 | 0.26 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3382 | 1/1 | 0.90 | 0.40 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3200 | 1/1 | 0.90 | 0.47 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3063 | 1/1 | 0.90 | 0.48 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3203 | 1/1 | 0.90 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | CA | 1875 | 1/1 | 0.90 | 1.09 | 267,267,267,267 | 0 |
| 56 | MG | DA | 2929 | 1/1 | 0.90 | 0.24 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3391 | 1/1 | 0.90 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3014 | 1/1 | 0.90 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | AA | 1958 | 1/1 | 0.90 | 0.29 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3466 | 1/1 | 0.90 | 0.40 | 39,39,39,39 | 0 |
| 56 | MG | CA | 1791 | 1/1 | 0.90 | 0.64 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3376 | 1/1 | 0.90 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1883 | 1/1 | 0.90 | 0.28 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3066 | 1/1 | 0.90 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3246 | 1/1 | 0.90 | 0.64 | 51,51,51,51 | 0 |
| 56 | MG | DA | 2941 | 1/1 | 0.90 | 0.20 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3470 | 1/1 | 0.90 | 0.50 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3048 | 1/1 | 0.90 | 0.64 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3413 | 1/1 | 0.90 | 0.71 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1962 | 1/1 | 0.90 | 0.30 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3420 | 1/1 | 0.90 | 0.24 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3259 | 1/1 | 0.90 | 0.30 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3422 | 1/1 | 0.90 | 0.26 | 77,77,77,77 | 0 |
| 56 | MG | DA | 2947 | 1/1 | 0.90 | 0.38 | 192,192,192,192 | 0 |
| 56 | MG | BA | 3552 | 1/1 | 0.90 | 0.23 | 29,29,29,29 | 0 |
| 56 | MG | AA | 1965 | 1/1 | 0.90 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | CA | 1799 | 1/1 | 0.90 | 0.38 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3268 | 1/1 | 0.90 | 0.34 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3269 | 1/1 | 0.90 | 0.25 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1883 | 1/1 | 0.90 | 0.38 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3294 | 1/1 | 0.90 | 0.53 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3296 | 1/1 | 0.90 | 0.58 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3283 | 1/1 | 0.90 | 0.32 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3435 | 1/1 | 0.90 | 0.73 | 68,68,68,68 | 0 |
| 56 | MG | CA | 1803 | 1/1 | 0.90 | 0.25 | 146,146,146,146 | 0 |
| 56 | MG | DA | 3437 | 1/1 | 0.90 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3724 | 1/1 | 0.90 | 0.75 | 119,119,119,119 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3440 | 1/1 | 0.90 | 0.48 | 58,58,58,58 | 0 |
| 56 | MG | BA | 2902 | 1/1 | 0.90 | 0.19 | 86,86,86,86 | 0 |
| 56 | MG | DA | 2957 | 1/1 | 0.90 | 0.23 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3065 | 1/1 | 0.90 | 0.30 | 88,88,88,88 | 0 |
| 56 | MG | AW | 103 | 1/1 | 0.90 | 0.22 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3027 | 1/1 | 0.90 | 0.24 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3634 | 1/1 | 0.90 | 0.37 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3394 | 1/1 | 0.90 | 0.49 | 56,56,56,56 | 0 |
| 56 | MG | CA | 1906 | 1/1 | 0.90 | 0.11 | 114,114,114,114 | 0 |
| 56 | MG | DB | 215 | 1/1 | 0.90 | 0.14 | 79,79,79,79 | 0 |
| 56 | MG | DB | 217 | 1/1 | 0.90 | 0.16 | 121,121,121,121 | 0 |
| 56 | MG | BA | 3155 | 1/1 | 0.90 | 0.61 | 93,93,93,93 | 0 |
| 56 | MG | DA | 2969 | 1/1 | 0.90 | 0.14 | 68,68,68,68 | 0 |
| 56 | MG | DB | 220 | 1/1 | 0.90 | 0.30 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3301 | 1/1 | 0.90 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | AA | 1940 | 1/1 | 0.90 | 0.17 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3305 | 1/1 | 0.90 | 0.38 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3306 | 1/1 | 0.90 | 0.55 | 48,48,48,48 | 0 |
| 56 | MG | DA | 2973 | 1/1 | 0.90 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | CA | 1910 | 1/1 | 0.90 | 0.34 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1901 | 1/1 | 0.90 | 0.27 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1888 | 1/1 | 0.90 | 0.41 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1913 | 1/1 | 0.90 | 0.47 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3475 | 1/1 | 0.90 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | DW | 202 | 1/1 | 0.90 | 0.25 | 50,50,50,50 | 0 |
| 56 | MG | DA | 2981 | 1/1 | 0.90 | 0.41 | 105,105,105,105 | 0 |
| 56 | MG | BA | 3646 | 1/1 | 0.90 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | AA | 1769 | 1/1 | 0.90 | 0.35 | 79,79,79,79 | 0 |
| 56 | MG | D5 | 102 | 1/1 | 0.90 | 0.10 | 68,68,68,68 | 0 |
| 56 | MG | DA | 2985 | 1/1 | 0.90 | 0.18 | 107,107,107,107 | 0 |
| 56 | MG | BA | 3254 | 1/1 | 0.90 | 0.24 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3226 | 1/1 | 0.91 | 0.25 | 58,58,58,58 | 0 |
| 56 | MG | CA | 1824 | 1/1 | 0.91 | 0.55 | 118,118,118,118 | 0 |
| 56 | MG | DA | 3036 | 1/1 | 0.91 | 0.10 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3288 | 1/1 | 0.91 | 0.27 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1800 | 1/1 | 0.91 | 0.42 | 87,87,87,87 | 0 |
| 56 | MG | AA | 1833 | 1/1 | 0.91 | 0.26 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1834 | 1/1 | 0.91 | 0.25 | 178,178,178,178 | 0 |
| 56 | MG | DA | 3273 | 1/1 | 0.91 | 0.54 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3462 | 1/1 | 0.91 | 0.66 | 55,55,55,55 | 0 |
| 56 | MG | AA | 1862 | 1/1 | 0.91 | 0.79 | 212,212,212,212 | 0 |
| 56 | MG | DA | 3276 | 1/1 | 0.91 | 0.18 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3281 | 1/1 | 0.91 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3282 | 1/1 | 0.91 | 0.41 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3572 | 1/1 | 0.91 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3669 | 1/1 | 0.91 | 0.65 | 53,53,53,53 | 0 |
| 56 | MG | AA | 1737 | 1/1 | 0.91 | 0.30 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3286 | 1/1 | 0.91 | 0.29 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1838 | 1/1 | 0.91 | 0.48 | 66,66,66,66 | 0 |
| 56 | MG | BA | 2963 | 1/1 | 0.91 | 0.38 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3576 | 1/1 | 0.91 | 0.41 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3675 | 1/1 | 0.91 | 0.26 | 145,145,145,145 | 0 |
| 56 | MG | DA | 3050 | 1/1 | 0.91 | 0.55 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3293 | 1/1 | 0.91 | 0.28 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1949 | 1/1 | 0.91 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1715 | 1/1 | 0.91 | 0.15 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3492 | 1/1 | 0.91 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | DA | 2919 | 1/1 | 0.91 | 0.62 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3298 | 1/1 | 0.91 | 0.35 | 46,46,46,46 | 0 |
| 56 | MG | DA | 2920 | 1/1 | 0.91 | 0.21 | 83,83,83,83 | 0 |
| 56 | MG | CA | 1627 | 1/1 | 0.91 | 0.56 | 85,85,85,85 | 0 |
| 56 | MG | DA | 2924 | 1/1 | 0.91 | 0.56 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3303 | 1/1 | 0.91 | 0.68 | 53,53,53,53 | 0 |
| 56 | MG | CA | 1845 | 1/1 | 0.91 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3681 | 1/1 | 0.91 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1848 | 1/1 | 0.91 | 0.32 | 113,113,113,113 | 0 |
| 56 | MG | BA | 3401 | 1/1 | 0.91 | 0.42 | 28,28,28,28 | 0 |
| 56 | MG | DA | 2932 | 1/1 | 0.91 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1733 | 1/1 | 0.91 | 0.23 | 197,197,197,197 | 0 |
| 56 | MG | DA | 3310 | 1/1 | 0.91 | 0.49 | 52,52,52,52 | 0 |
| 56 | MG | AA | 1924 | 1/1 | 0.91 | 0.47 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1853 | 1/1 | 0.91 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3514 | 1/1 | 0.91 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3056 | 1/1 | 0.91 | 0.47 | 117,117,117,117 | 0 |
| 56 | MG | BA | 3495 | 1/1 | 0.91 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3071 | 1/1 | 0.91 | 0.12 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3520 | 1/1 | 0.91 | 0.63 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3145 | 1/1 | 0.91 | 0.38 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3006 | 1/1 | 0.91 | 0.21 | 107,107,107,107 | 0 |
| 56 | MG | BA | 3691 | 1/1 | 0.91 | 0.28 | 45,45,45,45 | 0 |
| 56 | MG | CA | 1641 | 1/1 | 0.91 | 0.13 | 135,135,135,135 | 0 |
| 56 | MG | AA | 1677 | 1/1 | 0.91 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3061 | 1/1 | 0.91 | 0.61 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3529 | 1/1 | 0.91 | 0.29 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1991 | 1/1 | 0.91 | 0.09 | 96,96,96,96 | 0 |
| 56 | MG | CA | 1744 | 1/1 | 0.91 | 0.21 | 95,95,95,95 | 0 |
| 56 | MG | BA | 3413 | 1/1 | 0.91 | 0.13 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3102 | 1/1 | 0.91 | 0.18 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3195 | 1/1 | 0.91 | 0.18 | 97,97,97,97 | 0 |
| 56 | MG | DA | 3085 | 1/1 | 0.91 | 0.22 | 49,49,49,49 | 0 |
| 56 | MG | AA | 1926 | 1/1 | 0.91 | 0.39 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3703 | 1/1 | 0.91 | 0.97 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1771 | 1/1 | 0.91 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3547 | 1/1 | 0.91 | 0.38 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1930 | 1/1 | 0.91 | 0.45 | 198,198,198,198 | 0 |
| 56 | MG | DA | 3557 | 1/1 | 0.91 | 0.19 | 16,16,16,16 | 0 |
| 56 | MG | CA | 1652 | 1/1 | 0.91 | 0.91 | 193,193,193,193 | 0 |
| 56 | MG | BA | 3512 | 1/1 | 0.91 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1760 | 1/1 | 0.91 | 0.18 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3565 | 1/1 | 0.91 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3513 | 1/1 | 0.91 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1674 | 1/1 | 0.91 | 0.27 | 126,126,126,126 | 0 |
| 56 | MG | AA | 1707 | 1/1 | 0.91 | 0.11 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1847 | 1/1 | 0.91 | 0.32 | 209,209,209,209 | 0 |
| 56 | MG | DA | 3101 | 1/1 | 0.91 | 0.31 | 101,101,101,101 | 0 |
| 56 | MG | DA | 3102 | 1/1 | 0.91 | 0.53 | 126,126,126,126 | 0 |
| 56 | MG | BA | 2909 | 1/1 | 0.91 | 0.34 | 114,114,114,114 | 0 |
| 56 | MG | AA | 1743 | 1/1 | 0.91 | 0.41 | 81,81,81,81 | 0 |
| 56 | MG | BA | 3521 | 1/1 | 0.91 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | CA | 1771 | 1/1 | 0.91 | 0.20 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3359 | 1/1 | 0.91 | 0.35 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3108 | 1/1 | 0.91 | 0.41 | 74,74,74,74 | 0 |
| 56 | MG | DA | 2977 | 1/1 | 0.91 | 0.68 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3110 | 1/1 | 0.91 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3719 | 1/1 | 0.91 | 0.09 | 125,125,125,125 | 0 |
| 56 | MG | BA | 3324 | 1/1 | 0.91 | 0.34 | 15,15,15,15 | 0 |
| 56 | MG | BA | 2945 | 1/1 | 0.91 | 0.40 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3437 | 1/1 | 0.91 | 0.72 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3525 | 1/1 | 0.91 | 0.44 | 40,40,40,40 | 0 |
| 56 | MG | BA | 2911 | 1/1 | 0.91 | 0.54 | 91,91,91,91 | 0 |
| 56 | MG | CA | 1899 | 1/1 | 0.91 | 0.44 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3439 | 1/1 | 0.91 | 0.37 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3441 | 1/1 | 0.91 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | AA | 1736 | 1/1 | 0.91 | 0.47 | 83,83,83,83 | 0 |
| 56 | MG | BA | 3443 | 1/1 | 0.91 | 0.38 | 18,18,18,18 | 0 |
| 56 | MG | BA | 3535 | 1/1 | 0.91 | 0.33 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3619 | 1/1 | 0.91 | 0.28 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3615 | 1/1 | 0.91 | 0.27 | 57,57,57,57 | 0 |
| 56 | MG | BB | 210 | 1/1 | 0.91 | 0.11 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3341 | 1/1 | 0.91 | 0.29 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3619 | 1/1 | 0.91 | 0.49 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3446 | 1/1 | 0.91 | 0.22 | 93,93,93,93 | 0 |
| 56 | MG | DA | 3156 | 1/1 | 0.91 | 0.35 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3624 | 1/1 | 0.91 | 0.25 | 35,35,35,35 | 0 |
| 56 | MG | BA | 2948 | 1/1 | 0.91 | 0.59 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3344 | 1/1 | 0.91 | 0.53 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3624 | 1/1 | 0.91 | 0.27 | 83,83,83,83 | 0 |
| 56 | MG | BA | 3269 | 1/1 | 0.91 | 0.27 | 66,66,66,66 | 0 |
| 56 | MG | CA | 1797 | 1/1 | 0.91 | 0.91 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3631 | 1/1 | 0.91 | 0.23 | 85,85,85,85 | 0 |
| 56 | MG | BB | 217 | 1/1 | 0.91 | 0.19 | 99,99,99,99 | 0 |
| 56 | MG | BB | 220 | 1/1 | 0.91 | 0.13 | 123,123,123,123 | 0 |
| 56 | MG | AW | 108 | 1/1 | 0.91 | 0.39 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3356 | 1/1 | 0.91 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3271 | 1/1 | 0.91 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3406 | 1/1 | 0.91 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3272 | 1/1 | 0.91 | 0.40 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3547 | 1/1 | 0.91 | 0.17 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1924 | 1/1 | 0.91 | 0.54 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3415 | 1/1 | 0.91 | 0.37 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3207 | 1/1 | 0.91 | 0.47 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3417 | 1/1 | 0.91 | 0.29 | 145,145,145,145 | 0 |
| 56 | MG | DA | 3419 | 1/1 | 0.91 | 0.24 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3210 | 1/1 | 0.91 | 0.32 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3212 | 1/1 | 0.91 | 0.53 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3213 | 1/1 | 0.91 | 0.26 | 60,60,60,60 | 0 |
| 56 | MG | CA | 1925 | 1/1 | 0.91 | 0.33 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3125 | 1/1 | 0.91 | 0.36 | 106,106,106,106 | 0 |
| 56 | MG | BA | 3549 | 1/1 | 0.91 | 0.12 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3643 | 1/1 | 0.91 | 0.49 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3226 | 1/1 | 0.91 | 0.31 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1755 | 1/1 | 0.91 | 0.13 | 123,123,123,123 | 0 |
| 56 | MG | AA | 1853 | 1/1 | 0.91 | 0.24 | 69,69,69,69 | 0 |
| 56 | MG | DP | 202 | 1/1 | 0.91 | 0.40 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3036 | 1/1 | 0.91 | 0.34 | 131,131,131,131 | 0 |
| 56 | MG | DA | 3242 | 1/1 | 0.91 | 0.48 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3020 | 1/1 | 0.91 | 0.17 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1766 | 1/1 | 0.91 | 0.34 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3172 | 1/1 | 0.91 | 0.29 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1816 | 1/1 | 0.91 | 0.25 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3174 | 1/1 | 0.91 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | DA | 3255 | 1/1 | 0.91 | 0.30 | 44,44,44,44 | 0 |
| 56 | MG | AW | 114 | 1/1 | 0.91 | 0.19 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3445 | 1/1 | 0.91 | 0.27 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3474 | 1/1 | 0.91 | 0.40 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1821 | 1/1 | 0.91 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3657 | 1/1 | 0.91 | 0.27 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3425 | 1/1 | 0.92 | 0.33 | 202,202,202,202 | 0 |
| 56 | MG | DA | 3487 | 1/1 | 0.92 | 0.61 | 108,108,108,108 | 0 |
| 56 | MG | BA | 3426 | 1/1 | 0.92 | 0.29 | 28,28,28,28 | 0 |
| 56 | MG | CA | 1775 | 1/1 | 0.92 | 0.20 | 47,47,47,47 | 0 |
| 56 | MG | CA | 1666 | 1/1 | 0.92 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3429 | 1/1 | 0.92 | 0.61 | 43,43,43,43 | 0 |
| 56 | MG | BA | 2912 | 1/1 | 0.92 | 0.37 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3134 | 1/1 | 0.92 | 0.85 | 122,122,122,122 | 0 |
| 56 | MG | DA | 3495 | 1/1 | 0.92 | 0.12 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1747 | 1/1 | 0.92 | 0.29 | 109,109,109,109 | 0 |
| 56 | MG | BA | 3136 | 1/1 | 0.92 | 0.64 | 205,205,205,205 | 0 |
| 56 | MG | BA | 3183 | 1/1 | 0.92 | 0.20 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3105 | 1/1 | 0.92 | 0.42 | 94,94,94,94 | 0 |
| 56 | MG | BB | 204 | 1/1 | 0.92 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3526 | 1/1 | 0.92 | 0.36 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1703 | 1/1 | 0.92 | 0.40 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3503 | 1/1 | 0.92 | 0.13 | 92,92,92,92 | 0 |
| 56 | MG | AA | 1663 | 1/1 | 0.92 | 0.25 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3530 | 1/1 | 0.92 | 0.38 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3507 | 1/1 | 0.92 | 0.43 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3187 | 1/1 | 0.92 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3249 | 1/1 | 0.92 | 0.24 | 84,84,84,84 | 0 |
| 56 | MG | AA | 1886 | 1/1 | 0.92 | 0.40 | 65,65,65,65 | 0 |
| 56 | MG | DA | 2992 | 1/1 | 0.92 | 0.28 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3534 | 1/1 | 0.92 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1618 | 1/1 | 0.92 | 0.41 | 104,104,104,104 | 0 |
| 56 | MG | BA | 3627 | 1/1 | 0.92 | 0.28 | 100,100,100,100 | 0 |
| 56 | MG | DA | 3344 | 1/1 | 0.92 | 0.33 | 29,29,29,29 | 0 |
| 56 | MG | AA | 1859 | 1/1 | 0.92 | 0.33 | 177,177,177,177 | 0 |
| 56 | MG | AA | 1812 | 1/1 | 0.92 | 0.39 | 273,273,273,273 | 0 |
| 56 | MG | BB | 218 | 1/1 | 0.92 | 0.45 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3124 | 1/1 | 0.92 | 0.29 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3524 | 1/1 | 0.92 | 0.18 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3091 | 1/1 | 0.92 | 0.20 | 125,125,125,125 | 0 |
| 56 | MG | BA | 3336 | 1/1 | 0.92 | 0.34 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3144 | 1/1 | 0.92 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | BA | 2955 | 1/1 | 0.92 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | CA | 1694 | 1/1 | 0.92 | 0.64 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3051 | 1/1 | 0.92 | 0.31 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3005 | 1/1 | 0.92 | 0.47 | 89,89,89,89 | 0 |
| 56 | MG | AA | 1944 | 1/1 | 0.92 | 0.42 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3454 | 1/1 | 0.92 | 0.24 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3537 | 1/1 | 0.92 | 0.33 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3363 | 1/1 | 0.92 | 0.18 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1761 | 1/1 | 0.92 | 0.30 | 118,118,118,118 | 0 |
| 56 | MG | CV | 101 | 1/1 | 0.92 | 0.28 | 87,87,87,87 | 0 |
| 56 | MG | AA | 1843 | 1/1 | 0.92 | 0.24 | 124,124,124,124 | 0 |
| 56 | MG | AA | 1865 | 1/1 | 0.92 | 0.42 | 98,98,98,98 | 0 |
| 56 | MG | BA | 2961 | 1/1 | 0.92 | 0.24 | 83,83,83,83 | 0 |
| 56 | MG | CW | 103 | 1/1 | 0.92 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3190 | 1/1 | 0.92 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | B5 | 101 | 1/1 | 0.92 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3266 | 1/1 | 0.92 | 0.33 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3362 | 1/1 | 0.92 | 0.26 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3566 | 1/1 | 0.92 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | AA | 1948 | 1/1 | 0.92 | 0.95 | 103,103,103,103 | 0 |
| 56 | MG | BA | 3203 | 1/1 | 0.92 | 0.49 | 98,98,98,98 | 0 |
| 56 | MG | BA | 3656 | 1/1 | 0.92 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3208 | 1/1 | 0.92 | 0.59 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3024 | 1/1 | 0.92 | 0.27 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3211 | 1/1 | 0.92 | 0.32 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3103 | 1/1 | 0.92 | 0.36 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3658 | 1/1 | 0.92 | 0.43 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3388 | 1/1 | 0.92 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1983 | 1/1 | 0.92 | 1.07 | 76,76,76,76 | 0 |
| 56 | MG | CA | 1826 | 1/1 | 0.92 | 0.36 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3220 | 1/1 | 0.92 | 0.29 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1715 | 1/1 | 0.92 | 0.32 | 79,79,79,79 | 0 |
| 56 | MG | CA | 1716 | 1/1 | 0.92 | 0.21 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3396 | 1/1 | 0.92 | 0.24 | 18,18,18,18 | 0 |
| 56 | MG | BA | 3471 | 1/1 | 0.92 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3227 | 1/1 | 0.92 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | AA | 1984 | 1/1 | 0.92 | 0.23 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1834 | 1/1 | 0.92 | 0.33 | 108,108,108,108 | 0 |
| 56 | MG | BA | 3007 | 1/1 | 0.92 | 0.46 | 170,170,170,170 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3373 | 1/1 | 0.92 | 0.49 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1845 | 1/1 | 0.92 | 0.49 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1670 | 1/1 | 0.92 | 0.35 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3378 | 1/1 | 0.92 | 0.39 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3160 | 1/1 | 0.92 | 0.34 | 51,51,51,51 | 0 |
| 56 | MG | CA | 1726 | 1/1 | 0.92 | 0.26 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3251 | 1/1 | 0.92 | 0.29 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3252 | 1/1 | 0.92 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1730 | 1/1 | 0.92 | 0.20 | 78,78,78,78 | 0 |
| 56 | MG | AA | 1871 | 1/1 | 0.92 | 0.18 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3216 | 1/1 | 0.92 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3116 | 1/1 | 0.92 | 0.16 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3622 | 1/1 | 0.92 | 0.22 | 50,50,50,50 | 0 |
| 56 | MG | BA | 2933 | 1/1 | 0.92 | 0.22 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3579 | 1/1 | 0.92 | 0.46 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3580 | 1/1 | 0.92 | 0.54 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3263 | 1/1 | 0.92 | 0.35 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3051 | 1/1 | 0.92 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | CA | 1628 | 1/1 | 0.92 | 0.16 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3219 | 1/1 | 0.92 | 0.62 | 78,78,78,78 | 0 |
| 56 | MG | CA | 1852 | 1/1 | 0.92 | 0.25 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3489 | 1/1 | 0.92 | 0.22 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3433 | 1/1 | 0.92 | 0.17 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3220 | 1/1 | 0.92 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1754 | 1/1 | 0.92 | 0.58 | 72,72,72,72 | 0 |
| 56 | MG | AA | 1954 | 1/1 | 0.92 | 0.29 | 142,142,142,142 | 0 |
| 56 | MG | DA | 3278 | 1/1 | 0.92 | 0.30 | 83,83,83,83 | 0 |
| 56 | MG | CA | 1858 | 1/1 | 0.92 | 0.22 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3398 | 1/1 | 0.92 | 0.61 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3399 | 1/1 | 0.92 | 0.55 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3695 | 1/1 | 0.92 | 0.10 | 95,95,95,95 | 0 |
| 56 | MG | AA | 1611 | 1/1 | 0.92 | 0.18 | 109,109,109,109 | 0 |
| 56 | MG | DB | 211 | 1/1 | 0.92 | 0.31 | 35,35,35,35 | 0 |
| 56 | MG | DA | 2942 | 1/1 | 0.92 | 0.19 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3018 | 1/1 | 0.92 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3293 | 1/1 | 0.92 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3699 | 1/1 | 0.92 | 0.31 | 70,70,70,70 | 0 |
| 56 | MG | BA | 2937 | 1/1 | 0.92 | 0.23 | 71,71,71,71 | 0 |
| 56 | MG | BA | 2906 | 1/1 | 0.92 | 0.27 | 84,84,84,84 | 0 |
| 56 | MG | AA | 1832 | 1/1 | 0.92 | 0.15 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3505 | 1/1 | 0.92 | 1.25 | 101,101,101,101 | 0 |
| 56 | MG | BA | 3506 | 1/1 | 0.92 | 0.42 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3707 | 1/1 | 0.92 | 0.05 | 84,84,84,84 | 0 |
| 56 | MG | AA | 1821 | 1/1 | 0.92 | 0.13 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1880 | 1/1 | 0.92 | 0.32 | 43,43,43,43 | 0 |
| 56 | MG | DI | 201 | 1/1 | 0.92 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | DI | 202 | 1/1 | 0.92 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3466 | 1/1 | 0.92 | 0.26 | 90,90,90,90 | 0 |
| 56 | MG | AA | 1959 | 1/1 | 0.92 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3510 | 1/1 | 0.92 | 0.34 | 86,86,86,86 | 0 |
| 56 | MG | DA | 2958 | 1/1 | 0.92 | 0.85 | 95,95,95,95 | 0 |
| 56 | MG | CA | 1880 | 1/1 | 0.92 | 0.82 | 118,118,118,118 | 0 |
| 56 | MG | BA | 3235 | 1/1 | 0.92 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | BA | 2982 | 1/1 | 0.92 | 0.31 | 86,86,86,86 | 0 |
| 56 | MG | AA | 1961 | 1/1 | 0.92 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3477 | 1/1 | 0.92 | 0.66 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3716 | 1/1 | 0.92 | 0.07 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3238 | 1/1 | 0.92 | 0.37 | 61,61,61,61 | 0 |
| 56 | MG | BA | 2984 | 1/1 | 0.92 | 0.48 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3312 | 1/1 | 0.92 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3485 | 1/1 | 0.92 | 0.79 | 120,120,120,120 | 0 |
| 56 | MG | DA | 3412 | 1/1 | 0.93 | 0.26 | 60,60,60,60 | 0 |
| 56 | MG | CA | 1774 | 1/1 | 0.93 | 0.26 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3414 | 1/1 | 0.93 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3299 | 1/1 | 0.93 | 0.41 | 38,38,38,38 | 0 |
| 56 | MG | AA | 1889 | 1/1 | 0.93 | 0.20 | 81,81,81,81 | 0 |
| 56 | MG | CA | 1707 | 1/1 | 0.93 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3538 | 1/1 | 0.93 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1741 | 1/1 | 0.93 | 0.29 | 91,91,91,91 | 0 |
| 56 | MG | DA | 3159 | 1/1 | 0.93 | 0.32 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1985 | 1/1 | 0.93 | 0.32 | 108,108,108,108 | 0 |
| 56 | MG | DA | 3543 | 1/1 | 0.93 | 0.17 | 88,88,88,88 | 0 |
| 56 | MG | DA | 2968 | 1/1 | 0.93 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3280 | 1/1 | 0.93 | 0.16 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3164 | 1/1 | 0.93 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | AA | 1936 | 1/1 | 0.93 | 0.77 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3175 | 1/1 | 0.93 | 0.33 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3464 | 1/1 | 0.93 | 0.33 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3562 | 1/1 | 0.93 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3563 | 1/1 | 0.93 | 0.48 | 62,62,62,62 | 0 |
| 56 | MG | CA | 1784 | 1/1 | 0.93 | 0.50 | 96,96,96,96 | 0 |
| 56 | MG | AA | 1781 | 1/1 | 0.93 | 0.34 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3201 | 1/1 | 0.93 | 0.29 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3567 | 1/1 | 0.93 | 0.20 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3408 | 1/1 | 0.93 | 0.28 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1671 | 1/1 | 0.93 | 0.30 | 87,87,87,87 | 0 |
| 56 | MG | CA | 1862 | 1/1 | 0.93 | 0.31 | 117,117,117,117 | 0 |
| 56 | MG | BA | 3411 | 1/1 | 0.93 | 0.36 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3573 | 1/1 | 0.93 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | AA | 1636 | 1/1 | 0.93 | 0.20 | 97,97,97,97 | 0 |
| 56 | MG | BY | 201 | 1/1 | 0.93 | 0.21 | 30,30,30,30 | 0 |
| 56 | MG | AA | 1918 | 1/1 | 0.93 | 0.21 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3001 | 1/1 | 0.93 | 0.08 | 86,86,86,86 | 0 |
| 56 | MG | AO | 101 | 1/1 | 0.93 | 0.33 | 110,110,110,110 | 0 |
| 56 | MG | DA | 3443 | 1/1 | 0.93 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3444 | 1/1 | 0.93 | 0.25 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3584 | 1/1 | 0.93 | 0.34 | 49,49,49,49 | 0 |
| 56 | MG | AA | 1785 | 1/1 | 0.93 | 0.32 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3630 | 1/1 | 0.93 | 0.36 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3448 | 1/1 | 0.93 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | B8 | 102 | 1/1 | 0.93 | 0.27 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3334 | 1/1 | 0.93 | 0.36 | 72,72,72,72 | 0 |
| 56 | MG | DA | 2901 | 1/1 | 0.93 | 0.27 | 47,47,47,47 | 0 |
| 56 | MG | AA | 1711 | 1/1 | 0.93 | 0.21 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3221 | 1/1 | 0.93 | 0.25 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3635 | 1/1 | 0.93 | 0.43 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3457 | 1/1 | 0.93 | 0.44 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3042 | 1/1 | 0.93 | 0.30 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3113 | 1/1 | 0.93 | 0.48 | 109,109,109,109 | 0 |
| 56 | MG | DA | 2908 | 1/1 | 0.93 | 0.28 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3230 | 1/1 | 0.93 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | AA | 1712 | 1/1 | 0.93 | 0.31 | 166,166,166,166 | 0 |
| 56 | MG | DA | 3237 | 1/1 | 0.93 | 0.47 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3586 | 1/1 | 0.93 | 0.26 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3045 | 1/1 | 0.93 | 1.47 | 103,103,103,103 | 0 |
| 56 | MG | DA | 3469 | 1/1 | 0.93 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3046 | 1/1 | 0.93 | 0.45 | 126,126,126,126 | 0 |
| 56 | MG | AA | 1875 | 1/1 | 0.93 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | BA | 2901 | 1/1 | 0.93 | 0.93 | 123,123,123,123 | 0 |
| 56 | MG | BA | 3372 | 1/1 | 0.93 | 0.27 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3087 | 1/1 | 0.93 | 0.74 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3648 | 1/1 | 0.93 | 0.29 | 54,54,54,54 | 0 |
| 56 | MG | AA | 1969 | 1/1 | 0.93 | 0.55 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1789 | 1/1 | 0.93 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1888 | 1/1 | 0.93 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3256 | 1/1 | 0.93 | 0.18 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3361 | 1/1 | 0.93 | 0.29 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3652 | 1/1 | 0.93 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | DA | 2922 | 1/1 | 0.93 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | CA | 1891 | 1/1 | 0.93 | 0.22 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1623 | 1/1 | 0.93 | 0.10 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1818 | 1/1 | 0.93 | 0.26 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1776 | 1/1 | 0.93 | 0.56 | 146,146,146,146 | 0 |
| 56 | MG | AA | 1756 | 1/1 | 0.93 | 0.14 | 87,87,87,87 | 0 |
| 56 | MG | AA | 1863 | 1/1 | 0.93 | 0.34 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3267 | 1/1 | 0.93 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3372 | 1/1 | 0.93 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3440 | 1/1 | 0.93 | 0.40 | 37,37,37,37 | 0 |
| 56 | MG | CA | 1749 | 1/1 | 0.93 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3385 | 1/1 | 0.93 | 0.35 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3660 | 1/1 | 0.93 | 0.36 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3272 | 1/1 | 0.93 | 0.25 | 53,53,53,53 | 0 |
| 56 | MG | AA | 1603 | 1/1 | 0.93 | 0.22 | 64,64,64,64 | 0 |
| 56 | MG | CA | 1903 | 1/1 | 0.93 | 0.26 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3057 | 1/1 | 0.93 | 0.34 | 65,65,65,65 | 0 |
| 56 | MG | AA | 1706 | 1/1 | 0.93 | 0.43 | 186,186,186,186 | 0 |
| 56 | MG | DA | 3279 | 1/1 | 0.93 | 0.27 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3280 | 1/1 | 0.93 | 0.49 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3387 | 1/1 | 0.93 | 0.22 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3228 | 1/1 | 0.93 | 0.13 | 83,83,83,83 | 0 |
| 56 | MG | BA | 3161 | 1/1 | 0.93 | 0.45 | 73,73,73,73 | 0 |
| 56 | MG | BA | 2989 | 1/1 | 0.93 | 0.33 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1763 | 1/1 | 0.93 | 0.19 | 46,46,46,46 | 0 |
| 56 | MG | DP | 201 | 1/1 | 0.93 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1697 | 1/1 | 0.93 | 0.74 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3034 | 1/1 | 0.93 | 0.60 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3518 | 1/1 | 0.93 | 0.44 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1635 | 1/1 | 0.93 | 0.18 | 119,119,119,119 | 0 |
| 56 | MG | BA | 3555 | 1/1 | 0.93 | 0.18 | 94,94,94,94 | 0 |
| 56 | MG | BA | 3231 | 1/1 | 0.93 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | CA | 1701 | 1/1 | 0.93 | 0.21 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3291 | 1/1 | 0.93 | 0.41 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1769 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3525 | 1/1 | 0.93 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3670 | 1/1 | 0.93 | 0.30 | 79,79,79,79 | 0 |
| 56 | MG | BA | 3609 | 1/1 | 0.93 | 0.57 | 149,149,149,149 | 0 |
| 56 | MG | BA | 3233 | 1/1 | 0.93 | 0.30 | 55,55,55,55 | 0 |
| 56 | MG | AA | 1910 | 1/1 | 0.93 | 0.56 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 2916 | 1/1 | 0.94 | 0.32 | 37,37,37,37 | 0 |
| 56 | MG | CA | 1692 | 1/1 | 0.94 | 0.27 | 62,62,62,62 | 0 |
| 56 | MG | AW | 106 | 1/1 | 0.94 | 0.20 | 87,87,87,87 | 0 |
| 56 | MG | DA | 3228 | 1/1 | 0.94 | 0.39 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3515 | 1/1 | 0.94 | 0.09 | 76,76,76,76 | 0 |
| 56 | MG | BA | 3283 | 1/1 | 0.94 | 0.21 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3370 | 1/1 | 0.94 | 0.42 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3677 | 1/1 | 0.94 | 0.40 | 18,18,18,18 | 0 |
| 56 | MG | DA | 2943 | 1/1 | 0.94 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | BA | 2956 | 1/1 | 0.94 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3239 | 1/1 | 0.94 | 0.44 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3232 | 1/1 | 0.94 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3377 | 1/1 | 0.94 | 0.32 | 58,58,58,58 | 0 |
| 56 | MG | BA | 2998 | 1/1 | 0.94 | 0.31 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3447 | 1/1 | 0.94 | 0.20 | 64,64,64,64 | 0 |
| 56 | MG | CA | 1612 | 1/1 | 0.94 | 0.30 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1963 | 1/1 | 0.94 | 0.21 | 80,80,80,80 | 0 |
| 56 | MG | AA | 1964 | 1/1 | 0.94 | 0.16 | 84,84,84,84 | 0 |
| 56 | MG | AA | 1673 | 1/1 | 0.94 | 0.20 | 104,104,104,104 | 0 |
| 56 | MG | AA | 1685 | 1/1 | 0.94 | 0.15 | 199,199,199,199 | 0 |
| 56 | MG | CA | 1894 | 1/1 | 0.94 | 0.07 | 89,89,89,89 | 0 |
| 56 | MG | BA | 3690 | 1/1 | 0.94 | 0.12 | 66,66,66,66 | 0 |
| 56 | MG | AW | 111 | 1/1 | 0.94 | 0.12 | 91,91,91,91 | 0 |
| 56 | MG | DA | 3389 | 1/1 | 0.94 | 0.21 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1649 | 1/1 | 0.94 | 0.90 | 110,110,110,110 | 0 |
| 56 | MG | AA | 1696 | 1/1 | 0.94 | 0.22 | 96,96,96,96 | 0 |
| 56 | MG | DA | 2959 | 1/1 | 0.94 | 0.51 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3457 | 1/1 | 0.94 | 0.24 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3383 | 1/1 | 0.94 | 0.34 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3384 | 1/1 | 0.94 | 0.09 | 71,71,71,71 | 0 |
| 56 | MG | CA | 1804 | 1/1 | 0.94 | 0.37 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3546 | 1/1 | 0.94 | 0.34 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3264 | 1/1 | 0.94 | 0.23 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1805 | 1/1 | 0.94 | 0.25 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1625 | 1/1 | 0.94 | 0.36 | 125,125,125,125 | 0 |
| 56 | MG | BA | 3295 | 1/1 | 0.94 | 0.65 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3106 | 1/1 | 0.94 | 0.22 | 57,57,57,57 | 0 |
| 56 | MG | AA | 1784 | 1/1 | 0.94 | 0.07 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3109 | 1/1 | 0.94 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3084 | 1/1 | 0.94 | 0.35 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1851 | 1/1 | 0.94 | 0.28 | 111,111,111,111 | 0 |
| 56 | MG | BA | 3615 | 1/1 | 0.94 | 0.22 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1876 | 1/1 | 0.94 | 0.50 | 123,123,123,123 | 0 |
| 56 | MG | AA | 1602 | 1/1 | 0.94 | 0.24 | 163,163,163,163 | 0 |
| 56 | MG | DA | 2978 | 1/1 | 0.94 | 0.46 | 64,64,64,64 | 0 |
| 56 | MG | AA | 1628 | 1/1 | 0.94 | 0.64 | 213,213,213,213 | 0 |
| 56 | MG | BA | 3395 | 1/1 | 0.94 | 0.75 | 107,107,107,107 | 0 |
| 56 | MG | BA | 3396 | 1/1 | 0.94 | 0.34 | 43,43,43,43 | 0 |
| 56 | MG | AA | 1708 | 1/1 | 0.94 | 0.23 | 103,103,103,103 | 0 |
| 56 | MG | BA | 2970 | 1/1 | 0.94 | 0.25 | 93,93,93,93 | 0 |
| 56 | MG | BA | 3714 | 1/1 | 0.94 | 0.12 | 94,94,94,94 | 0 |
| 56 | MG | DA | 3096 | 1/1 | 0.94 | 0.31 | 82,82,82,82 | 0 |
| 56 | MG | AA | 1731 | 1/1 | 0.94 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3581 | 1/1 | 0.94 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | BA | 3551 | 1/1 | 0.94 | 0.26 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3625 | 1/1 | 0.94 | 0.38 | 117,117,117,117 | 0 |
| 56 | MG | BA | 3400 | 1/1 | 0.94 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1980 | 1/1 | 0.94 | 0.66 | 76,76,76,76 | 0 |
| 56 | MG | AA | 1856 | 1/1 | 0.94 | 0.46 | 134,134,134,134 | 0 |
| 56 | MG | DA | 3431 | 1/1 | 0.94 | 0.27 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3207 | 1/1 | 0.94 | 0.19 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3556 | 1/1 | 0.94 | 0.63 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3483 | 1/1 | 0.94 | 0.13 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3558 | 1/1 | 0.94 | 0.23 | 71,71,71,71 | 0 |
| 56 | MG | BB | 201 | 1/1 | 0.94 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3019 | 1/1 | 0.94 | 0.20 | 109,109,109,109 | 0 |
| 56 | MG | CA | 1656 | 1/1 | 0.94 | 0.48 | 52,52,52,52 | 0 |
| 56 | MG | CW | 106 | 1/1 | 0.94 | 0.20 | 59,59,59,59 | 0 |
| 56 | MG | AA | 1885 | 1/1 | 0.94 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | CW | 108 | 1/1 | 0.94 | 0.37 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3311 | 1/1 | 0.94 | 0.40 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3562 | 1/1 | 0.94 | 0.34 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3446 | 1/1 | 0.94 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3614 | 1/1 | 0.94 | 0.29 | 50,50,50,50 | 0 |
| 56 | MG | CA | 1745 | 1/1 | 0.94 | 0.20 | 115,115,115,115 | 0 |
| 56 | MG | BA | 3210 | 1/1 | 0.94 | 0.10 | 76,76,76,76 | 0 |
| 56 | MG | CW | 114 | 1/1 | 0.94 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | AA | 1719 | 1/1 | 0.94 | 0.13 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3452 | 1/1 | 0.94 | 0.28 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3565 | 1/1 | 0.94 | 0.30 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1887 | 1/1 | 0.94 | 0.09 | 70,70,70,70 | 0 |
| 56 | MG | CY | 402 | 1/1 | 0.94 | 0.26 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3316 | 1/1 | 0.94 | 0.23 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1846 | 1/1 | 0.94 | 0.39 | 101,101,101,101 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3129 | 1/1 | 0.94 | 0.35 | 104,104,104,104 | 0 |
| 56 | MG | AA | 1791 | 1/1 | 0.94 | 0.37 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3493 | 1/1 | 0.94 | 0.23 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3141 | 1/1 | 0.94 | 0.44 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3649 | 1/1 | 0.94 | 0.27 | 104,104,104,104 | 0 |
| 56 | MG | DA | 3323 | 1/1 | 0.94 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3465 | 1/1 | 0.94 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1987 | 1/1 | 0.94 | 0.58 | 121,121,121,121 | 0 |
| 56 | MG | AA | 1720 | 1/1 | 0.94 | 0.36 | 86,86,86,86 | 0 |
| 56 | MG | DA | 3468 | 1/1 | 0.94 | 0.38 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1793 | 1/1 | 0.94 | 0.36 | 127,127,127,127 | 0 |
| 56 | MG | CA | 1758 | 1/1 | 0.94 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3330 | 1/1 | 0.94 | 0.40 | 36,36,36,36 | 0 |
| 56 | MG | BA | 2942 | 1/1 | 0.94 | 0.51 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3268 | 1/1 | 0.94 | 0.50 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3025 | 1/1 | 0.94 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3167 | 1/1 | 0.94 | 0.18 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3575 | 1/1 | 0.94 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1861 | 1/1 | 0.94 | 0.52 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3480 | 1/1 | 0.94 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3176 | 1/1 | 0.94 | 0.41 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3340 | 1/1 | 0.94 | 0.33 | 31,31,31,31 | 0 |
| 56 | MG | DA | 2913 | 1/1 | 0.94 | 0.73 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1709 | 1/1 | 0.94 | 0.23 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3427 | 1/1 | 0.94 | 0.38 | 35,35,35,35 | 0 |
| 56 | MG | DE | 301 | 1/1 | 0.94 | 0.29 | 29,29,29,29 | 0 |
| 56 | MG | AA | 1893 | 1/1 | 0.94 | 0.52 | 48,48,48,48 | 0 |
| 56 | MG | CA | 1679 | 1/1 | 0.94 | 0.19 | 81,81,81,81 | 0 |
| 56 | MG | AA | 1927 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3345 | 1/1 | 0.94 | 0.24 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1795 | 1/1 | 0.94 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | AW | 101 | 1/1 | 0.94 | 0.33 | 105,105,105,105 | 0 |
| 56 | MG | DA | 3204 | 1/1 | 0.94 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3354 | 1/1 | 0.94 | 0.32 | 38,38,38,38 | 0 |
| 56 | MG | AA | 1655 | 1/1 | 0.94 | 0.52 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3209 | 1/1 | 0.94 | 0.21 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3277 | 1/1 | 0.94 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | AA | 1840 | 1/1 | 0.94 | 1.44 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1683 | 1/1 | 0.94 | 0.15 | 249,249,249,249 | 0 |
| 56 | MG | CA | 1873 | 1/1 | 0.94 | 0.21 | 207,207,207,207 | 0 |
| 56 | MG | CA | 1778 | 1/1 | 0.94 | 0.45 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3218 | 1/1 | 0.94 | 0.18 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1799 | 1/1 | 0.94 | 0.78 | 85,85,85,85 | 0 |
| 56 | MG | D5 | 101 | 1/1 | 0.94 | 0.28 | 71,71,71,71 | 0 |
| 56 | MG | DA | 2933 | 1/1 | 0.94 | 0.34 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3363 | 1/1 | 0.94 | 0.44 | 19,19,19,19 | 0 |
| 56 | MG | CA | 1781 | 1/1 | 0.94 | 0.50 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1915 | 1/1 | 0.95 | 0.70 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3365 | 1/1 | 0.95 | 0.34 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3404 | 1/1 | 0.95 | 0.54 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3595 | 1/1 | 0.95 | 0.27 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1911 | 1/1 | 0.95 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3131 | 1/1 | 0.95 | 0.55 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3408 | 1/1 | 0.95 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3536 | 1/1 | 0.95 | 0.55 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3132 | 1/1 | 0.95 | 0.46 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3134 | 1/1 | 0.95 | 0.44 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3135 | 1/1 | 0.95 | 0.49 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3120 | 1/1 | 0.95 | 0.51 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3484 | 1/1 | 0.95 | 0.34 | 104,104,104,104 | 0 |
| 56 | MG | DA | 3295 | 1/1 | 0.95 | 0.33 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3659 | 1/1 | 0.95 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3418 | 1/1 | 0.95 | 0.20 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3146 | 1/1 | 0.95 | 0.74 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3148 | 1/1 | 0.95 | 0.53 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3554 | 1/1 | 0.95 | 0.44 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3150 | 1/1 | 0.95 | 0.44 | 17,17,17,17 | 0 |
| 56 | MG | AA | 1768 | 1/1 | 0.95 | 0.19 | 183,183,183,183 | 0 |
| 56 | MG | CA | 1923 | 1/1 | 0.95 | 0.14 | 77,77,77,77 | 0 |
| 56 | MG | BA | 2944 | 1/1 | 0.95 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3544 | 1/1 | 0.95 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | DA | 2961 | 1/1 | 0.95 | 0.37 | 143,143,143,143 | 0 |
| 56 | MG | DA | 2962 | 1/1 | 0.95 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1638 | 1/1 | 0.95 | 0.17 | 118,118,118,118 | 0 |
| 56 | MG | CA | 1639 | 1/1 | 0.95 | 0.09 | 100,100,100,100 | 0 |
| 56 | MG | AA | 1704 | 1/1 | 0.95 | 0.45 | 186,186,186,186 | 0 |
| 56 | MG | AA | 1608 | 1/1 | 0.95 | 0.76 | 108,108,108,108 | 0 |
| 56 | MG | AA | 1915 | 1/1 | 0.95 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3375 | 1/1 | 0.95 | 0.32 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3181 | 1/1 | 0.95 | 0.36 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3183 | 1/1 | 0.95 | 0.38 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3056 | 1/1 | 0.95 | 0.21 | 77,77,77,77 | 0 |
| 56 | MG | CA | 1855 | 1/1 | 0.95 | 0.27 | 197,197,197,197 | 0 |
| 56 | MG | AA | 1878 | 1/1 | 0.95 | 0.28 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3193 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3194 | 1/1 | 0.95 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3090 | 1/1 | 0.95 | 0.43 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1982 | 1/1 | 0.95 | 0.14 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3199 | 1/1 | 0.95 | 0.53 | 36,36,36,36 | 0 |
| 56 | MG | CA | 1713 | 1/1 | 0.95 | 0.19 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3379 | 1/1 | 0.95 | 0.39 | 23,23,23,23 | 0 |
| 56 | MG | CA | 1787 | 1/1 | 0.95 | 0.28 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3028 | 1/1 | 0.95 | 0.48 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3206 | 1/1 | 0.95 | 0.42 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3029 | 1/1 | 0.95 | 0.27 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3593 | 1/1 | 0.95 | 0.15 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1749 | 1/1 | 0.95 | 0.29 | 114,114,114,114 | 0 |
| 56 | MG | AA | 1662 | 1/1 | 0.95 | 0.27 | 108,108,108,108 | 0 |
| 56 | MG | BA | 2905 | 1/1 | 0.95 | 0.35 | 54,54,54,54 | 0 |
| 56 | MG | BB | 221 | 1/1 | 0.95 | 0.10 | 65,65,65,65 | 0 |
| 56 | MG | CA | 1654 | 1/1 | 0.95 | 0.27 | 106,106,106,106 | 0 |
| 56 | MG | BA | 3386 | 1/1 | 0.95 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3605 | 1/1 | 0.95 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3215 | 1/1 | 0.95 | 0.54 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3680 | 1/1 | 0.95 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | AA | 1813 | 1/1 | 0.95 | 0.29 | 134,134,134,134 | 0 |
| 56 | MG | BA | 3388 | 1/1 | 0.95 | 0.59 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3613 | 1/1 | 0.95 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | AA | 1814 | 1/1 | 0.95 | 0.48 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3101 | 1/1 | 0.95 | 0.16 | 106,106,106,106 | 0 |
| 56 | MG | DA | 3078 | 1/1 | 0.95 | 0.19 | 75,75,75,75 | 0 |
| 56 | MG | CA | 1661 | 1/1 | 0.95 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3686 | 1/1 | 0.95 | 0.43 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3037 | 1/1 | 0.95 | 0.18 | 101,101,101,101 | 0 |
| 56 | MG | BA | 3327 | 1/1 | 0.95 | 0.33 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3330 | 1/1 | 0.95 | 0.31 | 27,27,27,27 | 0 |
| 56 | MG | AA | 1838 | 1/1 | 0.95 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3005 | 1/1 | 0.95 | 0.23 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3354 | 1/1 | 0.95 | 0.47 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3335 | 1/1 | 0.95 | 0.73 | 49,49,49,49 | 0 |
| 56 | MG | AA | 1884 | 1/1 | 0.95 | 0.39 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3337 | 1/1 | 0.95 | 0.52 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3458 | 1/1 | 0.95 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3338 | 1/1 | 0.95 | 0.21 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3360 | 1/1 | 0.95 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3483 | 1/1 | 0.95 | 0.33 | 96,96,96,96 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1773 | 1/1 | 0.95 | 0.49 | 281,281,281,281 | 0 |
| 56 | MG | DA | 3245 | 1/1 | 0.95 | 0.48 | 45,45,45,45 | 0 |
| 56 | MG | CA | 1814 | 1/1 | 0.95 | 0.25 | 156,156,156,156 | 0 |
| 56 | MG | DA | 3247 | 1/1 | 0.95 | 0.19 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3633 | 1/1 | 0.95 | 0.48 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3249 | 1/1 | 0.95 | 0.48 | 120,120,120,120 | 0 |
| 56 | MG | BA | 3461 | 1/1 | 0.95 | 0.50 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3108 | 1/1 | 0.95 | 0.38 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3637 | 1/1 | 0.95 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3342 | 1/1 | 0.95 | 0.20 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3706 | 1/1 | 0.95 | 0.46 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3099 | 1/1 | 0.95 | 0.07 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3012 | 1/1 | 0.95 | 0.34 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3374 | 1/1 | 0.95 | 0.29 | 54,54,54,54 | 0 |
| 56 | MG | AA | 1659 | 1/1 | 0.95 | 0.23 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3009 | 1/1 | 0.95 | 0.18 | 86,86,86,86 | 0 |
| 56 | MG | AA | 1904 | 1/1 | 0.95 | 0.42 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3378 | 1/1 | 0.95 | 0.37 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3253 | 1/1 | 0.95 | 0.13 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3528 | 1/1 | 0.95 | 0.54 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3018 | 1/1 | 0.95 | 0.08 | 83,83,83,83 | 0 |
| 56 | MG | CA | 1685 | 1/1 | 0.95 | 0.18 | 104,104,104,104 | 0 |
| 56 | MG | AA | 1869 | 1/1 | 0.95 | 0.56 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3022 | 1/1 | 0.95 | 0.21 | 80,80,80,80 | 0 |
| 56 | MG | BA | 3047 | 1/1 | 0.95 | 0.30 | 50,50,50,50 | 0 |
| 56 | MG | DA | 2939 | 1/1 | 0.95 | 0.63 | 66,66,66,66 | 0 |
| 56 | MG | CA | 1829 | 1/1 | 0.95 | 0.68 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3115 | 1/1 | 0.95 | 0.16 | 60,60,60,60 | 0 |
| 56 | MG | AY | 402 | 1/1 | 0.95 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1665 | 1/1 | 0.95 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | AA | 1842 | 1/1 | 0.95 | 0.20 | 98,98,98,98 | 0 |
| 56 | MG | CA | 1762 | 1/1 | 0.95 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1657 | 1/1 | 0.95 | 0.28 | 112,112,112,112 | 0 |
| 56 | MG | DA | 2946 | 1/1 | 0.95 | 0.58 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3260 | 1/1 | 0.95 | 0.25 | 109,109,109,109 | 0 |
| 56 | MG | DA | 3397 | 1/1 | 0.95 | 0.36 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3123 | 1/1 | 0.95 | 0.63 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3399 | 1/1 | 0.95 | 0.09 | 85,85,85,85 | 0 |
| 56 | MG | BA | 3417 | 1/1 | 0.95 | 0.25 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3118 | 1/1 | 0.95 | 0.44 | 132,132,132,132 | 0 |
| 56 | MG | DA | 3166 | 1/1 | 0.96 | 0.25 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3351 | 1/1 | 0.96 | 0.54 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3173 | 1/1 | 0.96 | 0.60 | 46,46,46,46 | 0 |
| 56 | MG | AA | 1968 | 1/1 | 0.96 | 0.89 | 86,86,86,86 | 0 |
| 56 | MG | BA | 3467 | 1/1 | 0.96 | 0.16 | 103,103,103,103 | 0 |
| 56 | MG | BA | 3428 | 1/1 | 0.96 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | DA | 2902 | 1/1 | 0.96 | 0.25 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3179 | 1/1 | 0.96 | 0.21 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3094 | 1/1 | 0.96 | 0.43 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3355 | 1/1 | 0.96 | 0.26 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1805 | 1/1 | 0.96 | 0.24 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3516 | 1/1 | 0.96 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3317 | 1/1 | 0.96 | 0.39 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3191 | 1/1 | 0.96 | 0.37 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3192 | 1/1 | 0.96 | 0.25 | 38,38,38,38 | 0 |
| 56 | MG | AA | 1610 | 1/1 | 0.96 | 0.19 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3360 | 1/1 | 0.96 | 0.54 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3475 | 1/1 | 0.96 | 0.61 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1601 | 1/1 | 0.96 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | DA | 2974 | 1/1 | 0.96 | 0.18 | 90,90,90,90 | 0 |
| 56 | MG | BA | 3159 | 1/1 | 0.96 | 0.20 | 151,151,151,151 | 0 |
| 56 | MG | DA | 3587 | 1/1 | 0.96 | 0.10 | 90,90,90,90 | 0 |
| 56 | MG | DA | 3100 | 1/1 | 0.96 | 0.42 | 97,97,97,97 | 0 |
| 56 | MG | BA | 3058 | 1/1 | 0.96 | 0.38 | 60,60,60,60 | 0 |
| 56 | MG | CA | 1751 | 1/1 | 0.96 | 0.58 | 163,163,163,163 | 0 |
| 56 | MG | BA | 3023 | 1/1 | 0.96 | 0.54 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3040 | 1/1 | 0.96 | 0.32 | 102,102,102,102 | 0 |
| 56 | MG | AA | 1626 | 1/1 | 0.96 | 0.09 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3325 | 1/1 | 0.96 | 0.55 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3481 | 1/1 | 0.96 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1859 | 1/1 | 0.96 | 0.60 | 132,132,132,132 | 0 |
| 56 | MG | AA | 1633 | 1/1 | 0.96 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3488 | 1/1 | 0.96 | 0.07 | 70,70,70,70 | 0 |
| 56 | MG | DA | 2984 | 1/1 | 0.96 | 0.26 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3606 | 1/1 | 0.96 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3607 | 1/1 | 0.96 | 0.19 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3394 | 1/1 | 0.96 | 0.28 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3111 | 1/1 | 0.96 | 0.28 | 84,84,84,84 | 0 |
| 56 | MG | CA | 1609 | 1/1 | 0.96 | 0.19 | 100,100,100,100 | 0 |
| 56 | MG | DA | 2923 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | CA | 1759 | 1/1 | 0.96 | 0.41 | 65,65,65,65 | 0 |
| 56 | MG | DA | 2925 | 1/1 | 0.96 | 0.55 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3311 | 1/1 | 0.96 | 0.30 | 54,54,54,54 | 0 |
| 56 | MG | BA | 3044 | 1/1 | 0.96 | 0.35 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3617 | 1/1 | 0.96 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3314 | 1/1 | 0.96 | 0.36 | 65,65,65,65 | 0 |
| 56 | MG | DA | 2927 | 1/1 | 0.96 | 0.30 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3402 | 1/1 | 0.96 | 0.33 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3225 | 1/1 | 0.96 | 0.39 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3274 | 1/1 | 0.96 | 0.12 | 105,105,105,105 | 0 |
| 56 | MG | AA | 1844 | 1/1 | 0.96 | 0.26 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3673 | 1/1 | 0.96 | 0.24 | 133,133,133,133 | 0 |
| 56 | MG | DA | 3409 | 1/1 | 0.96 | 0.32 | 102,102,102,102 | 0 |
| 56 | MG | DA | 3506 | 1/1 | 0.96 | 0.20 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3229 | 1/1 | 0.96 | 0.28 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3445 | 1/1 | 0.96 | 0.16 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3232 | 1/1 | 0.96 | 0.61 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3324 | 1/1 | 0.96 | 0.48 | 13,13,13,13 | 0 |
| 56 | MG | AA | 1974 | 1/1 | 0.96 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3235 | 1/1 | 0.96 | 0.59 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3334 | 1/1 | 0.96 | 0.35 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3490 | 1/1 | 0.96 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3126 | 1/1 | 0.96 | 0.71 | 65,65,65,65 | 0 |
| 56 | MG | BA | 2938 | 1/1 | 0.96 | 0.21 | 81,81,81,81 | 0 |
| 56 | MG | BA | 3374 | 1/1 | 0.96 | 0.24 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3030 | 1/1 | 0.96 | 0.45 | 64,64,64,64 | 0 |
| 56 | MG | AA | 1905 | 1/1 | 0.96 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3452 | 1/1 | 0.96 | 0.67 | 53,53,53,53 | 0 |
| 56 | MG | AW | 117 | 1/1 | 0.96 | 0.14 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3133 | 1/1 | 0.96 | 0.36 | 20,20,20,20 | 0 |
| 56 | MG | BA | 2914 | 1/1 | 0.96 | 0.32 | 122,122,122,122 | 0 |
| 56 | MG | BA | 3498 | 1/1 | 0.96 | 0.07 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3137 | 1/1 | 0.96 | 0.29 | 23,23,23,23 | 0 |
| 56 | MG | DB | 216 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | AA | 1693 | 1/1 | 0.96 | 0.33 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3140 | 1/1 | 0.96 | 0.41 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3253 | 1/1 | 0.96 | 0.36 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3254 | 1/1 | 0.96 | 0.31 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1788 | 1/1 | 0.96 | 0.28 | 175,175,175,175 | 0 |
| 56 | MG | BA | 3072 | 1/1 | 0.96 | 0.17 | 88,88,88,88 | 0 |
| 56 | MG | DA | 3347 | 1/1 | 0.96 | 0.21 | 23,23,23,23 | 0 |
| 56 | MG | CW | 109 | 1/1 | 0.96 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3438 | 1/1 | 0.96 | 0.28 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3147 | 1/1 | 0.96 | 0.23 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3418 | 1/1 | 0.96 | 0.20 | 27,27,27,27 | 0 |
| 56 | MG | DN | 201 | 1/1 | 0.96 | 0.14 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3540 | 1/1 | 0.96 | 0.20 | 85,85,85,85 | 0 |
| 56 | MG | CA | 1832 | 1/1 | 0.96 | 0.19 | 65,65,65,65 | 0 |
| 56 | MG | DA | 3442 | 1/1 | 0.96 | 0.40 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3152 | 1/1 | 0.96 | 0.39 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3153 | 1/1 | 0.96 | 0.48 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3285 | 1/1 | 0.96 | 0.24 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3694 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | AA | 1818 | 1/1 | 0.96 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1889 | 1/1 | 0.96 | 0.06 | 92,92,92,92 | 0 |
| 56 | MG | DA | 3555 | 1/1 | 0.96 | 0.28 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3556 | 1/1 | 0.96 | 0.23 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3347 | 1/1 | 0.96 | 0.23 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3558 | 1/1 | 0.96 | 0.34 | 14,14,14,14 | 0 |
| 56 | MG | BA | 3463 | 1/1 | 0.96 | 0.30 | 106,106,106,106 | 0 |
| 56 | MG | BA | 3349 | 1/1 | 0.96 | 0.39 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3165 | 1/1 | 0.96 | 0.47 | 25,25,25,25 | 0 |
| 57 | ZN | CN | 101 | 1/1 | 0.96 | 0.15 | 111,111,111,111 | 0 |
| 56 | MG | BA | 3518 | 1/1 | 0.97 | 0.25 | 27,27,27,27 | 0 |
| 56 | MG | CA | 1632 | 1/1 | 0.97 | 0.17 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3021 | 1/1 | 0.97 | 0.48 | 66,66,66,66 | 0 |
| 56 | MG | BD | 301 | 1/1 | 0.97 | 0.23 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3705 | 1/1 | 0.97 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3453 | 1/1 | 0.97 | 0.47 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1849 | 1/1 | 0.97 | 0.12 | 95,95,95,95 | 0 |
| 56 | MG | BA | 2978 | 1/1 | 0.97 | 0.67 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3597 | 1/1 | 0.97 | 0.41 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3214 | 1/1 | 0.97 | 0.39 | 22,22,22,22 | 0 |
| 56 | MG | BX | 101 | 1/1 | 0.97 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3424 | 1/1 | 0.97 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3603 | 1/1 | 0.97 | 0.09 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3217 | 1/1 | 0.97 | 0.40 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3136 | 1/1 | 0.97 | 0.45 | 12,12,12,12 | 0 |
| 56 | MG | AA | 1798 | 1/1 | 0.97 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | BA | 2980 | 1/1 | 0.97 | 0.25 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3608 | 1/1 | 0.97 | 0.57 | 50,50,50,50 | 0 |
| 56 | MG | CA | 1830 | 1/1 | 0.97 | 0.15 | 80,80,80,80 | 0 |
| 56 | MG | DA | 2928 | 1/1 | 0.97 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3214 | 1/1 | 0.97 | 0.23 | 85,85,85,85 | 0 |
| 56 | MG | AA | 1919 | 1/1 | 0.97 | 0.56 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3631 | 1/1 | 0.97 | 0.34 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3632 | 1/1 | 0.97 | 0.39 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3015 | 1/1 | 0.97 | 0.33 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | AA | 1976 | 1/1 | 0.97 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | DA | 2935 | 1/1 | 0.97 | 0.14 | 89,89,89,89 | 0 |
| 56 | MG | DA | 3231 | 1/1 | 0.97 | 0.42 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3154 | 1/1 | 0.97 | 0.28 | 12,12,12,12 | 0 |
| 56 | MG | BA | 3339 | 1/1 | 0.97 | 0.28 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3234 | 1/1 | 0.97 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3157 | 1/1 | 0.97 | 0.21 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3236 | 1/1 | 0.97 | 0.64 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3636 | 1/1 | 0.97 | 0.47 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1664 | 1/1 | 0.97 | 0.30 | 64,64,64,64 | 0 |
| 56 | MG | AA | 1978 | 1/1 | 0.97 | 0.30 | 129,129,129,129 | 0 |
| 56 | MG | DA | 3534 | 1/1 | 0.97 | 0.52 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3240 | 1/1 | 0.97 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3566 | 1/1 | 0.97 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1877 | 1/1 | 0.97 | 0.49 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1943 | 1/1 | 0.97 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3642 | 1/1 | 0.97 | 0.35 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3312 | 1/1 | 0.97 | 0.52 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3021 | 1/1 | 0.97 | 0.13 | 111,111,111,111 | 0 |
| 56 | MG | DA | 3464 | 1/1 | 0.97 | 0.60 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3168 | 1/1 | 0.97 | 0.40 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3172 | 1/1 | 0.97 | 0.58 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3545 | 1/1 | 0.97 | 0.19 | 91,91,91,91 | 0 |
| 56 | MG | BA | 3314 | 1/1 | 0.97 | 0.49 | 13,13,13,13 | 0 |
| 56 | MG | AA | 1902 | 1/1 | 0.97 | 0.22 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3100 | 1/1 | 0.97 | 0.22 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3550 | 1/1 | 0.97 | 0.39 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3553 | 1/1 | 0.97 | 0.45 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3352 | 1/1 | 0.97 | 0.25 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3177 | 1/1 | 0.97 | 0.31 | 21,21,21,21 | 0 |
| 56 | MG | AA | 1870 | 1/1 | 0.97 | 0.42 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3328 | 1/1 | 0.97 | 0.52 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3692 | 1/1 | 0.97 | 0.36 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3180 | 1/1 | 0.97 | 0.45 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3476 | 1/1 | 0.97 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3561 | 1/1 | 0.97 | 0.18 | 16,16,16,16 | 0 |
| 56 | MG | AA | 1735 | 1/1 | 0.97 | 0.36 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3182 | 1/1 | 0.97 | 0.50 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3479 | 1/1 | 0.97 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3184 | 1/1 | 0.97 | 0.29 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3578 | 1/1 | 0.97 | 0.27 | 32,32,32,32 | 0 |
| 56 | MG | DA | 2904 | 1/1 | 0.97 | 0.60 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3025 | 1/1 | 0.97 | 0.30 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1601 | 1/1 | 0.97 | 0.36 | 92,92,92,92 | 0 |
| 56 | MG | CA | 1623 | 1/1 | 0.97 | 0.17 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3410 | 1/1 | 0.97 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3572 | 1/1 | 0.97 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3416 | 1/1 | 0.97 | 0.42 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1694 | 1/1 | 0.97 | 0.28 | 165,165,165,165 | 0 |
| 56 | MG | AA | 1960 | 1/1 | 0.97 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3197 | 1/1 | 0.97 | 0.22 | 21,21,21,21 | 0 |
| 56 | MG | BB | 219 | 1/1 | 0.97 | 0.30 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3328 | 1/1 | 0.97 | 0.57 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3580 | 1/1 | 0.97 | 0.49 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3069 | 1/1 | 0.97 | 0.23 | 32,32,32,32 | 0 |
| 56 | MG | CA | 1721 | 1/1 | 0.97 | 0.12 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3202 | 1/1 | 0.97 | 0.40 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3420 | 1/1 | 0.97 | 0.39 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3277 | 1/1 | 0.97 | 0.38 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3421 | 1/1 | 0.97 | 0.21 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1906 | 1/1 | 0.98 | 0.70 | 38,38,38,38 | 0 |
| 56 | MG | BA | 2990 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3143 | 1/1 | 0.98 | 0.48 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3144 | 1/1 | 0.98 | 0.41 | 14,14,14,14 | 0 |
| 56 | MG | BA | 3667 | 1/1 | 0.98 | 0.37 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3628 | 1/1 | 0.98 | 0.21 | 295,295,295,295 | 0 |
| 56 | MG | BB | 207 | 1/1 | 0.98 | 0.14 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3357 | 1/1 | 0.98 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3265 | 1/1 | 0.98 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3184 | 1/1 | 0.98 | 0.38 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3185 | 1/1 | 0.98 | 0.17 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3186 | 1/1 | 0.98 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3187 | 1/1 | 0.98 | 0.27 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3319 | 1/1 | 0.98 | 0.41 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3313 | 1/1 | 0.98 | 0.39 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3149 | 1/1 | 0.98 | 0.41 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3320 | 1/1 | 0.98 | 0.39 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3345 | 1/1 | 0.98 | 0.29 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3274 | 1/1 | 0.98 | 0.36 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3545 | 1/1 | 0.98 | 0.51 | 245,245,245,245 | 0 |
| 56 | MG | DA | 3588 | 1/1 | 0.98 | 0.26 | 24,24,24,24 | 0 |
| 56 | MG | B3 | 101 | 1/1 | 0.98 | 0.43 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3155 | 1/1 | 0.98 | 0.39 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3450 | 1/1 | 0.98 | 0.15 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | DA | 3195 | 1/1 | 0.98 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1810 | 1/1 | 0.98 | 0.06 | 87,87,87,87 | 0 |
| 56 | MG | DA | 2971 | 1/1 | 0.98 | 0.15 | 132,132,132,132 | 0 |
| 56 | MG | AA | 1647 | 1/1 | 0.98 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3596 | 1/1 | 0.98 | 0.43 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3410 | 1/1 | 0.98 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3598 | 1/1 | 0.98 | 0.36 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3599 | 1/1 | 0.98 | 0.31 | 14,14,14,14 | 0 |
| 56 | MG | CA | 1878 | 1/1 | 0.98 | 0.35 | 66,66,66,66 | 0 |
| 56 | MG | BA | 3033 | 1/1 | 0.98 | 0.24 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3350 | 1/1 | 0.98 | 0.38 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3549 | 1/1 | 0.98 | 0.34 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3163 | 1/1 | 0.98 | 0.29 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3551 | 1/1 | 0.98 | 0.38 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3552 | 1/1 | 0.98 | 0.50 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3678 | 1/1 | 0.98 | 0.30 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3205 | 1/1 | 0.98 | 0.24 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3053 | 1/1 | 0.98 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | BA | 3104 | 1/1 | 0.98 | 0.15 | 120,120,120,120 | 0 |
| 56 | MG | BA | 3381 | 1/1 | 0.98 | 0.34 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3509 | 1/1 | 0.98 | 0.22 | 142,142,142,142 | 0 |
| 56 | MG | BA | 3243 | 1/1 | 0.98 | 0.25 | 149,149,149,149 | 0 |
| 56 | MG | DA | 3170 | 1/1 | 0.98 | 0.11 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3171 | 1/1 | 0.98 | 0.23 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3513 | 1/1 | 0.98 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3315 | 1/1 | 0.98 | 0.19 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3368 | 1/1 | 0.98 | 0.28 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3684 | 1/1 | 0.98 | 0.29 | 47,47,47,47 | 0 |
| 56 | MG | D5 | 103 | 1/1 | 0.98 | 0.33 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3620 | 1/1 | 0.98 | 0.48 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3138 | 1/1 | 0.98 | 0.36 | 12,12,12,12 | 0 |
| 57 | ZN | CD | 301 | 1/1 | 0.98 | 0.34 | 109,109,109,109 | 0 |
| 56 | MG | BA | 3316 | 1/1 | 0.98 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3151 | 1/1 | 0.99 | 0.22 | 12,12,12,12 | 0 |
| 56 | MG | CA | 1757 | 1/1 | 0.99 | 0.45 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3222 | 1/1 | 0.99 | 0.35 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3575 | 1/1 | 0.99 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3329 | 1/1 | 0.99 | 0.46 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3333 | 1/1 | 0.99 | 0.42 | 12,12,12,12 | 0 |
| 56 | MG | AA | 1928 | 1/1 | 0.99 | 0.08 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3502 | 1/1 | 0.99 | 0.23 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3250 | 1/1 | 0.99 | 0.17 | 269,269,269,269 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | BA | 3348 | 1/1 | 0.99 | 0.43 | 25,25,25,25 | 0 |
| 57 | ZN | AD | 301 | 1/1 | 0.99 | 0.29 | 71,71,71,71 | 0 |
| 57 | ZN | AN | 101 | 1/1 | 0.99 | 0.17 | 115,115,115,115 | 0 |
| 56 | MG | DA | 3142 | 1/1 | 0.99 | 0.42 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3169 | 1/1 | 0.99 | 0.31 | 33,33,33,33 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.