



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:23 PM GMT

PDB ID : 4V7K  
Title : Structure of RelE nuclease bound to the 70S ribosome (postcleavage state)  
Authors : Neubauer, C.; Gao, Y.-G.; Andersen, K.R.; Dunham, C.M.; Kelley, A.C.;  
Hentschel, J.; Gerdes, K.; Ramakrishnan, V.; Brodersen, D.E.  
Deposited on : 2009-11-02  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

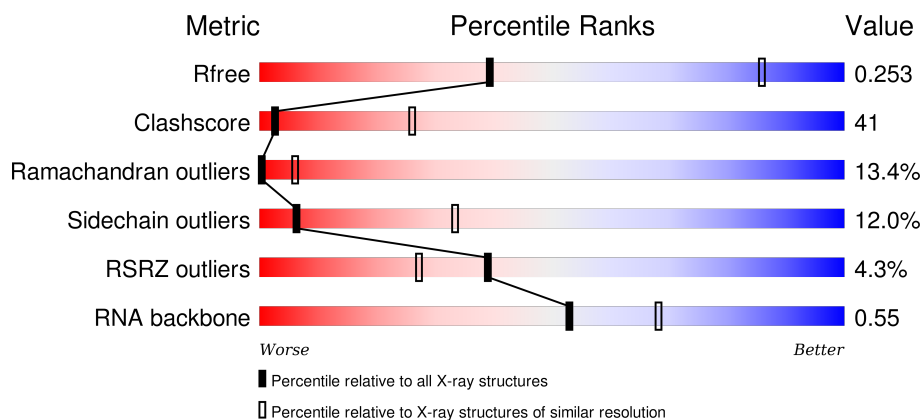
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 91344                       | 1408 (3.80-3.40)                                      |
| Clashscore            | 102246                      | 1010 (3.74-3.46)                                      |
| Ramachandran outliers | 100387                      | 1007 (3.76-3.44)                                      |
| Sidechain outliers    | 100360                      | 1007 (3.76-3.44)                                      |
| RSRZ outliers         | 91569                       | 1003 (3.78-3.42)                                      |
| RNA backbone          | 2183                        | 1058 (4.40-2.80)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 1   | Ab    | 256    | <div> <div>3%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>9%</div> </div> </div>  |
| 1   | Bb    | 256    | <div> <div>3%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>9%</div> </div> </div>  |
| 2   | Ac    | 239    | <div> <div>5%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>14%</div> </div> </div> |
| 2   | Bc    | 239    | <div> <div>3%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>14%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | Ad    | 209    |    |
| 3   | Bd    | 209    |    |
| 4   | Ae    | 162    |    |
| 4   | Be    | 162    |    |
| 5   | Af    | 101    |    |
| 5   | Bf    | 101    |    |
| 6   | Ag    | 156    |    |
| 6   | Bg    | 156    |    |
| 7   | Ah    | 138    |    |
| 7   | Bh    | 138    |    |
| 8   | Ai    | 128    |    |
| 8   | Bi    | 128    |   |
| 9   | Aj    | 105    |  |
| 9   | Bj    | 105    |  |
| 10  | Ak    | 129    |  |
| 10  | Bk    | 129    |  |
| 11  | Al    | 132    |  |
| 11  | Bl    | 132    |  |
| 12  | Am    | 126    |  |
| 12  | Bm    | 126    |  |
| 13  | An    | 61     |  |
| 13  | Bn    | 61     |  |
| 14  | Ao    | 89     |  |
| 14  | Bo    | 89     |  |
| 15  | Ap    | 88     |  |

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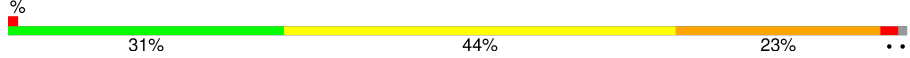
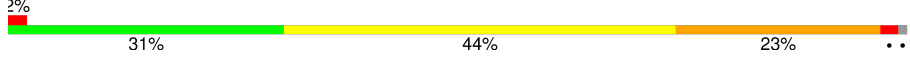
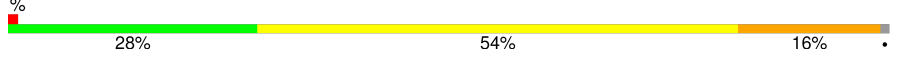

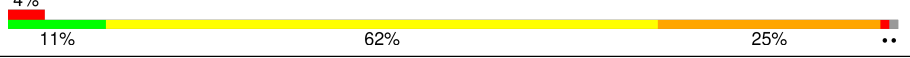
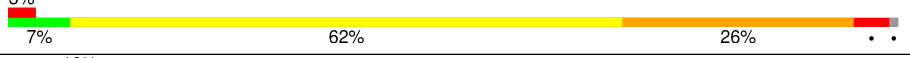
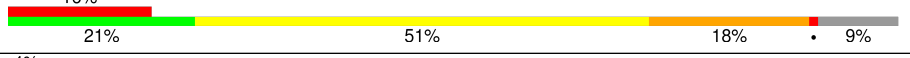
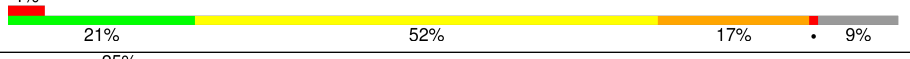
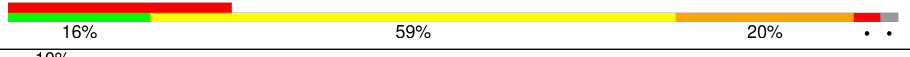
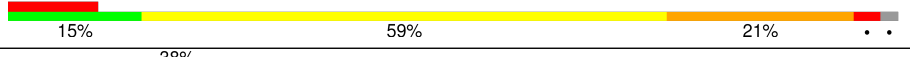
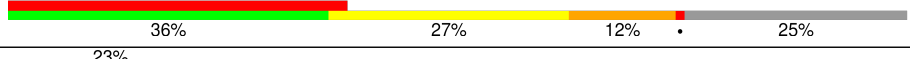
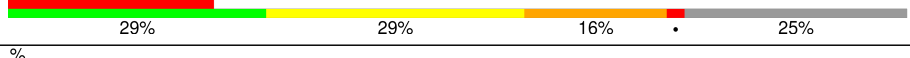
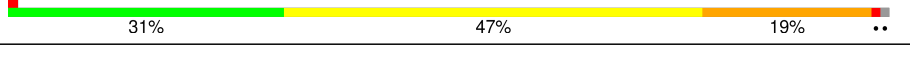
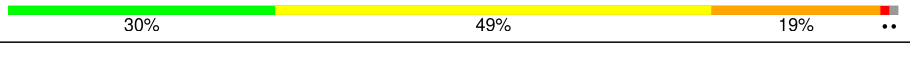
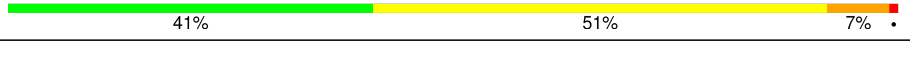
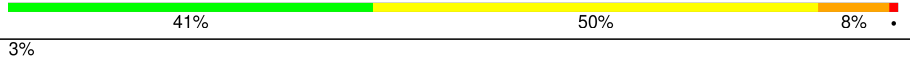
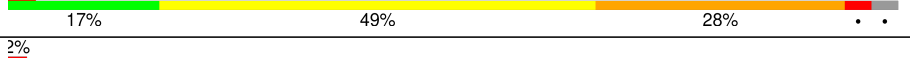
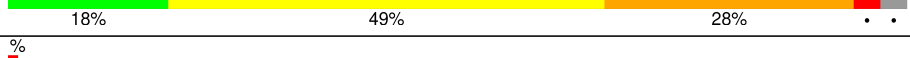


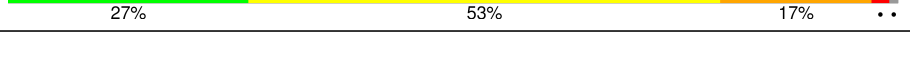
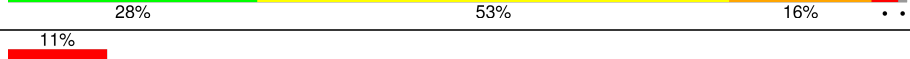

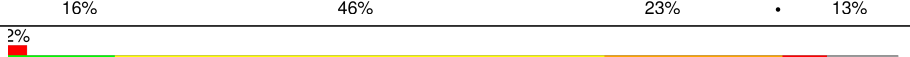

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | Bp    | 88     |                  |
| 16  | Aq    | 105    |                  |
| 16  | Bq    | 105    |                  |
| 17  | Ar    | 88     |                  |
| 17  | Br    | 88     |                  |
| 18  | As    | 93     |                  |
| 18  | Bs    | 93     |                  |
| 19  | At    | 106    |                  |
| 19  | Bt    | 106    |                  |
| 20  | Au    | 27     |                  |
| 20  | Bu    | 27     |                  |
| 21  | Ay    | 95     |                  |
| 21  | By    | 95     |                  |
| 22  | Aa    | 1504   |                  |
| 22  | Ba    | 1504   |                  |
| 23  | Ax    | 14     |                  |
| 23  | Bx    | 14     |                  |
| 24  | Av    | 77     |                  |
| 24  | Bv    | 77     |                  |
| 25  | Aw    | 77     |                  |
| 25  | Bw    | 77     |                  |
| 26  | AC    | 229    |                  |
| 26  | BC    | 229    |                  |
| 27  | AD    | 276    |                  |
| 27  | BD    | 276    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28  | AE    | 206    |    |
| 28  | BE    | 206    |    |
| 29  | AF    | 210    |    |
| 29  | BF    | 210    |    |
| 30  | AG    | 182    |    |
| 30  | BG    | 182    |    |
| 31  | AH    | 180    |    |
| 31  | BH    | 180    |    |
| 32  | AI    | 148    |    |
| 32  | BI    | 148    |    |
| 33  | AJ    | 173    |    |
| 33  | BJ    | 173    |   |
| 34  | AN    | 140    |  |
| 34  | BN    | 140    |  |
| 35  | AO    | 122    |  |
| 35  | BO    | 122    |  |
| 36  | AP    | 150    |  |
| 36  | BP    | 150    |  |
| 37  | AQ    | 141    |  |
| 37  | BQ    | 141    |  |
| 38  | AR    | 118    |  |
| 38  | BR    | 118    |  |
| 39  | AS    | 112    |  |
| 39  | BS    | 112    |  |
| 40  | AT    | 146    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | BT    | 146    |                  |
| 41  | AU    | 118    |                  |
| 41  | BU    | 118    |                  |
| 42  | AV    | 101    |                  |
| 42  | BV    | 101    |                  |
| 43  | AW    | 113    |                  |
| 43  | BW    | 113    |                  |
| 44  | AX    | 96     |                  |
| 44  | BX    | 96     |                  |
| 45  | AY    | 110    |                  |
| 45  | BY    | 110    |                  |
| 46  | AZ    | 206    |                  |
| 46  | BZ    | 206    |                  |
| 47  | A0    | 85     |                  |
| 47  | B0    | 85     |                  |
| 48  | A1    | 98     |                  |
| 48  | B1    | 98     |                  |
| 49  | A2    | 72     |                  |
| 49  | B2    | 72     |                  |
| 50  | A3    | 60     |                  |
| 50  | B3    | 60     |                  |
| 51  | A4    | 71     |                  |
| 51  | B4    | 71     |                  |
| 52  | A5    | 60     |                  |
| 52  | B5    | 60     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | A6    | 54     |                  |
| 53  | B6    | 54     |                  |
| 54  | A7    | 49     |                  |
| 54  | B7    | 49     |                  |
| 55  | A8    | 65     |                  |
| 55  | B8    | 65     |                  |
| 56  | A9    | 37     |                  |
| 56  | B9    | 37     |                  |
| 57  | AA    | 2848   |                  |
| 57  | BA    | 2848   |                  |
| 58  | AB    | 119    |                  |
| 58  | BB    | 119    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60  | MG   | A7    | 101  | -         | -        | -       | X                |
| 60  | MG   | AA    | 2906 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2907 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2909 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2913 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2914 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2915 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2918 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2919 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2920 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2921 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2925 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2928 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2929 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2931 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2932 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2943 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60  | MG   | AA    | 2949 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2951 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2953 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2960 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2964 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2965 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2968 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2969 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2976 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2980 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2981 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2985 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2987 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2988 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2991 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2996 | -         | -        | -       | X                |
| 60  | MG   | AA    | 2997 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3011 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3012 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3019 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3023 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3025 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3028 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3029 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3035 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3038 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3039 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3044 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3046 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3051 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3054 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3056 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3061 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3069 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3070 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3072 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3083 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3088 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3095 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3096 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3097 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3099 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60  | MG   | AA    | 3101 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3102 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3121 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3124 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3126 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3128 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3133 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3134 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3138 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3147 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3150 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3158 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3163 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3172 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3175 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3177 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3179 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3190 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3194 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3195 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3197 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3205 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3219 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3221 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3231 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3233 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3236 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3243 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3245 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3247 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3256 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3259 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3261 | -         | -        | -       | X                |
| 60  | MG   | AA    | 3265 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1611 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1613 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1622 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1624 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1628 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1631 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1633 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1635 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60  | MG   | Aa    | 1642 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1645 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1662 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1666 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1670 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1674 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1678 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1679 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1685 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1686 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1725 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1727 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1729 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1735 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1738 | -         | -        | -       | X                |
| 60  | MG   | Aa    | 1744 | -         | -        | -       | X                |
| 60  | MG   | Ae    | 202  | -         | -        | -       | X                |
| 60  | MG   | Av    | 102  | -         | -        | -       | X                |
| 60  | MG   | B0    | 101  | -         | -        | -       | X                |
| 60  | MG   | B7    | 101  | -         | -        | -       | X                |
| 60  | MG   | BA    | 2905 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2908 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2912 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2913 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2914 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2917 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2920 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2927 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2928 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2930 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2931 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2951 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2957 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2962 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2965 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2966 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2967 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2968 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2979 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2980 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2982 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2984 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60  | MG   | BA    | 2987 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2990 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2995 | -         | -        | -       | X                |
| 60  | MG   | BA    | 2996 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3010 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3011 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3013 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3018 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3022 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3024 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3027 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3028 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3029 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3034 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3035 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3037 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3038 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3043 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3045 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3052 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3053 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3055 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3060 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3069 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3070 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3084 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3088 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3091 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3093 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3094 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3095 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3097 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3100 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3101 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3102 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3105 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3120 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3123 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3127 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3131 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3133 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3134 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60  | MG   | BA    | 3138 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3147 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3150 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3156 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3160 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3165 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3171 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3172 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3176 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3183 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3187 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3191 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3194 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3211 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3217 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3231 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3234 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3236 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3241 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3254 | -         | -        | -       | X                |
| 60  | MG   | BA    | 3257 | -         | -        | -       | X                |
| 60  | MG   | BD    | 301  | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1608 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1609 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1621 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1630 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1634 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1644 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1654 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1668 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1671 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1684 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1685 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1691 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1695 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1724 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1726 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1728 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1731 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1739 | -         | -        | -       | X                |
| 60  | MG   | Ba    | 1742 | -         | -        | -       | X                |
| 60  | MG   | Bv    | 105  | -         | -        | -       | X                |



## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 297230 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 protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Ab    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |
| 1   | Bb    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | Ac    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |
| 2   | Bc    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | Ad    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 3   | Bd    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | Ae    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |
| 4   | Be    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | Af    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 5   | Bf    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | Ah    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 7   | Bh    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 8   | Ai    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |
| 8   | Bi    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | Aj    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 794   | 499 | 156 | 138 | 1 |         |         |       |
| 9   | Bj    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 794   | 499 | 156 | 138 | 1 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | Ak    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | Bk    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | Al    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |
| 11  | Bl    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | Am    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |
| 12  | Bm    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 13  | An    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 13  | Bn    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | Ao    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 14  | Bo    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | Ap    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |
| 15  | Bp    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | Aq    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |
| 16  | Bq    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 17  | Ar    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |
| 17  | Br    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | As    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 629   | 403 | 114 | 110 | 2 |         |         |       |
| 18  | Bs    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 629   | 403 | 114 | 110 | 2 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | At    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |
| 19  | Bt    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 20  | Au    | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |
| 20  | Bu    | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |

- Molecule 21 is a protein called Toxin relE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | Ay    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 782   | 502 | 139 | 139 | 2 |         |         |       |
| 21  | By    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 782   | 502 | 139 | 139 | 2 |         |         |       |

- Molecule 22 is a RNA chain called RNA (1504-MER).

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 22  | Aa    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32329 | 14390 | 5992 | 10444 | 1503 |         |         |       |
| 22  | Ba    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32329 | 14390 | 5992 | 10444 | 1503 |         |         |       |

- Molecule 23 is a RNA chain called RNA (5'-R(\*A\*AP\*GP\*UP\*AP\*AP\*AP\*AP\*AP\*UP\*GP\*UP\*A\*(CCC))-3').

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 23  | Ax    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 260   | 117 | 51 | 80 | 12 |         |         |       |
| 23  | Bx    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 260   | 117 | 51 | 80 | 12 |         |         |       |

- Molecule 24 is a RNA chain called RNA (77-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 24  | Av    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1641  | 733 | 297 | 535 | 76 |         |         |       |
| 24  | Bv    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1641  | 733 | 297 | 535 | 76 |         |         |       |

- Molecule 25 is a RNA chain called RNA (77-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 25  | Aw    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 25  | Bw    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | AC    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 590 | 174 | 172 | 1 |         |         |       |
| 26  | BC    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 590 | 174 | 172 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27  | AD    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2104  | 1329 | 416 | 356 | 3 |         |         |       |
| 27  | BD    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2104  | 1329 | 416 | 356 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | AE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1563  | 988 | 299 | 270 | 6 |         |         |       |
| 28  | BE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1563  | 988 | 299 | 270 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | AF    | 207      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1623  | 1035 | 303 | 282 | 3 |         |         |       |
| 29  | BF    | 207      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1623  | 1035 | 303 | 282 | 3 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | AH    | 164      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1259  | 800 | 233 | 225 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BH    | 164      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1259  | 800 | 233 | 225 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | AI    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1131  | 723 | 200 | 207 | 1 |         |         |       |
| 32  | BI    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1131  | 723 | 200 | 207 | 1 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | AJ    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 641   | 381 | 130 | 130 |   |         |         |       |
| 33  | BJ    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 641   | 381 | 130 | 130 |   |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | AN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 34  | BN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | AO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 35  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | AQ    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 710 | 210 | 185 | 7 |         |         |       |
| 37  | BQ    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 710 | 210 | 185 | 7 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 39  | AS    | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 770   | 486 | 154 | 130 |         |         |       |
| 39  | BS    | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 770   | 486 | 154 | 130 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | AT    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1123  | 699 | 230 | 193 | 1 |         |         |       |
| 40  | BT    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1123  | 699 | 230 | 193 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | AU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |
| 41  | BU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |

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



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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | AW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |
| 43  | BW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 44  | AX    | 92       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |  |         |         |       |
| 44  | BX    | 92       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | AY    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 500 | 148 | 123 | 4 |         |         |       |
| 45  | BY    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 500 | 148 | 123 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | AZ    | 184      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1467  | 936 | 261 | 268 | 2 |         |         |       |
| 46  | BZ    | 184      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1467  | 936 | 261 | 268 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | A0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | B0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | A1    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 731   | 460 | 145 | 125 | 1 |         |         |       |
| 48  | B1    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 731   | 460 | 145 | 125 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | A2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |
| 49  | B2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | A3    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 467   | 298 | 90 | 78 | 1 |         |         |       |
| 50  | B3    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 467   | 298 | 90 | 78 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | A4    | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 450   | 285 | 77 | 83 | 5 |         |         |       |
| 51  | B4    | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 450   | 285 | 77 | 83 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | A5    | 55       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 427   | 267 | 86 | 69 | 5 |         |         |       |
| 52  | B5    | 55       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 427   | 267 | 86 | 69 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | A6    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 433   | 270 | 88 | 71 | 4 |         |         |       |
| 53  | B6    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 433   | 270 | 88 | 71 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | A7    | 47       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 409   | 251 | 102 | 54 | 2 |         |         |       |
| 54  | B7    | 47       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 409   | 251 | 102 | 54 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55  | A8    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 326 | 101 | 78 | 2 |         |         |       |
| 55  | B8    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 326 | 101 | 78 | 2 |         |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 56  | A9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 56  | B9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 57 is a RNA chain called RNA (2848-MER).

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 57  | AA    | 2848     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61341 | 27300 | 11478 | 19716 | 2847 |         |         |       |
| 57  | BA    | 2848     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61341 | 27300 | 11478 | 19716 | 2847 |         |         |       |

- Molecule 58 is a RNA chain called RNA (119-MER).

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 58  | AB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |
| 58  | BB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | B4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | Ad    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | Bn    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | B9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | Bd    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | A4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | An    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | A9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 60  | BA    | 365      | Total | Mg  | 0       | 0       |
|     |       |          | 365   | 365 |         |         |
| 60  | AB    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 60  | Bd    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | AX    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | Bw    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | B5    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | BB    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 60  | Ba    | 143      | Total | Mg  | 0       | 0       |
|     |       |          | 143   | 143 |         |         |

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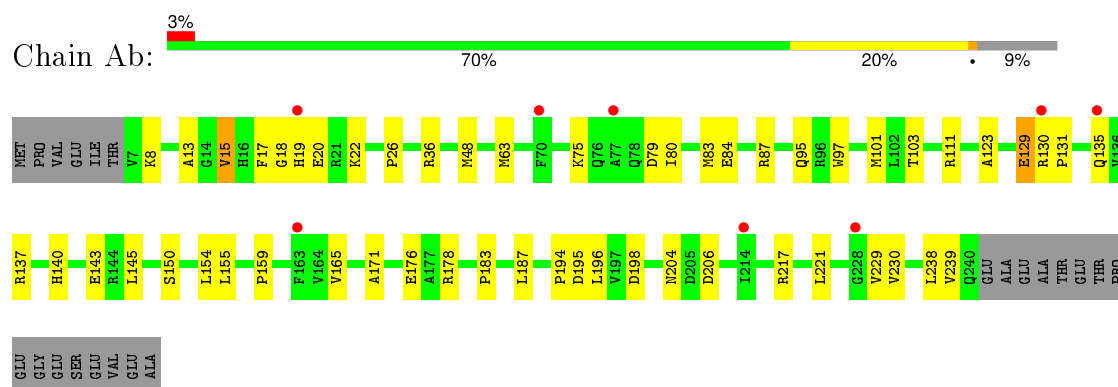
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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 60  | Bl    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | BF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | BX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | Aw    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | AA    | 367      | Total<br>367 | Mg<br>367 | 0       | 0       |
| 60  | A5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | A1    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | AD    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | Ae    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | Bm    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | Av    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 60  | Bx    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | Aa    | 145      | Total<br>145 | Mg<br>145 | 0       | 0       |
| 60  | B7    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | BO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | AQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | A7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 60  | BD    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | B0    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 60  | Bv    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 60  | AF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

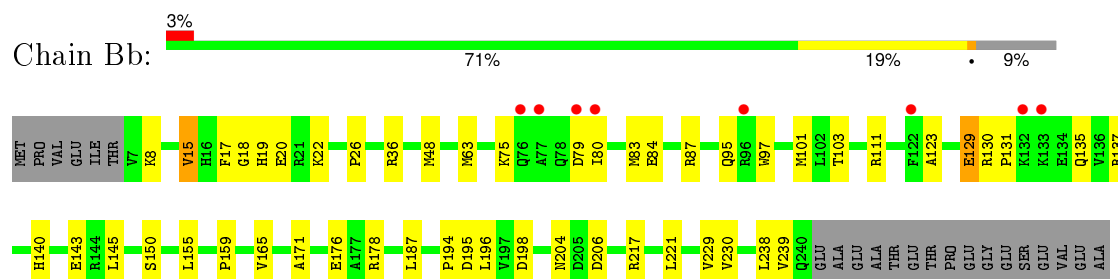
### 3 Residue-property plots

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

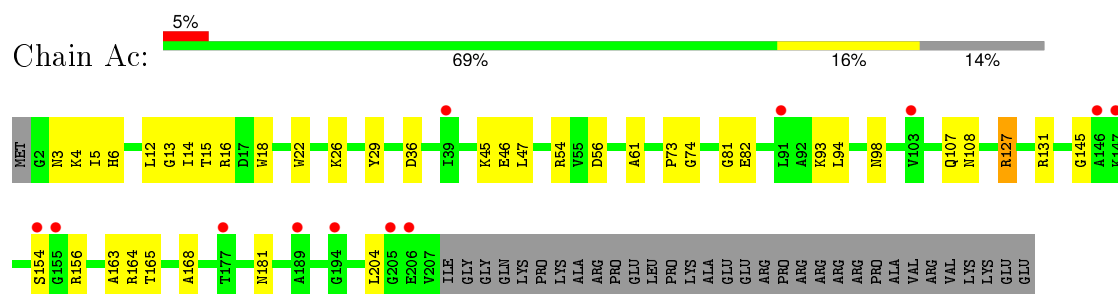
- Molecule 1: 30S ribosomal protein S2



- Molecule 1: 30S ribosomal protein S2

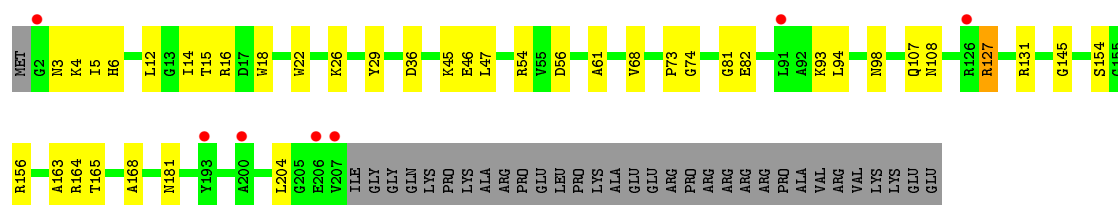


- Molecule 2: 30S ribosomal protein S3



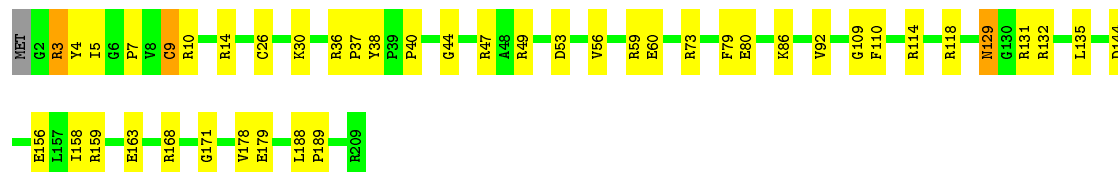
- Molecule 2: 30S ribosomal protein S3





- Molecule 3: 30S ribosomal protein S4

Chain Ad: 78% 20%



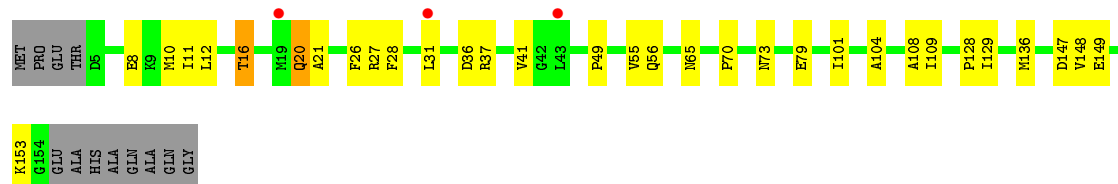
- Molecule 3: 30S ribosomal protein S4

Chain Bd: 78% 21%



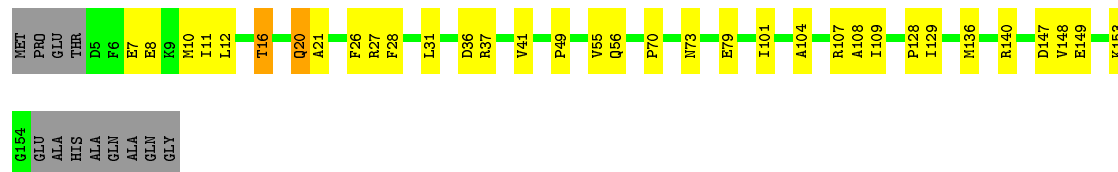
- Molecule 4: 30S ribosomal protein S5

Chain Ae: 73% 19% 7%



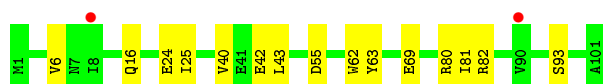
- Molecule 4: 30S ribosomal protein S5

Chain Be: 72% 20% 7%

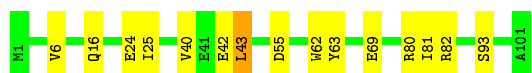
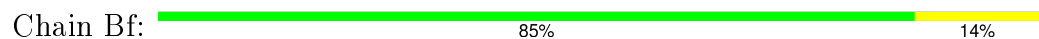


- Molecule 5: 30S ribosomal protein S6

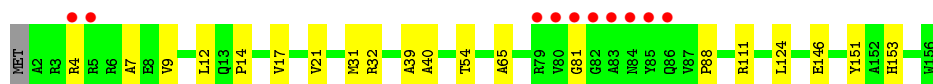
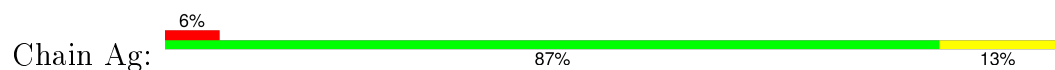
Chain Af: 85% 15%



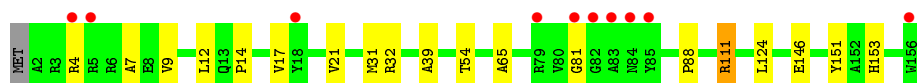
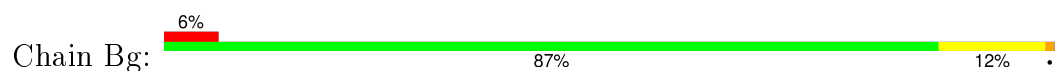
- Molecule 5: 30S ribosomal protein S6



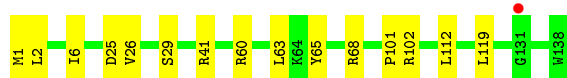
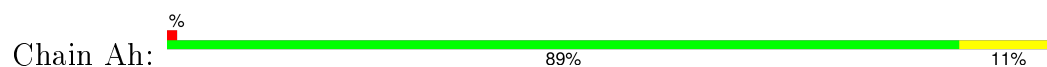
- Molecule 6: 30S ribosomal protein S7



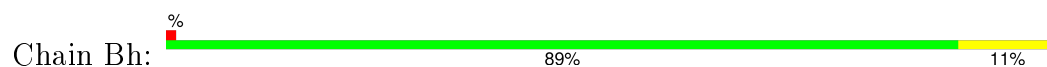
- Molecule 6: 30S ribosomal protein S7



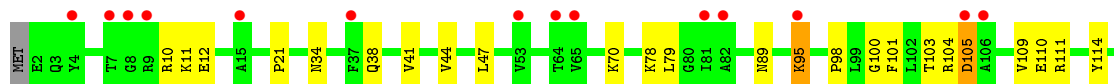
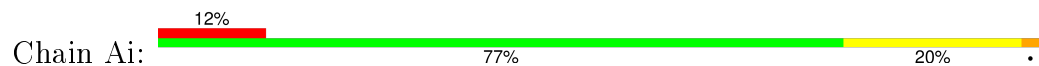
- Molecule 7: 30S ribosomal protein S8



- Molecule 7: 30S ribosomal protein S8

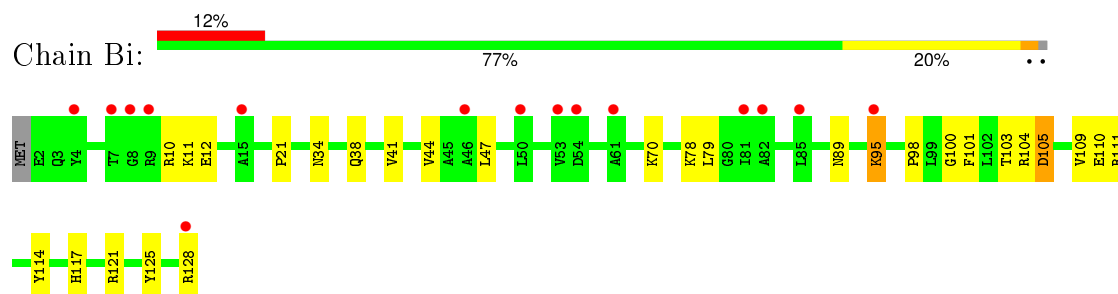


- Molecule 8: 30S ribosomal protein S9

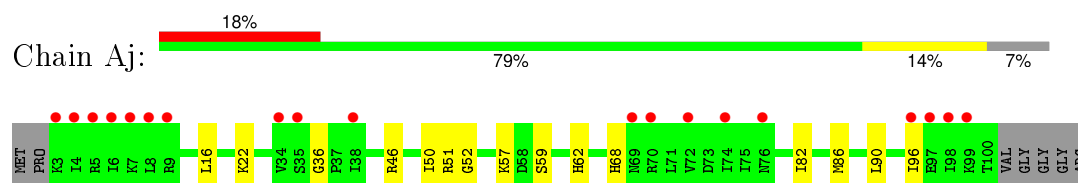




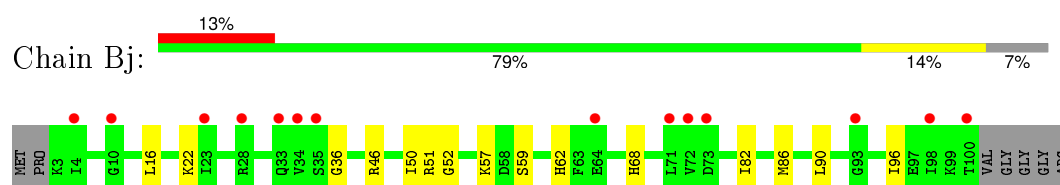
- Molecule 8: 30S ribosomal protein S9



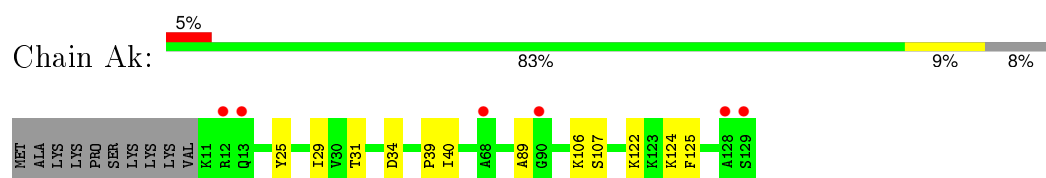
- Molecule 9: 30S ribosomal protein S10



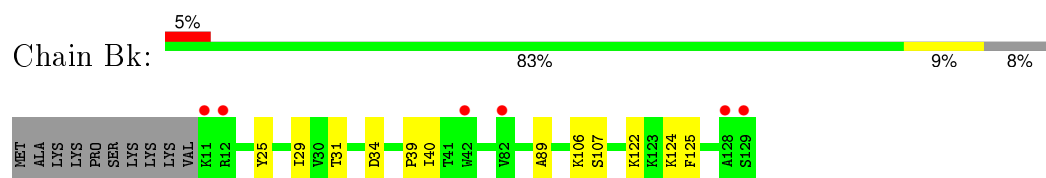
- Molecule 9: 30S ribosomal protein S10



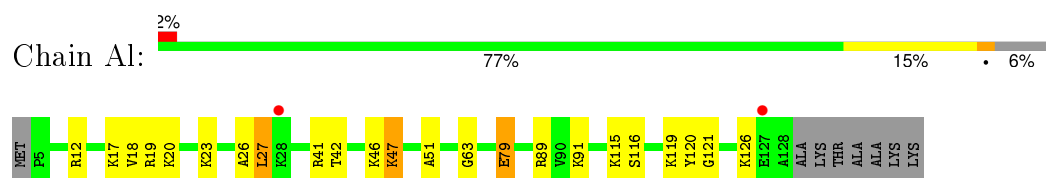
- Molecule 10: 30S ribosomal protein S11



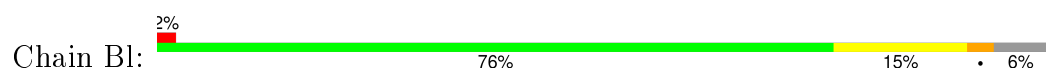
- Molecule 10: 30S ribosomal protein S11

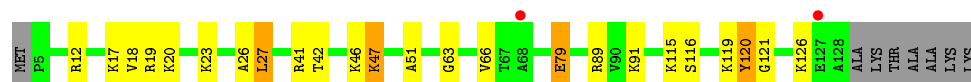


- Molecule 11: 30S ribosomal protein S12

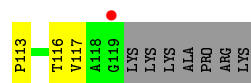


- Molecule 11: 30S ribosomal protein S12

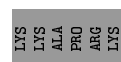




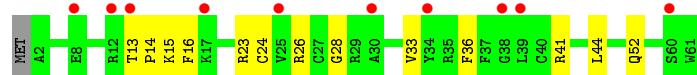
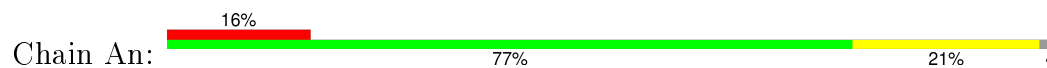
- Molecule 12: 30S ribosomal protein S13



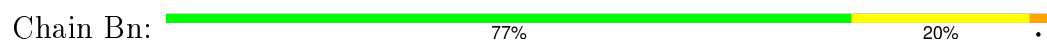
- Molecule 12: 30S ribosomal protein S13



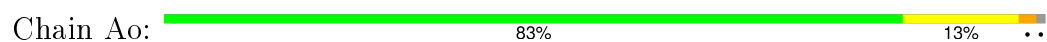
- Molecule 13: 30S ribosomal protein S14 type Z



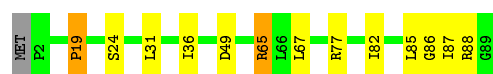
- Molecule 13: 30S ribosomal protein S14 type Z



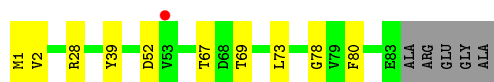
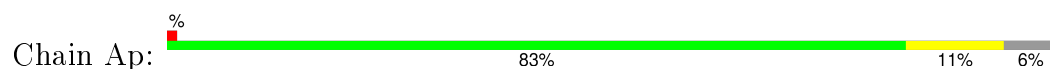
- Molecule 14: 30S ribosomal protein S15



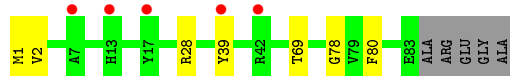
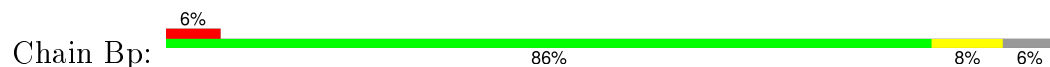
- Molecule 14: 30S ribosomal protein S15



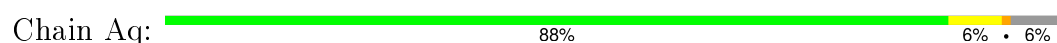
- Molecule 15: 30S ribosomal protein S16



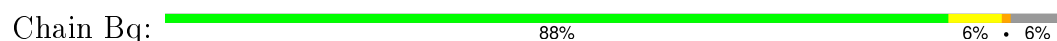
- Molecule 15: 30S ribosomal protein S16



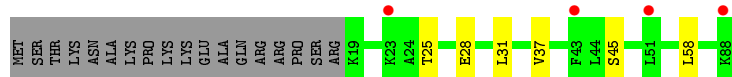
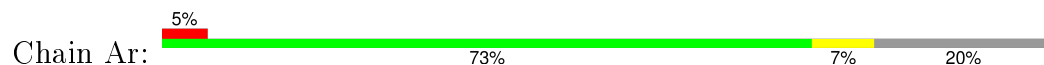
- Molecule 16: 30S ribosomal protein S17



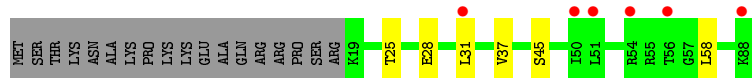
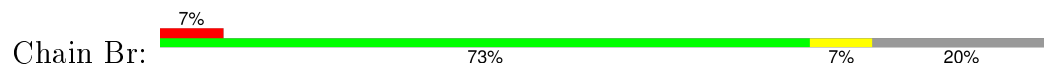
- Molecule 16: 30S ribosomal protein S17



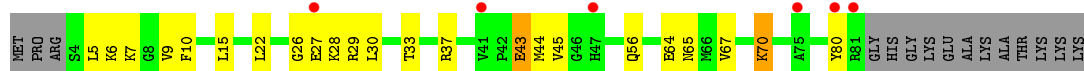
- Molecule 17: 30S ribosomal protein S18



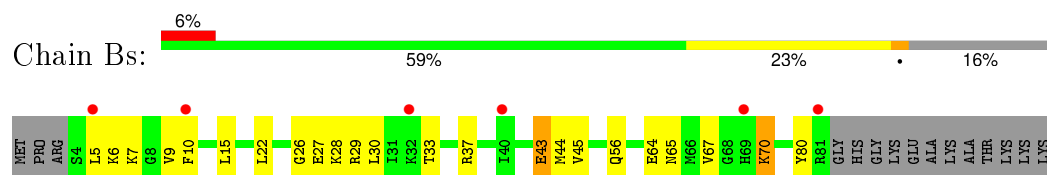
- Molecule 17: 30S ribosomal protein S18



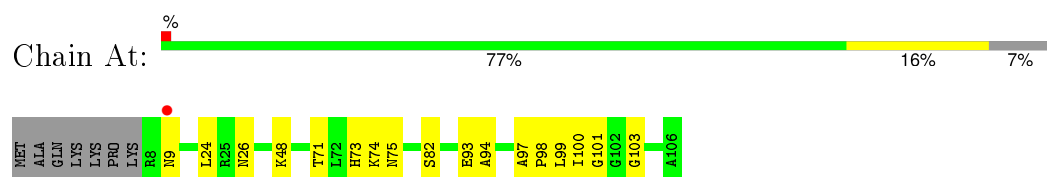
- Molecule 18: 30S ribosomal protein S19



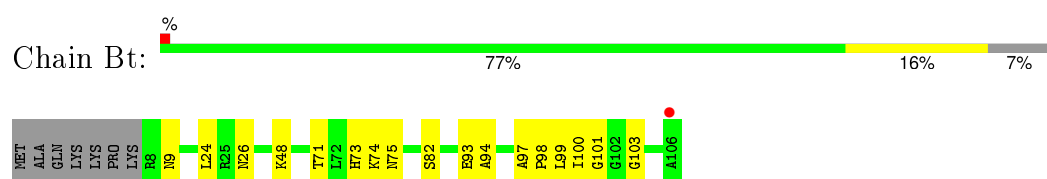
- Molecule 18: 30S ribosomal protein S19



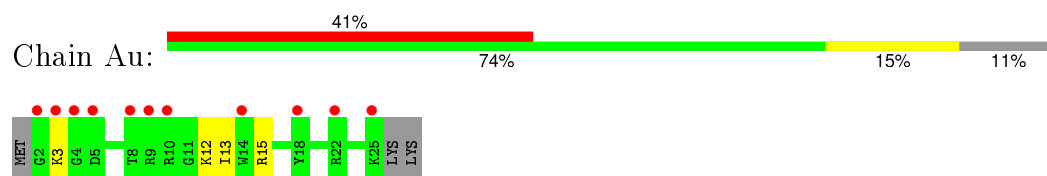
- Molecule 19: 30S ribosomal protein S20



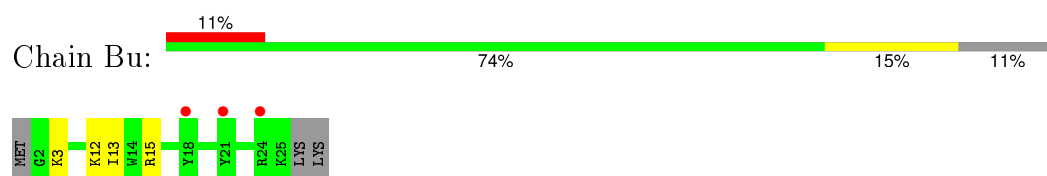
- Molecule 19: 30S ribosomal protein S20



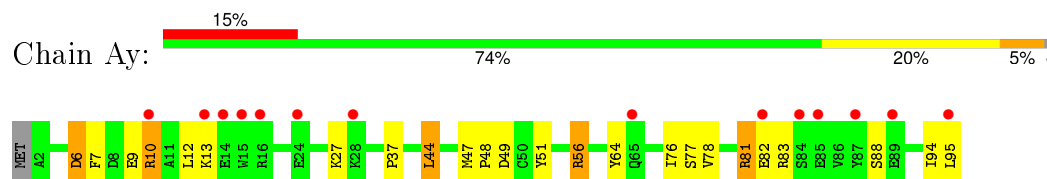
- Molecule 20: 30S ribosomal protein Thx



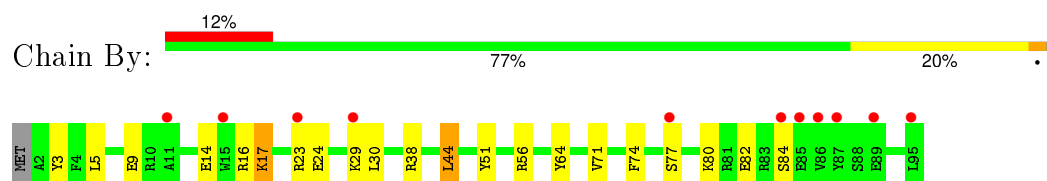
- Molecule 20: 30S ribosomal protein Thx



- Molecule 21: Toxin relE



- Molecule 21: Toxin relE



Chain Aa:

2% 85% 14%

U5  
G9  
G31  
A32  
G39  
C47  
C48  
A51  
A60  
G61  
G79  
G80  
U81  
U82  
U83  
U84  
A88  
C89  
U90  
C91  
G97  
A101  
G115  
A116  
A120  
C121  
C131  
G144  
C150  
A172  
U182  
G189H  
A195  
A196  
A197  
C201  
U202  
U203  
U204  
G216  
U244  
G247  
G251  
G266  
C267  
A279  
G289  
A321  
G328  
A329  
G332  
C345  
G352  
A353  
G354  
C366  
U367  
C372  
A373  
A397  
A412  
G413  
A414  
U421  
C422  
G428  
U429  
A430  
C435  
C436  
U437  
G438  
A439  
A441  
C442  
A452  
A453  
C454  
A461  
C482  
G485  
U494  
A495  
A496  
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A509  
A510  
C511  
C518  
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A547  
A559  
U560  
U561  
C562  
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A573  
A574  
G575  
G576  
G577  
G588  
G631  
A632  
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A665  
A687  
G688  
G724  
G731  
C749  
G755  
U793  
A794  
A816  
C817  
G818  
A819  
U820  
G821  
A828  
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U833  
U839  
A840  
U841  
C848  
A859  
U884  
G898  
G902  
A913  
A914  
G927  
C934  
A935  
U960  
U961  
G966  
C967  
A968  
A969  
C970  
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A974  
A975  
G976  
A977  
C978  
C979  
U991  
U992  
G993  
A996  
C999  
U1000  
A1001  
G1001A  
G1002  
U1003  
A1004  
A1005  
U1020  
G1024  
U1025  
G1026  
C1027  
C1028  
C1029  
C1030  
G1030A  
C1030B  
G1033  
A1034  
A1035  
G1036  
C1037  
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C1054  
A1067  
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G1077  
G1094  
U1095  
A1101  
G1108  
C1115  
C1116  
G1117  
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U1125  
U1126  
C1129  
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A1287  
A1288  
G1294  
G1300  
U1301  
U1302  
G1305  
C1317  
C1320  
G1321  
G1322  
G1323  
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A1398  
G1419

Chain Balance

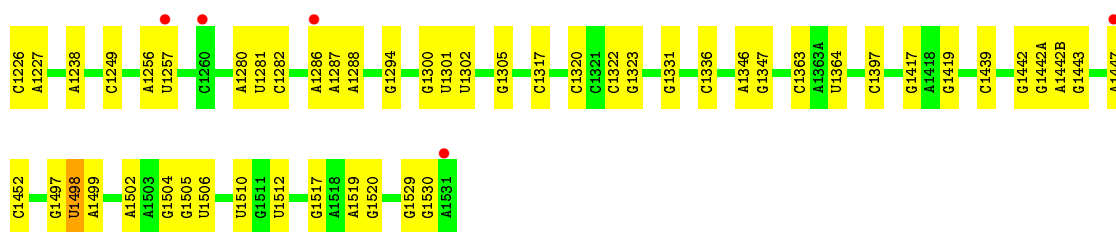
2% 85% 14%

Transactions (Y-axis):

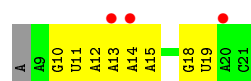
- U494
- U495
- A496
- U498
- A509
- A510
- C511
- C518
- G527
- A532
- A533
- U534
- A547
- A559
- U560
- U561
- C562
- A572
- A573
- G575
- G576
- G577
- G587
- G588
- G631
- A632
- A653
- A665
- A687
- G688
- G731
- C749
- G755
- A739
- A794
- A816
- G817
- G818
- A819
- U820
- G821
- A828
- G1030A
- C1030B
- C832
- U833
- U839
- C840
- C848
- A859
- U884
- G898
- G902
- A913
- A914
- G927
- C934
- A935
- U960
- U961
- G966
- G967
- A968
- A969
- G970
- G971
- A974
- A975
- G976
- A977
- A978
- G979
- C980
- A1152
- U1159
- G993
- G1001A
- G1002
- G1003
- A1004
- A1005
- G1024
- U1025
- G1026
- G1027
- G1028

Blocks (X-axis):

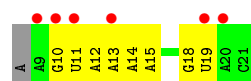
- U5
- G9
- G31
- A32
- G39
- C47
- C48
- A51
- A60
- G61
- G79
- G80
- U81
- U82
- U83
- U84
- A88
- C89
- C90
- C91
- G97
- A101
- G115
- A116
- A120
- C121
- C131
- G144
- C150
- A172
- U182
- G189H
- A195
- A196
- A197
- C201
- U202
- U203
- U204
- G216
- U244
- G247
- G251
- G266
- C267
- A279
- G289
- A321
- C328
- A329
- G332
- C345
- C352
- A355
- C354
- C366
- U367
- C372
- A373
- A397
- A412
- G413
- A414
- U421
- C422
- G428
- U429
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- A441
- C442
- A452
- A461
- G484
- G485



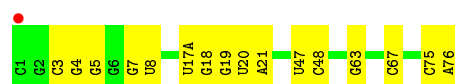
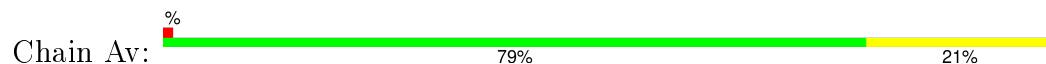
- Molecule 23: RNA (5'-R(\*A\*AP\*GP\*UP\*AP\*AP\*AP\*AP\*AP\*UP\*GP\*UP\*A\*(CCC))-3')



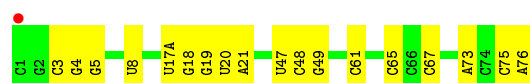
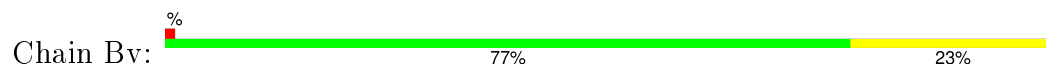
- Molecule 23: RNA (5'-R(\*A\*AP\*GP\*UP\*AP\*AP\*AP\*AP\*AP\*UP\*GP\*UP\*A\*(CCC))-3')



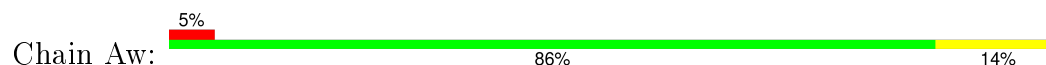
- Molecule 24: RNA (77-MER)



- Molecule 24: RNA (77-MER)

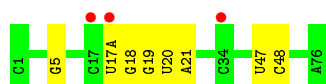


- Molecule 25: RNA (77-MER)

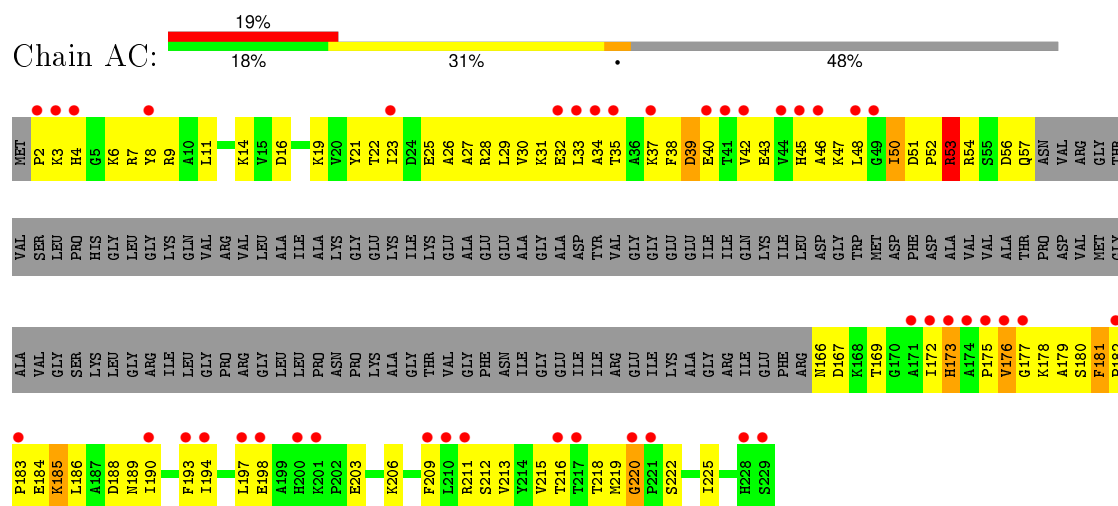


- Molecule 25: RNA (77-MER)

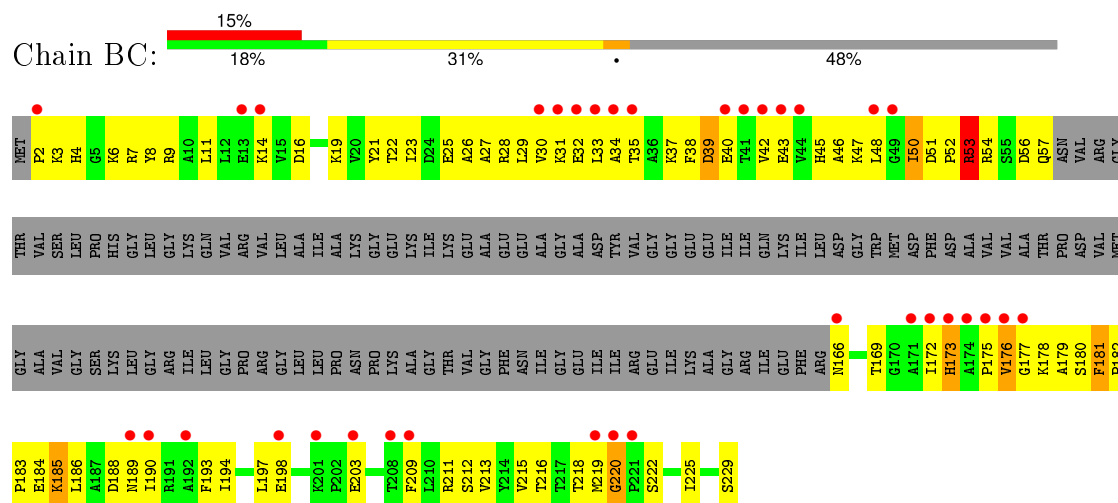




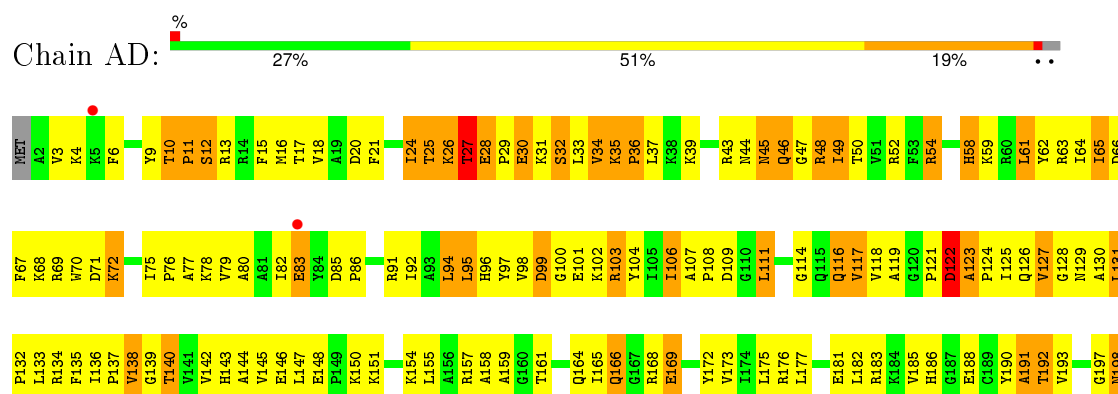
• Molecule 26: 50S ribosomal protein L1

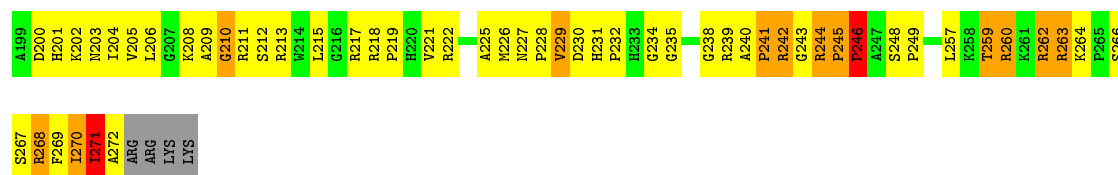


• Molecule 26: 50S ribosomal protein L1



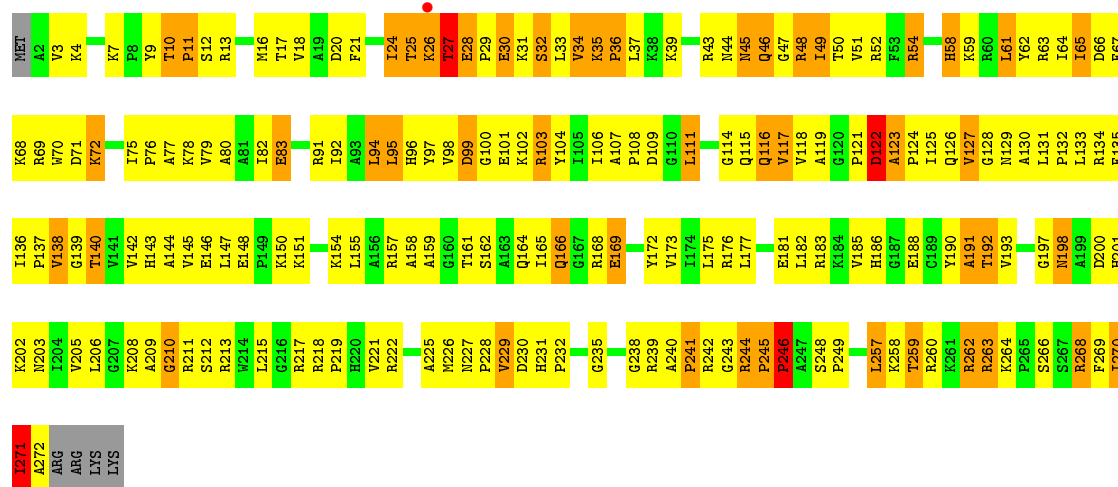
• Molecule 27: 50S ribosomal protein L2





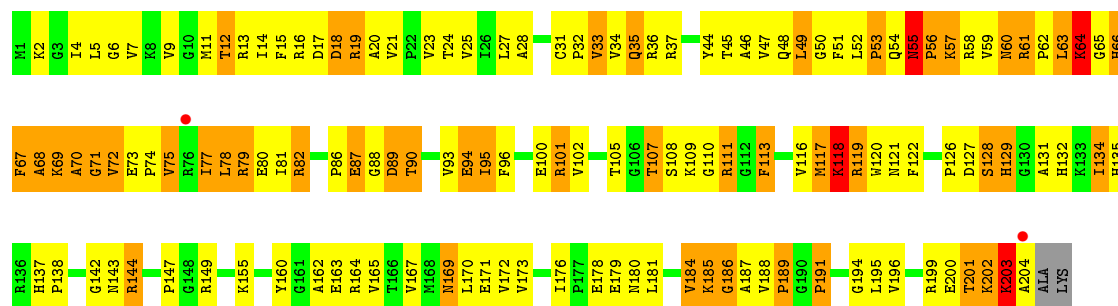
• Molecule 27: 50S ribosomal protein L2

Chain BD: 28% 51% 17%



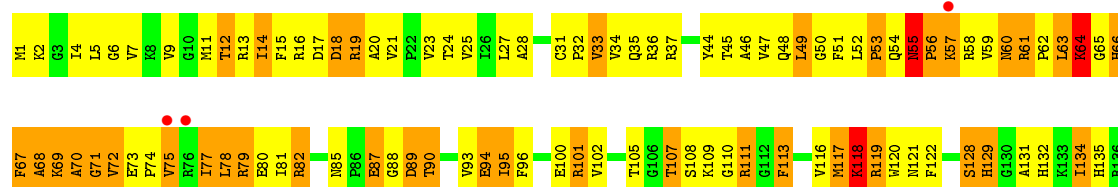
• Molecule 28: 50S ribosomal protein L3

Chain AE: 31% 44% 23%



• Molecule 28: 50S ribosomal protein L3

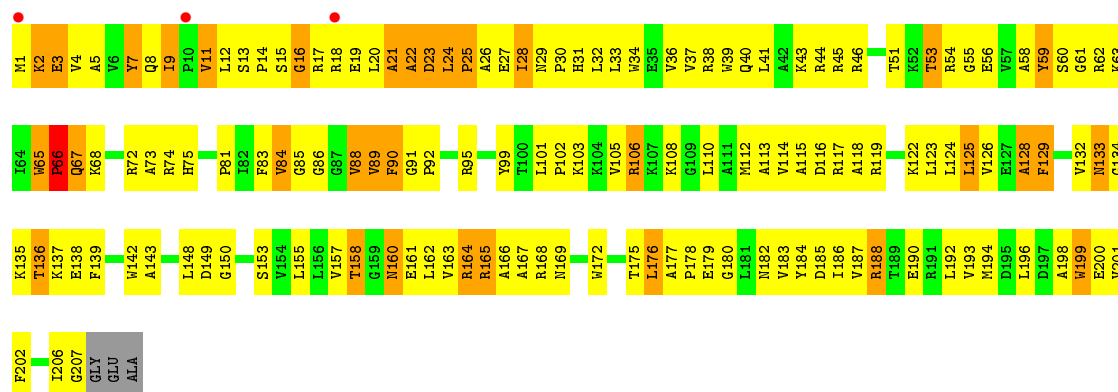
Chain BE: 31% 44% 23%



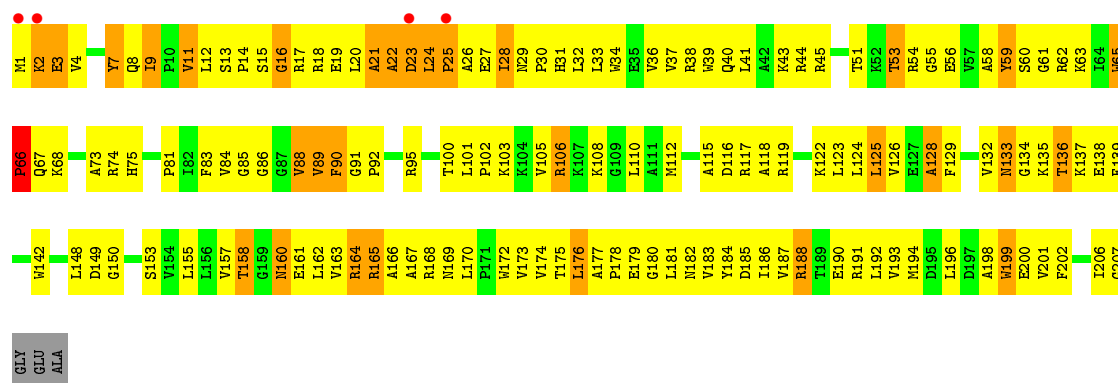




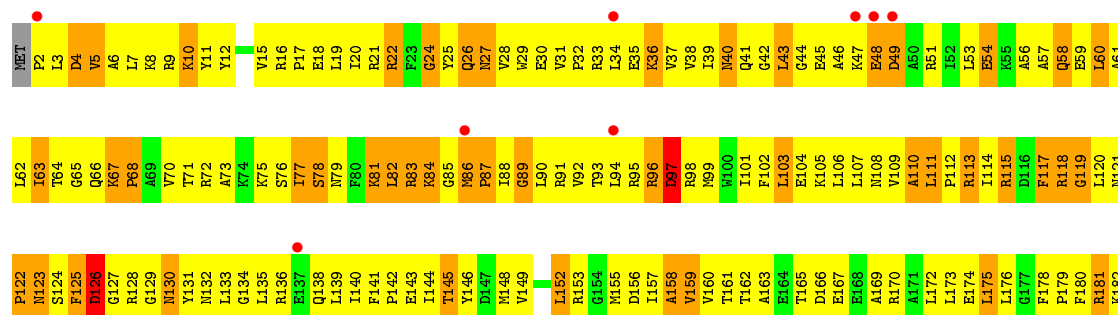
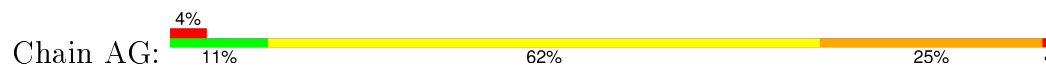
• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L5

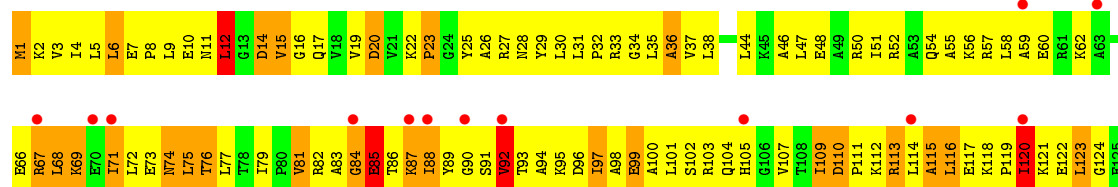
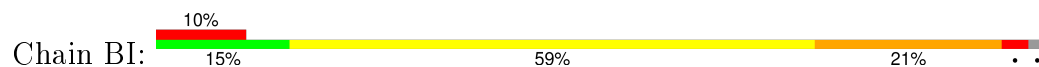


• Molecule 30: 50S ribosomal protein L5

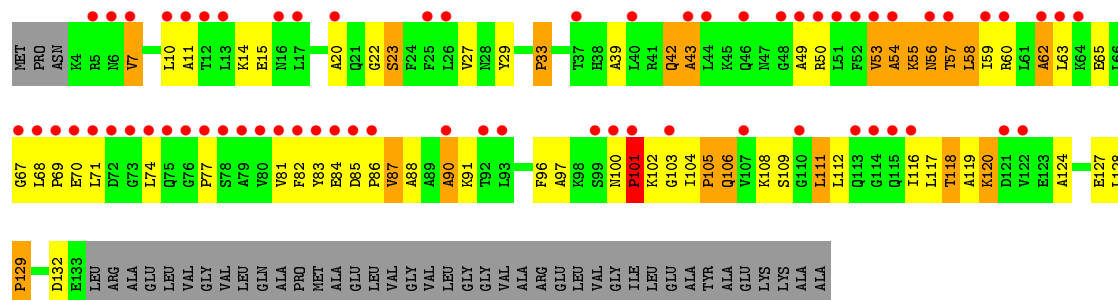




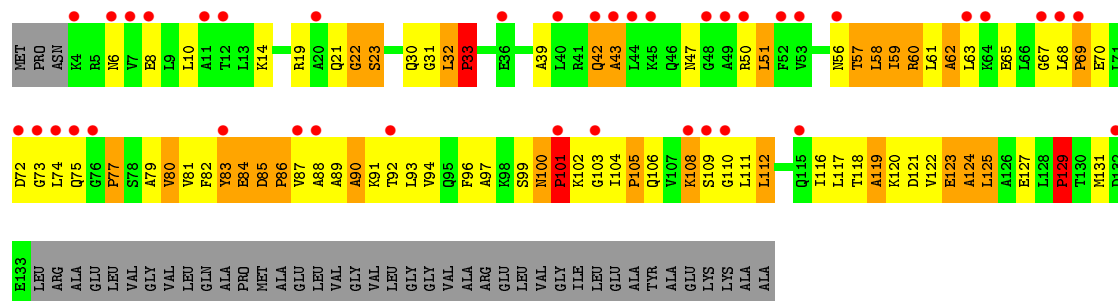
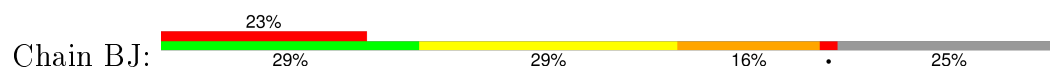
• Molecule 32: 50S ribosomal protein L9



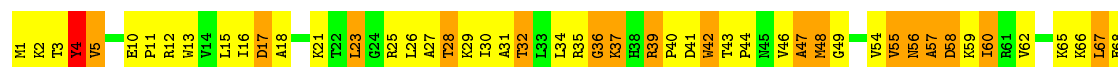
• Molecule 33: 50S ribosomal protein L10

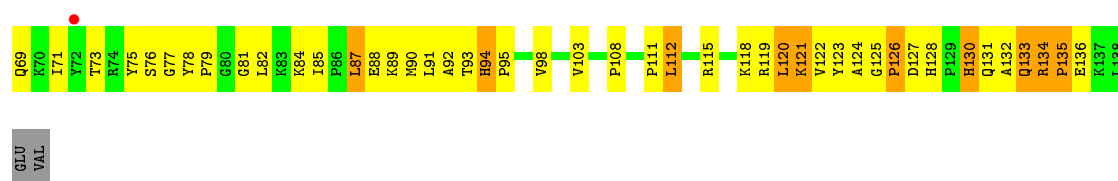


• Molecule 33: 50S ribosomal protein L10



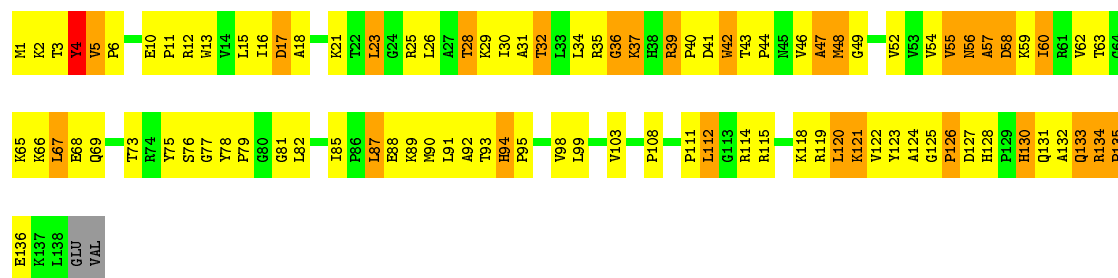
• Molecule 34: 50S ribosomal protein L13





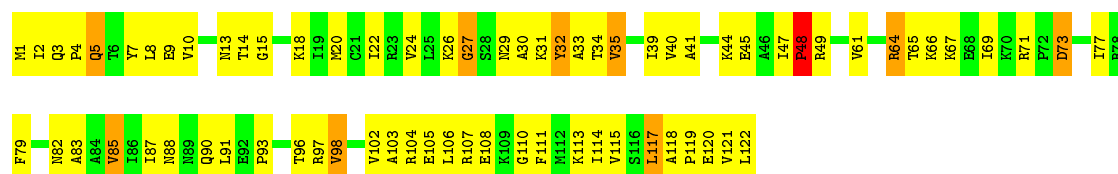
• Molecule 34: 50S ribosomal protein L13

Chain BN: 30% 49% 19% ..



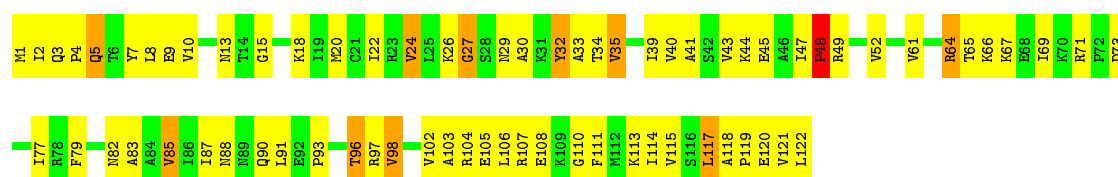
• Molecule 35: 50S ribosomal protein L14

Chain AO: 41% 51% 7% .



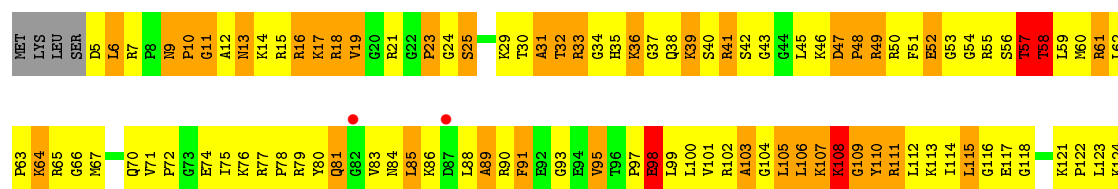
• Molecule 36: 50S ribosomal protein L15

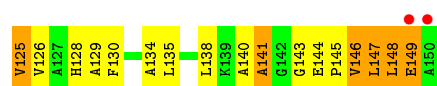
Chain BO: 41% 50% 8% .



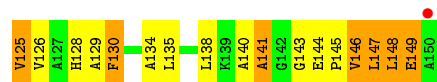
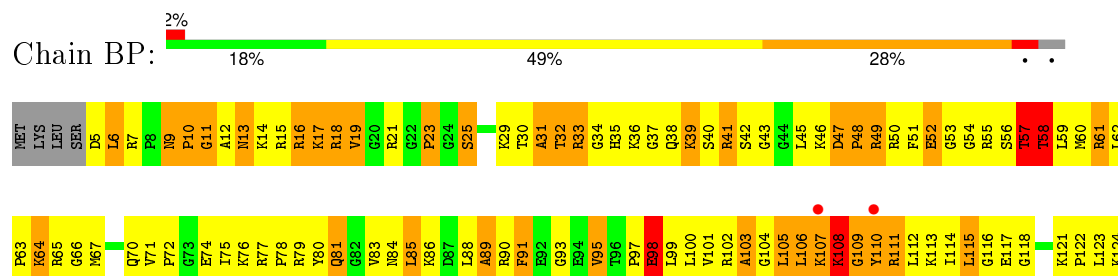
• Molecule 37: 50S ribosomal protein L16

Chain AP: 3% 17% 49% 28% . .

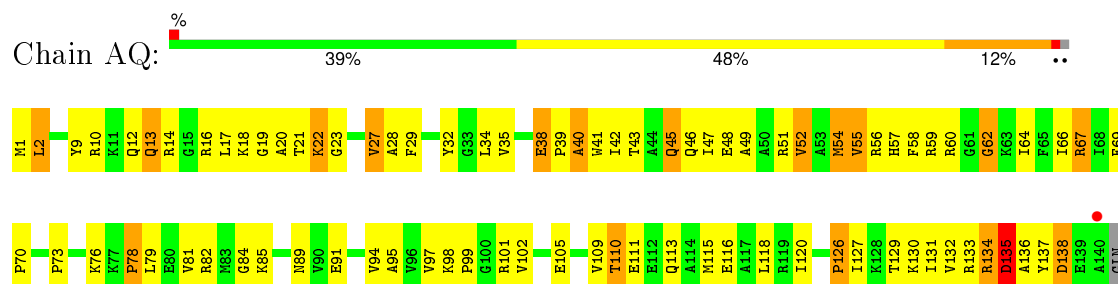




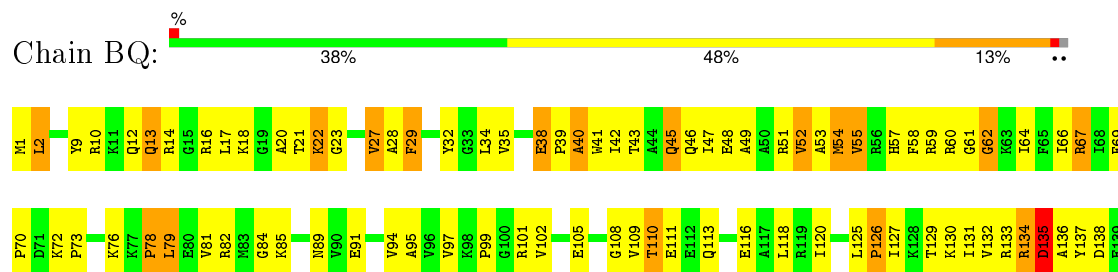
- Molecule 36: 50S ribosomal protein L15



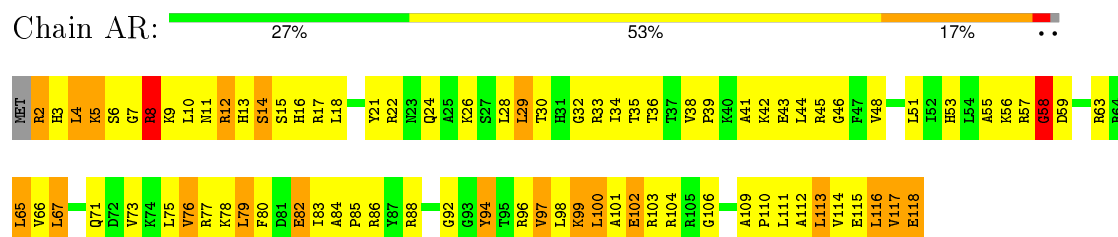
- Molecule 37: 50S ribosomal protein L16



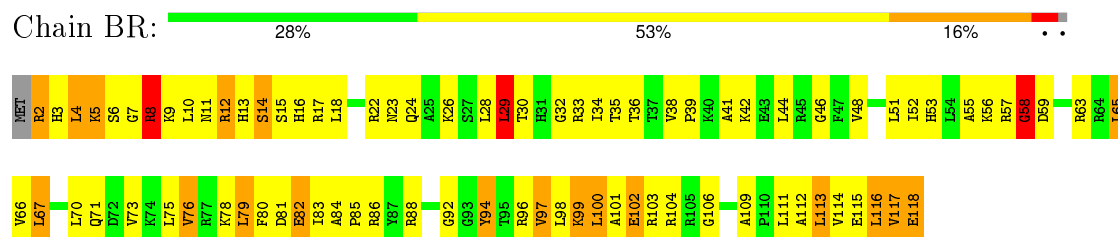
- Molecule 37: 50S ribosomal protein L16



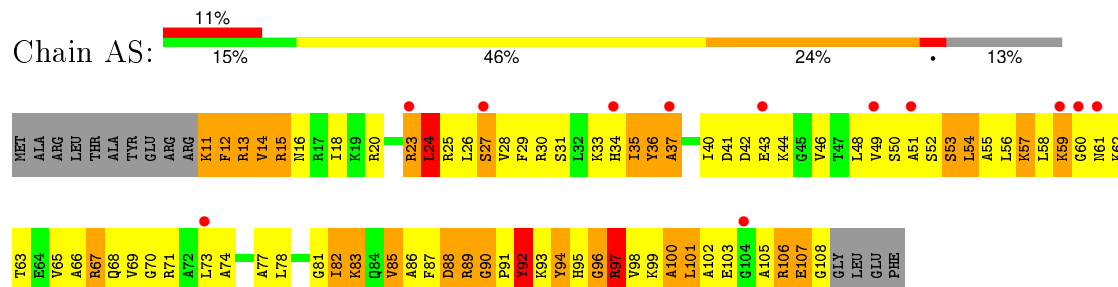
- Molecule 38: 50S ribosomal protein L17



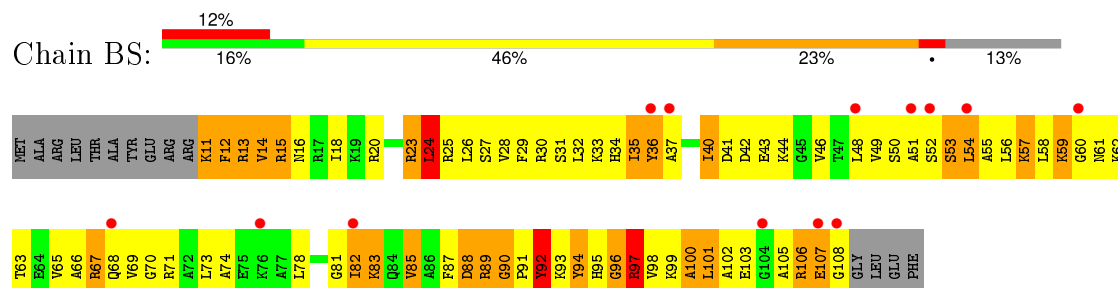
- Molecule 38: 50S ribosomal protein L17



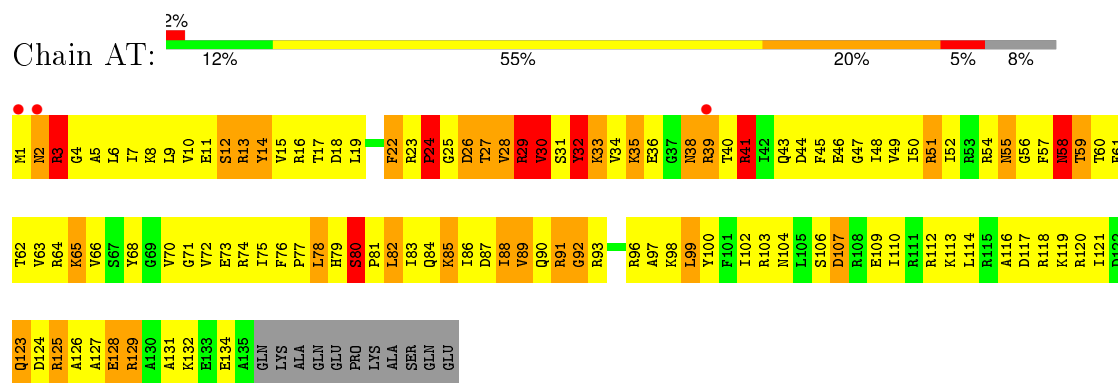
- Molecule 39: 50S ribosomal protein L18



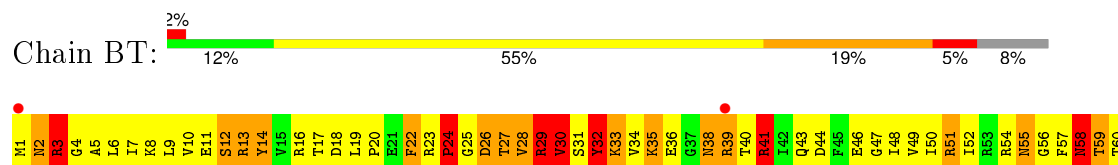
- Molecule 39: 50S ribosomal protein L18

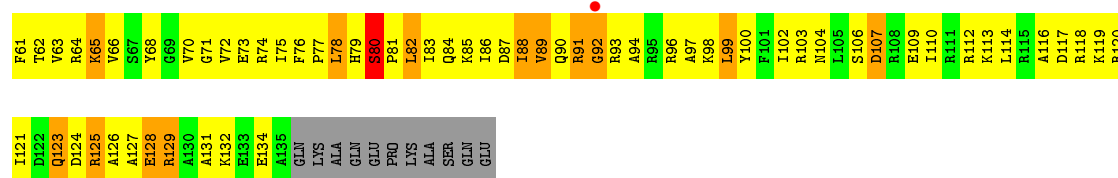


- Molecule 40: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L19





- Molecule 41: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21

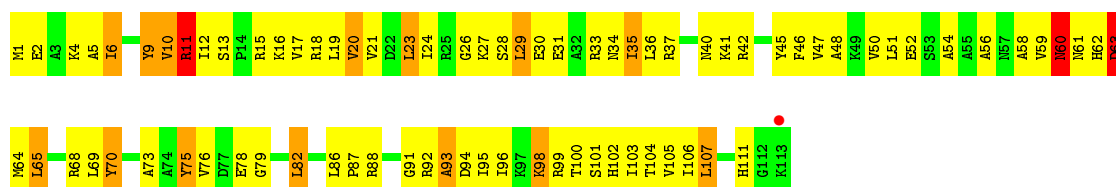


- Molecule 42: 50S ribosomal protein L21

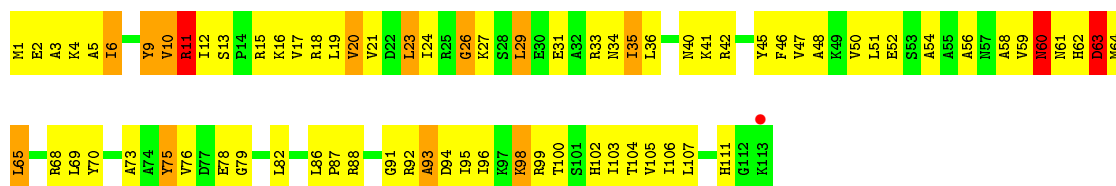


- Molecule 43: 50S ribosomal protein L22





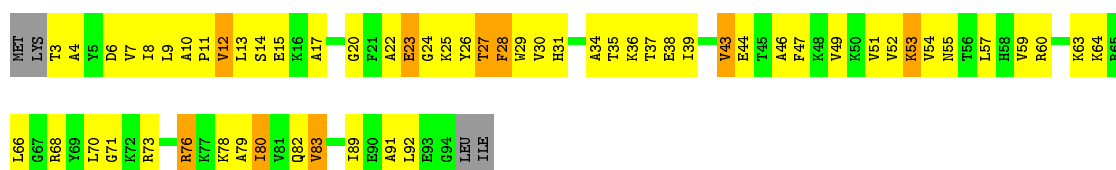
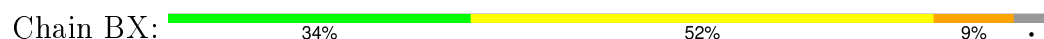
• Molecule 43: 50S ribosomal protein L22



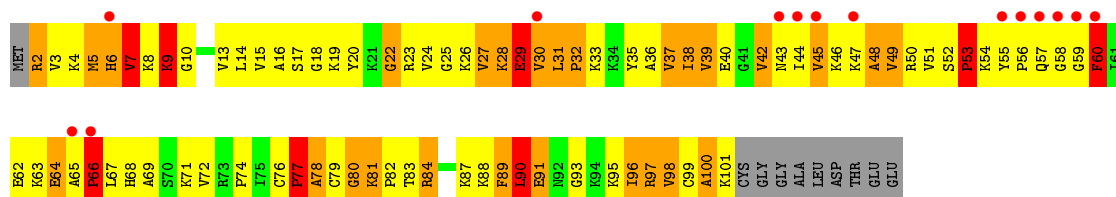
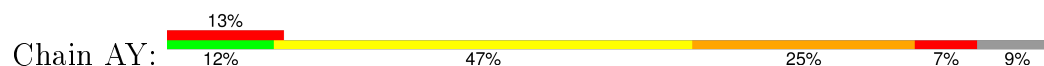
• Molecule 44: 50S ribosomal protein L23



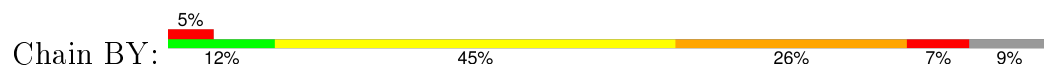
• Molecule 44: 50S ribosomal protein L23



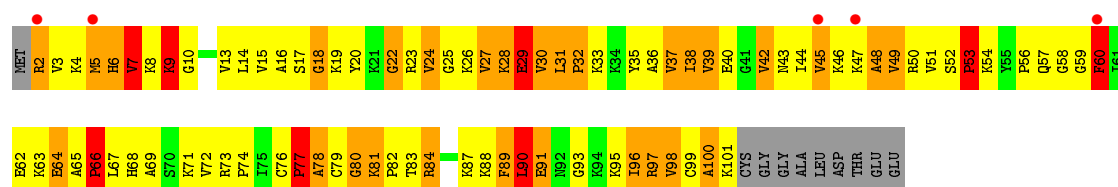
• Molecule 45: 50S ribosomal protein L24



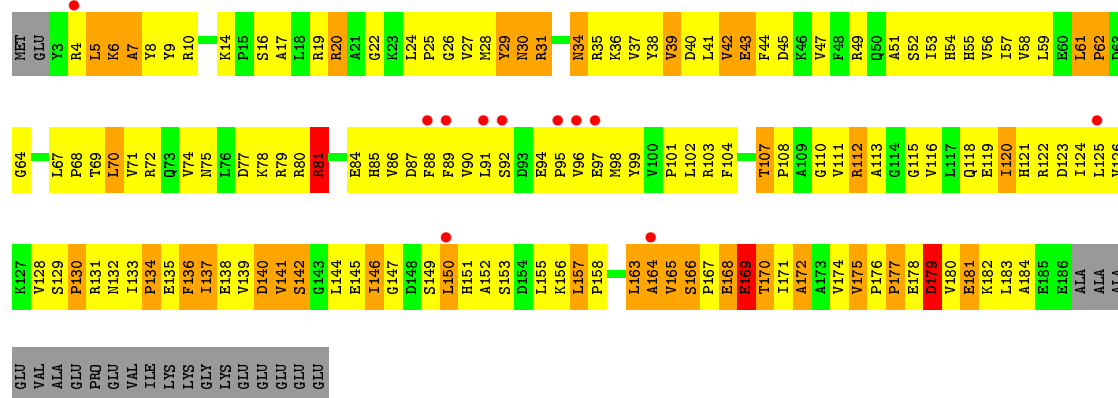
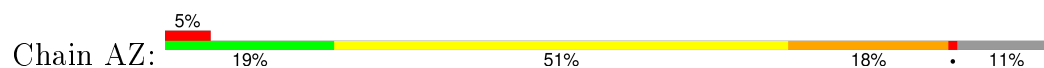
• Molecule 45: 50S ribosomal protein L24

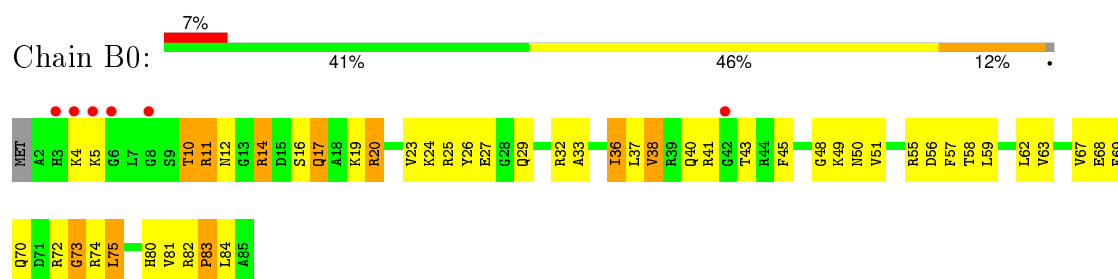




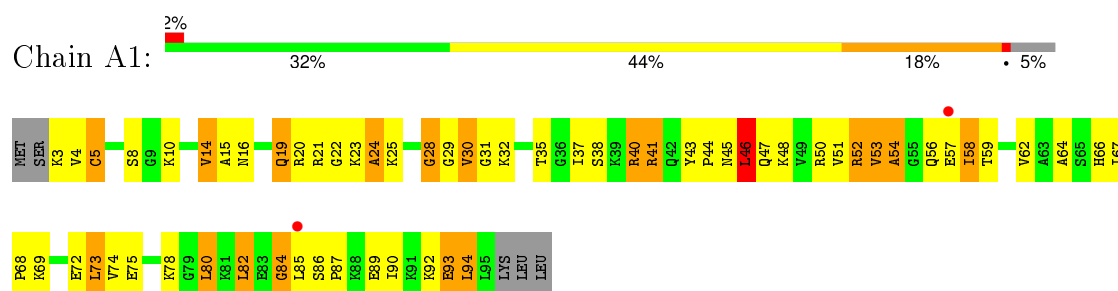


• Molecule 46: 50S ribosomal protein L25

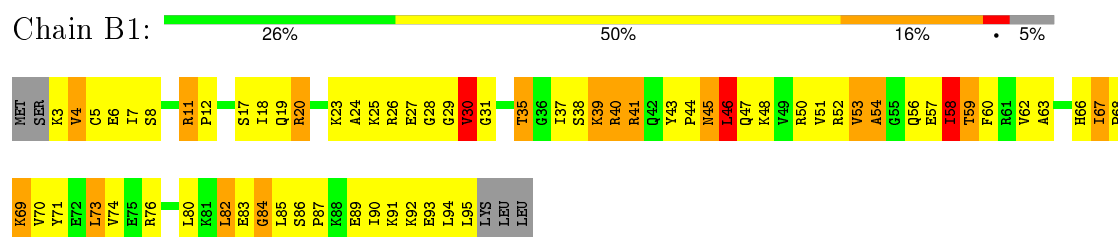




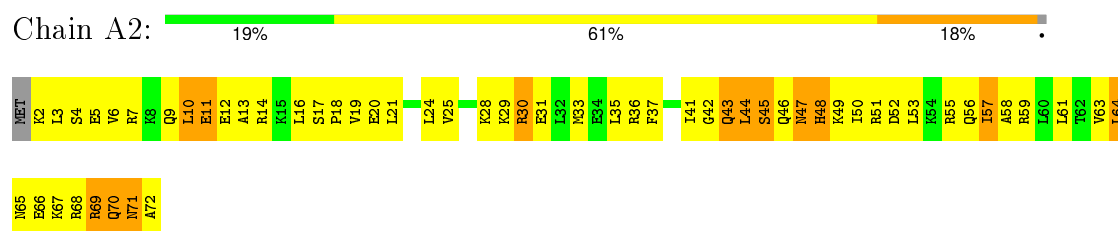
- Molecule 48: 50S ribosomal protein L28



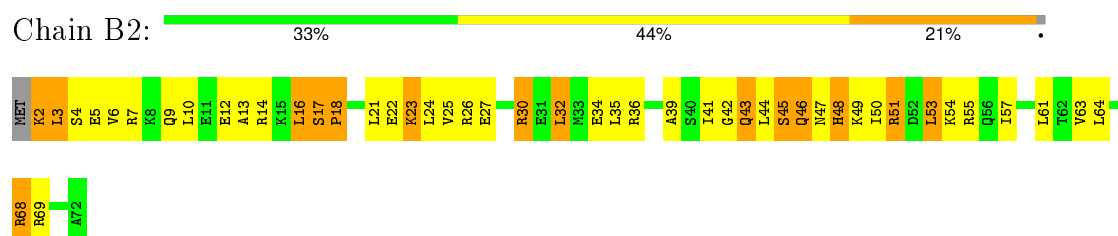
- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29

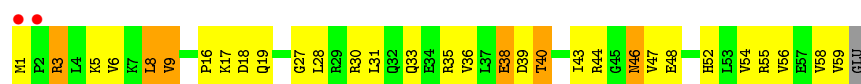


- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30

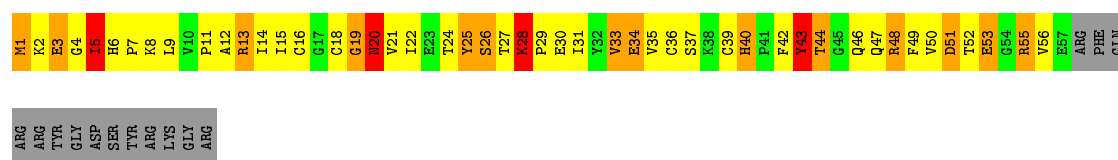




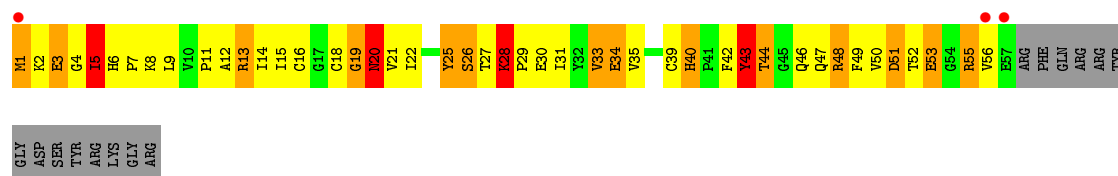
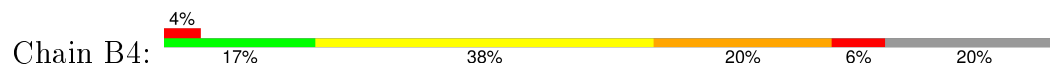
- Molecule 50: 50S ribosomal protein L30



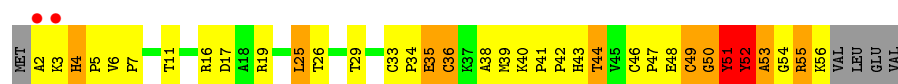
- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31



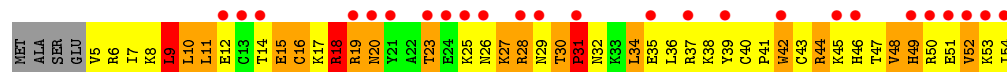
- Molecule 52: 50S ribosomal protein L32



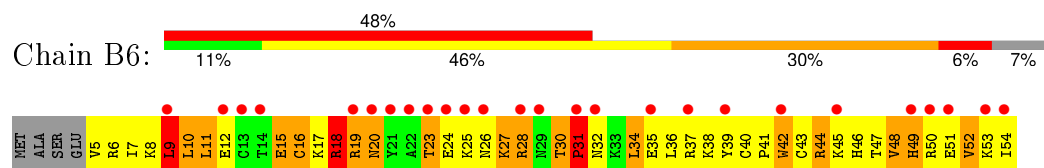
- Molecule 52: 50S ribosomal protein L32



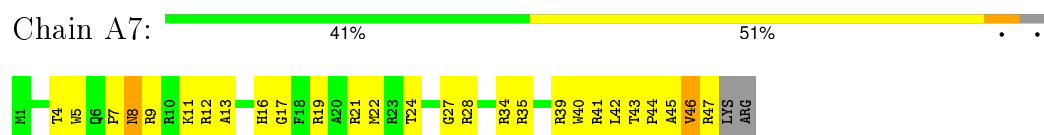
- Molecule 53: 50S ribosomal protein L33



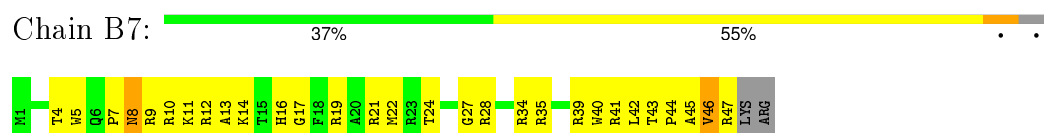
- Molecule 53: 50S ribosomal protein L33



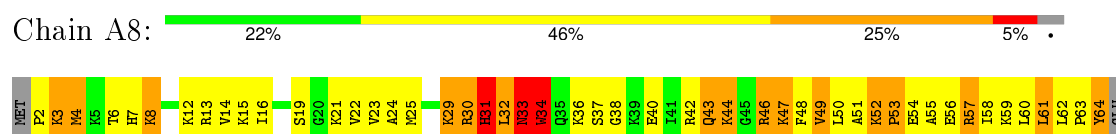
- Molecule 54: 50S ribosomal protein L34



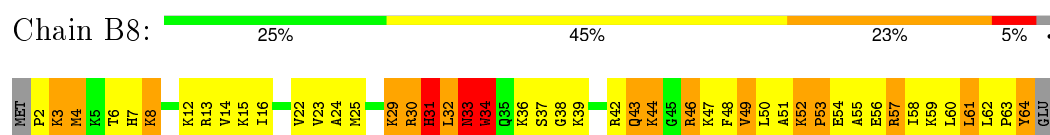
- Molecule 54: 50S ribosomal protein L34



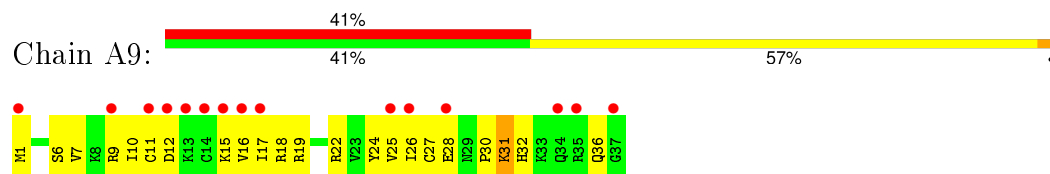
- Molecule 55: 50S ribosomal protein L35



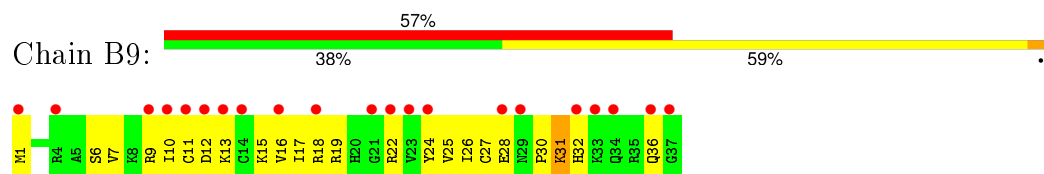
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



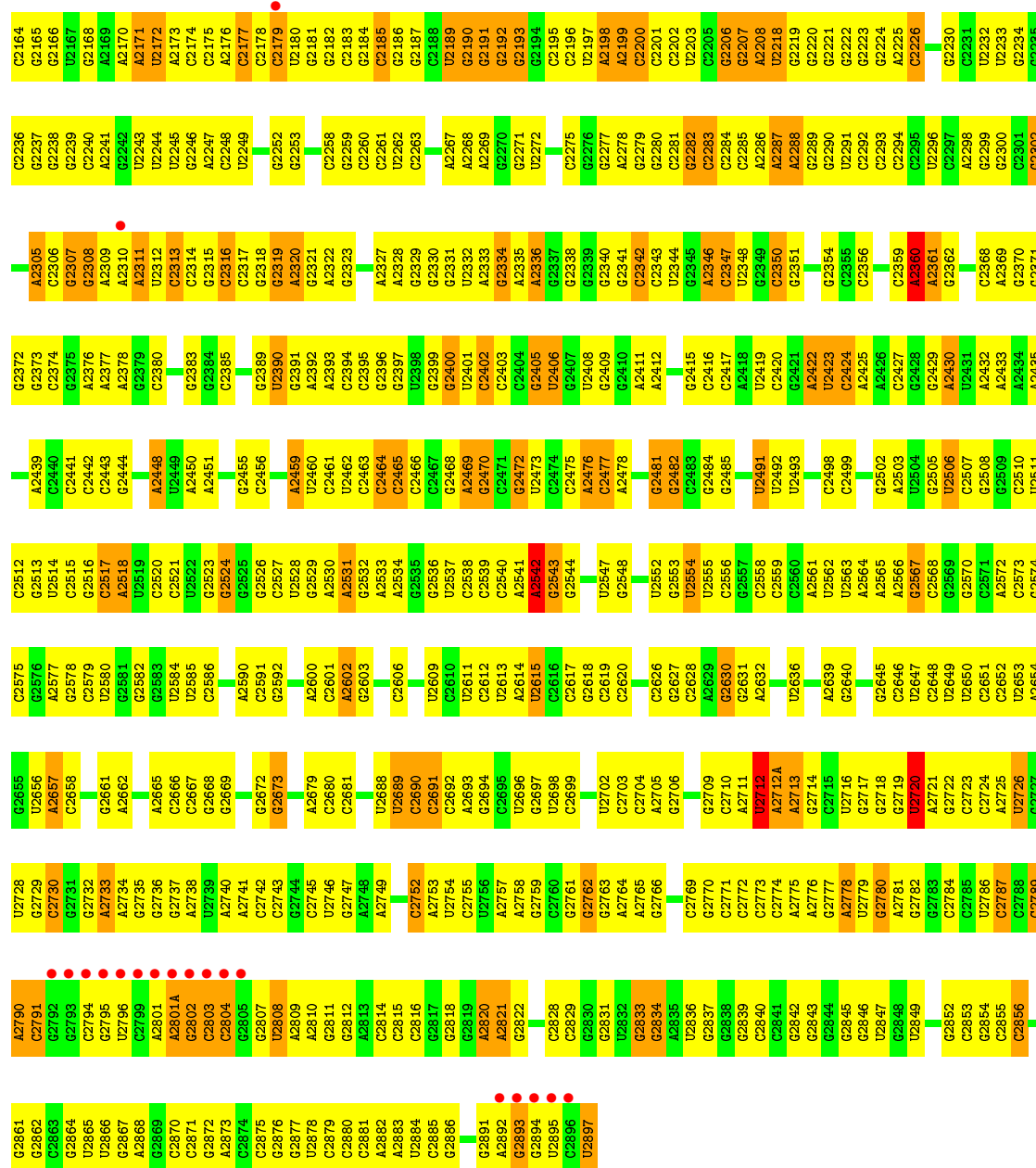
- Molecule 56: 50S ribosomal protein L36



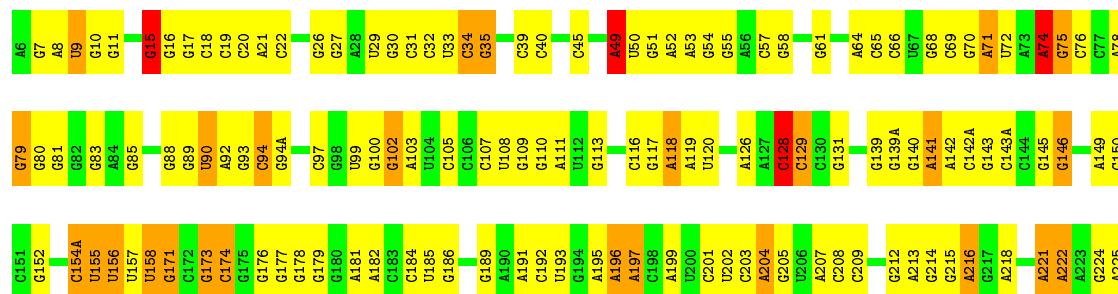
- Molecule 57: RNA (2848-MER)



|       |       |       |       |       |        |       |       |        |        |       |       |       |        |       |
|-------|-------|-------|-------|-------|--------|-------|-------|--------|--------|-------|-------|-------|--------|-------|
| G2101 | A2033 | U1963 | A1889 | A1810 | G1719  | G1649 | A1572 | U1497  | U1433  | C1363 | U1292 | C1218 | C1150  | A1027 |
| U2102 | U2034 | G1964 | A1890 | G1811 | U1720  | G1650 | G1573 | C1501  | A1434  | G1364 | C1293 | C1218 | G1150  | A1028 |
| C2103 | G2035 | G1965 | G1891 | A1812 | G1721  | G1651 | C1574 | C1502  | G1435  | A1365 | U1294 | C1221 | G1151  | U1033 |
| G2104 | C2036 | A1966 | C1892 | G1813 | A1722  | A1652 | C1577 | U1503  | G1436  | G1366 | C1297 | C1222 | C1152  | G1037 |
| G2105 | C2039 | G1968 | C1893 | G1814 | U1739  | G1653 | U1578 | C1504  | C1437  | A1367 | U1300 | G1227 | A1155  | G1038 |
| C2107 | C2040 | A1969 | C1898 | G1816 | A1741  | A1654 | A1579 | C1505  | A1439  | G1368 | A1301 | G1228 | A1156  | C1038 |
| C2108 | U2041 | A1970 | A1899 | G1817 | A1742  | C1657 | A1580 | G1506  | G1440  | G1369 | A1301 | G1228 | G1157  | C1039 |
| A2042 | C2043 | A1971 | A1900 | U1818 | G1743  | C1658 | G1581 | C1509  | G1441  | A1373 | C1305 | G1231 | G1158  | C1040 |
| G2110 | A2042 | A1972 | A1901 | A1819 | G1747A | C1659 | G1582 | C1509  | G1442  | G1374 | C1306 | G1232 | G1159  | C1041 |
| G2111 | C2043 | G1973 | G1902 | A1820 | G1748  | C1662 | A1583 | C1509B | G1443  | A1378 | A1307 | G1233 | G1160  | A1045 |
| G2112 | G2046 | C1978 | G1903 | A1821 | G1749  | A1664 | C1584 | A1510  | G1444  | A1379 | A1308 | G1234 | G1161  | A1046 |
| U2113 | G2062 | G1980 | G1904 | G1822 | G1750  | A1665 | A1587 | C1511  | C1445A | A1380 | G1309 | U1240 | G1162  | A1047 |
| A2114 | G2063 | A1981 | C1906 | G1824 | C1751  | A1666 | A1588 | C1516  | C1446  | G1310 | G1310 | U1240 | G1163  | A1048 |
| G2115 | A2064 | G1982 | G1907 | A1825 | G1752  | G1667 | C1589 | C1517  | G1447  | G1164 | A1311 | A1241 | U1165  | A1049 |
| A2117 | C2055 | G1983 | C1908 | G1826 | C1754  | A1668 | U1590 | G1517  | G1448  | G1165 | U1312 | A1242 | C1166  | A1050 |
| G2118 | G2056 | G1984 | C1909 | A1827 | A1755  | A1669 | G1591 | U1518  | A1449  | G1167 | U1313 | G1243 | U1167  | G1051 |
| A2119 | C2057 | G1985 | G1910 | G1828 | G1756  | C1670 | C1592 | G1519  | A1450  | G1168 | C1314 | G1244 | G1168  | C1052 |
| G2120 | A2059 | A1986 | U1911 | A1829 | U1757  | C1671 | G1593 | G1520  | C1450A | G1169 | C1315 | G1245 | C1053  | G1053 |
| G2121 | A2060 | G1987 | A1912 | C1830 | U1758  | U1673 | G1594 | U1523  | C1451  | G1170 | U1316 | A1246 | G1171  | A1106 |
| G2122 | G2061 | C1988 | A1913 | G1831 | C1767  | C1674 | G1595 | G1524  | A1452  | G1171 | A1317 | A1247 | G1172  | G1107 |
| G2123 | A2062 | G1989 | C1914 | C1832 | G1768  | C1675 | A1596 | C1525  | A1453  | G1172 | U1318 | G1248 | G1173  | U1108 |
| G2124 | C2063 | C1990 | A1916 | U1833 | G1769  | A1676 | A1597 | A1528  | G1459  | A1392 | G1319 | U1249 | A1174  | G1109 |
| G2125 | C2064 | U1917 | A1917 | U1834 | G1766  | A1677 | C1598 | A1528A | G1460  | A1393 | C1320 | G1250 | U1175  | G1110 |
| A2126 | C2065 | G1992 | A1918 | G1835 | C1765  | G1678 | C1599 | G1529  | A1461  | U1394 | A1321 | C1251 | G1176  | A1111 |
| G2127 | C2066 | U1993 | C1921 | C1838 | U1766  | A1679 | G1601 | C1530  | G1462  | A1395 | C1327 | G1252 | A1177  | G1112 |
| G2128 | G2067 | G1994 | U1922 | G1839 | C1767  | U1680 | U1602 | C1531  | C1463  | U1396 | U1328 | G1253 | G1178  | U1113 |
| G2129 | U2068 | G1995 | G1923 | G1845 | G1772  | G1682 | A1603 | G1532  | G1464  | U1397 | G1329 | G1256 | C1179  | G1114 |
| G2130 | C2069 | U1996 | C1924 | G1846 | A1773  | C1683 | C1605 | U1534  | G1465  | G1400 | C1330 | G1260 | C1180  | G1115 |
| A2071 | G2070 | G1997 | G1925 | G1847 | C1774  | C1684 | G1606 | A1535  | C1466  | G1401 | A1331 | G1261 | G1187  | G1116 |
| G2132 | A2072 | C1998 | U1926 | A1847 | U1775  | C1685 | C1607 | C1536  | C1468  | C1402 | G1332 | C1261 | G1188  | G1117 |
| G2133 | C2073 | G2000 | C1929 | A1848 | G1777  | G1686 | A1608 | G1537  | A1469  | C1403 | C1333 | G1264 | U1188  | G1119 |
| A2135 | U2074 | A2001 | G1929 | U1853 | U1777  | G1687 | A1609 | G1538  | G1470  | C1404 | A1336 | G1265 | U1189  | G1120 |
| G2136 | U2075 | G2002 | G1930 | A1854 | U1778  | U1688 | A1610 | U1539  | A1471  | U1405 | G1337 | A1266 | G1190  | G1123 |
| C2137 | U2076 | U1931 | U1931 | A1854 | U1779  | A1689 | A1613 | U1540  | A1472  | U1406 | G1337 | G1266 | G1191  | G1124 |
| C2138 | A2077 | A1932 | A1932 | G1855 | A1780  | A1690 | C1614 | G1541  | G1473  | C1407 | G1338 | U1267 | G1192  | G1125 |
| C2139 | U2079 | G1933 | G1933 | G1858 | A1784  | C1691 | A1614 | A1542  | C1474  | C1408 | G1339 | A1268 | G1193  | G1126 |
| G2143 | A2082 | U2011 | U2011 | A1859 | A1785  | C1694 | C1615 | C1543  | G1475  | C1409 | U1340 | A1269 | C1194  | G1127 |
| U2144 | C2083 | A2013 | A1936 | G1861 | A1786  | G1695 | C1616 | A1544  | C1476  | G1410 | U1341 | G1270 | A1194  | G1128 |
| C2145 | C2084 | A2014 | A1937 | G1862 | C1786  | G1696 | C1617 | C1547  | A1477  | G1411 | G1344 | A1272 | G1195  | G1129 |
| G2146 | C2085 | A2015 | U1938 | G1863 | U1790  | G1697 | A1618 | C1548  | G1478  | A1412 | G1345 | U1273 | G1199  | G1130 |
| G2147 | U2086 | U2016 | U1940 | U1864 | A1791  | A1698 | G1626 | C1549  | U1481  | G1416 | G1346 | A1274 | C1200  | G1131 |
| G2148 | C2087 | C1947 | C1947 | G1865 | U1794  | A1701 | G1627 | C1551  | G1482  | C1417 | G1347 | A1275 | C1201  | G1132 |
| U2150 | G2088 | A2020 | G1948 | C1866 | C1795  | G1702 | A1634 | A1554  | G1483  | G1418 | A1349 | A1278 | A1204  | G1133 |
| U2069 | U2069 | C2021 | A1948 | A1876 | U1796  | G1703 | G1635 | G1484  | G1485  | A1419 | U1205 | A1279 | U1205  | G1137 |
| G2090 | U2022 | G1949 | G1949 | A1877 | C1797  | G1704 | C1636 | A1486  | U1420  | U1420 | G1280 | G1280 | G1139  | G1138 |
| G2091 | G2023 | G1950 | G1950 | G1878 | U1798  | G1705 | A1637 | G1487  | G1422  | G1422 | A1353 | U1281 | G1207  | G1137 |
| U2092 | G2024 | U1951 | U1951 | C1881 | G1799  | U1706 | C1638 | G1488  | G1422  | G1422 | A1354 | U1282 | C1208  | G1136 |
| G2093 | C2025 | A1952 | A1952 | A1882 | C1800  | U1709 | U1639 | U1489  | G1422  | G1422 | A1355 | U1283 | G1209  | G1135 |
| G2094 | C2026 | G2093 | G2093 | G1883 | A1801  | G1710 | C1640 | A1490  | G1422  | G1422 | A1356 | U1284 | A1142  | U1141 |
| G2095 | C2027 | U1955 | U1955 | A1884 | A1802  | C1710 | A1641 | A1490  | G1422  | G1422 | G1356 | A1284 | A1142A | A1142 |
| U2096 | U2028 | U1956 | U1956 | A1885 | A1803  | C1711 | G1642 | G1491  | G1422  | G1422 | U1357 | G1285 | A1143  | G1144 |
| C2097 | G2029 | C1957 | C1957 | A1886 | C1804  | C1712 | G1643 | G1492  | G1422  | G1422 | U1358 | G1286 | G1212  | A1143 |
| U2098 | A2030 | U1958 | U1958 | C1887 | C1804  | C1713 | G1644 | G1493  | G1422  | G1422 | A1359 | A1287 | C1145  | G1145 |
| U2099 | C1958 | C1958 | C1958 | C1887 | U1714  | U1714 | G1647 | A1495  | A1495  | A1495 | A1360 | U1288 | G1216  | C1146 |
| G2100 | G2032 | C1962 | C1962 | G1888 | A1809  | U1714 | C1648 | A1571  | A1496  | C1432 | C1362 | C1291 | C1147  | C1147 |



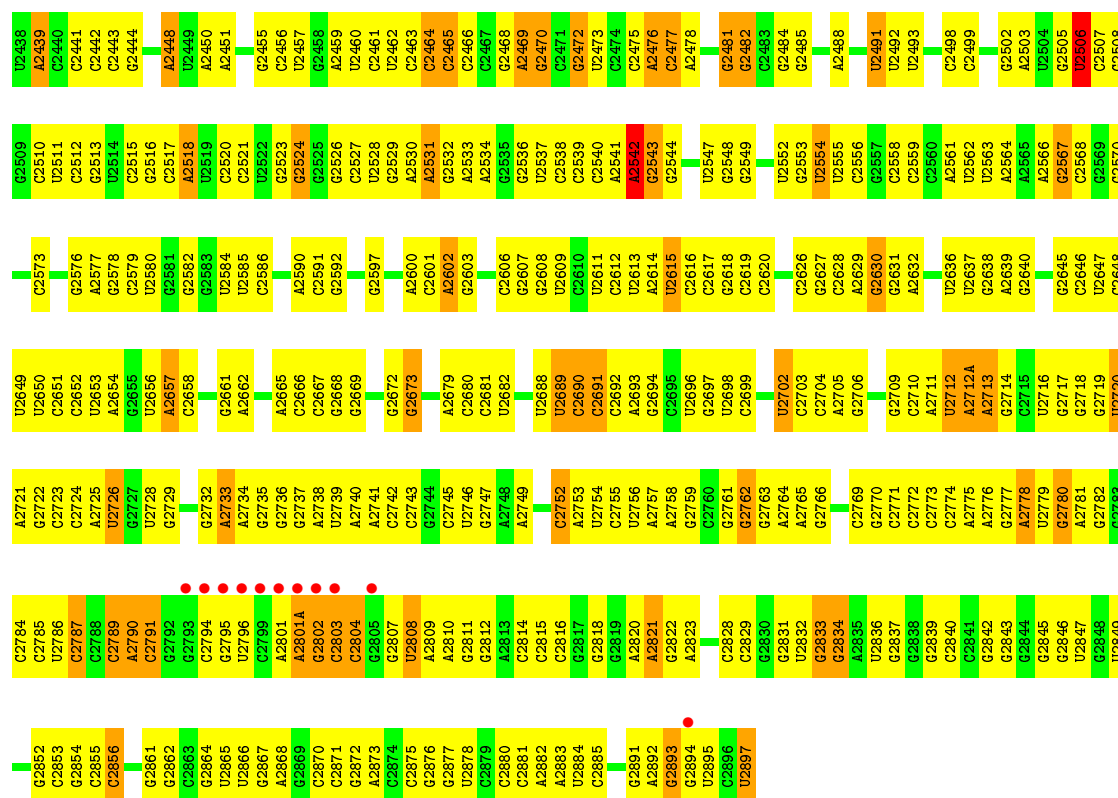
● Molecule 57: RNA (2848-MER)



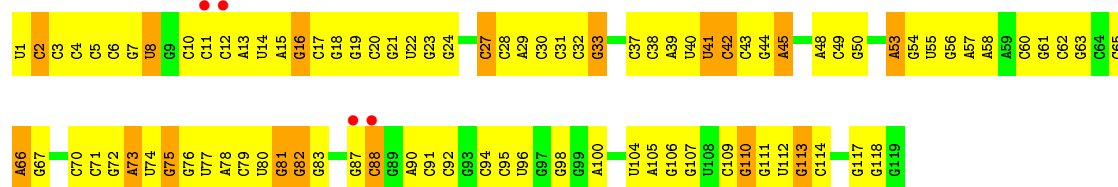
|       |       |       |       |       |      |      |      |      |       |       |      |      |       |       |       |
|-------|-------|-------|-------|-------|------|------|------|------|-------|-------|------|------|-------|-------|-------|
| A1286 | G1212 | G1144 | A1020 | C949  | A878 | C816 | U747 | G666 | A627  | G561  | A483 | G418 | A330  | G271U | G226  |
| A1287 | G1215 | C1145 | A1021 | G950  | G879 | C817 | G743 | U667 | U628  | U562  | C494 | C419 | A331  | G271V | A227  |
| U1288 | G1216 | C1146 | U1022 | G951  | G880 | G819 | A751 | G668 | G629  | G563  | C485 | C420 | A332  | G271W | A228  |
| G1291 | G1217 | C1147 | U1023 | G952  | G881 | A819 | A752 | G669 | G630  | C486  | C486 | C564 | G333  | G271X | A229  |
| U1292 | G1218 | G1150 | G1025 | G954  | G882 | A820 | G753 | A670 | A631  | C487  | C488 | U421 | C334  | U271Y | U230  |
| C1293 | C1219 | G1151 | U1026 | C955  | G883 | U822 | C754 | C672 | A632  | U569  | C489 | G424 | C335  | G271Z | C231  |
| U1294 | C1221 | G1152 | A1027 | C958  | A887 | G823 | C756 | C673 | A633  | G570  | C491 | G425 | C336  | G272  | G232  |
| C1297 | C1222 | G1153 | A1028 | U958  | C888 | A824 | C757 | C674 | C634  | A571  | A492 | G426 | C337  | G272B | A233  |
| U1300 | G1227 | A1155 | G1037 | A960  | A890 | U826 | G760 | A675 | A636  | A572  | C493 | U427 | A340  | G272C | C234  |
| A1301 | G1231 | G1156 | U1038 | C961  | G892 | U827 | A761 | A676 | G638  | G573  | C574 | A428 | G352  | G272E | U235  |
| C1305 | G1232 | G1157 | G1039 | G962  | C893 | U828 | G765 | G679 | U639  | C575  | C498 | U431 | G353  | G272F | C237  |
| A1307 | G1233 | G1158 | C1040 | U963  | C894 | A829 | G766 | G680 | U640  | U576  | U499 | A432 | G356  | G272G | C238  |
| A1308 | U1234 | A1161 | C1041 | C965  | A896 | G830 | U767 | G681 | G642  | A578  | G500 | C433 | G357  | G272H | G242  |
| G1309 | U1240 | G1162 | A1045 | U969  | C897 | G831 | U768 | G686 | A643  | G579  | A505 | U434 | A363A | G272J | U243  |
| G1310 | A1241 | G1163 | G1047 | C970  | A899 | G832 | G769 | U646 | A644  | C580  | C506 | C435 | G363B | G274  | A244  |
| G1311 | A1242 | G1164 | A1048 | C971  | A900 | G833 | G770 | G691 | G645  | C581  | C507 | C436 | G363C | G275  | G245  |
| U1312 | G1243 | G1165 | U1050 | G974  | A901 | G834 | G771 | G692 | A646  | C582  | C508 | G437 | G363D | A276  | C246  |
| U1313 | G1244 | G1166 | A1051 | C975  | C902 | C837 | G772 | C693 | G647  | G583  | G509 | G438 | G363E | G277  | G247  |
| U1314 | G1245 | G1167 | G1051 | C976  | C903 | C838 | G773 | G694 | G648  | G584  | C510 | U441 | A363F | G278  | G248  |
| G1315 | G1246 | G1168 | G1052 | C977  | C904 | U839 | G775 | G696 | G650  | A586  | U511 | G442 | C364  | G279  | C249  |
| U1316 | A1247 | G1169 | G1053 | G879  | U905 | C840 | G776 | A699 | G651  | C587  | C512 | A443 | C365  | A251  | A251  |
| A1317 | G1248 | G1170 | A1106 | A980  | U906 | G843 | A777 | A698 | G652  | U588  | A513 | A444 | C366  | G280  | G252  |
| C1318 | U1249 | G1171 | G1107 | C983  | C908 | G844 | G778 | A706 | A654  | C589  | U519 | G446 | A371  | C291  | A257  |
| G1319 | G1250 | A1174 | U1108 | A983  | A909 | C845 | U779 | G707 | G654A | C591  | G520 | U447 | G372  | C292  | G258  |
| C1320 | C1251 | G1175 | G1110 | C986  | A911 | G846 | A781 | U709 | G654B | G592  | C523 | U448 | U373  | U293  | G259  |
| A1321 | G1252 | G1176 | C1111 | G987  | C912 | U847 | A782 | G710 | G654C | G593  | U524 | A449 | A374  | C296  | C296  |
| A1283 | U1283 | G1177 | G1112 | C991  | U913 | G848 | A783 | G711 | G654E | C595  | U525 | G450 | U380  | C297  | A262  |
| U1285 | G1256 | A1178 | U1113 | C992  | C914 | A849 | A784 | G712 | G654F | G596  | A528 | A454 | G381  | C298  | C263  |
| C1326 | U1260 | G1179 | G1114 | C993  | C915 | C850 | G786 | G713 | G654H | U597  | A529 | C456 | U382  | C299  | C264  |
| G1328 | A1262 | G1183 | C1116 | C994  | A917 | G852 | U787 | A716 | G654I | G602  | C530 | A457 | U384  | A300  | A265  |
| A1331 | U1283 | G1187 | C1117 | A996  | G921 | G853 | A788 | G717 | C654J | A603  | C531 | G458 | C365  | G301  | G266  |
| G1332 | G1284 | U1188 | C1118 | C997  | U922 | G854 | A789 | A718 | C654K | G604  | A532 | U459 | C386  | C302  | C267  |
| C1333 | A1285 | G1189 | G1119 | C998  | C923 | G855 | C790 | C719 | G654L | G605  | G533 | A460 | U387  | U269  | C268  |
| U1336 | G1266 | A1189 | C1120 | U999  | C924 | C857 | G792 | C720 | G654M | G606  | U534 | C461 | G388  | A270  | A271  |
| A1337 | U1267 | G1190 | G1123 | A1000 | C924 | U858 | A793 | C721 | G654N | U607  | C535 | C462 | G389  | G307  | G307  |
| G1337 | A1268 | G1191 | C1124 | C1001 | G927 | G859 | G794 | A722 | G654O | A608  | A536 | G463 | A390  | G309  | A271A |
| C1338 | U1269 | G1192 | G1125 | G1002 | G928 | U860 | C795 | A727 | C654P | A609  | U464 | U464 | G391  | A310  | C271B |
| G1339 | G1270 | A1194 | A1129 | C1003 | U930 | A861 | C796 | G728 | G654Q | G610  | C465 | A466 | A394  | A311  | C271C |
| U1341 | A1271 | G1195 | U1130 | C1004 | G931 | G862 | C797 | G729 | G654R | C611  | A467 | U475 | U395  | A314  | G271D |
| U1344 | U1273 | U1199 | G1131 | C1005 | G932 | A863 | G798 | C730 | G654S | C612  | C543 | G469 | G396  | A315  | U271E |
| G1345 | A1274 | G1200 | A1132 | C1006 | A933 | G864 | A802 | C731 | A654T | G613  | C544 | U614 | G401  | C316  | G271F |
| C1346 | U1275 | C1201 | U1133 | C1007 | G934 | C865 | U803 | C732 | A654U | U614A | C545 | A470 | A401  | G271G | C271H |
| G1347 | A1278 | A1204 | G1136 | A1009 | C935 | A866 | U804 | G733 | A655  | G614B | A547 | A471 | A402  | G271I | G271I |
| U1348 | G1279 | U1205 | U1012 | C1010 | C936 | G869 | G805 | G738 | G656  | G615  | U549 | A472 | U403  | C319  | G271J |
| A1349 | G1280 | C1206 | G1138 | U1011 | A941 | A870 | C806 | G739 | U657  | G616  | G540 | G474 | C404  | G320  | G321  |
| U1352 | U1282 | G1207 | G1139 | U1012 | G942 | U871 | U807 | U740 | C658  | C620  | U554 | U475 | U405  | A322  | U271N |
| A1353 | G1283 | G1208 | A1141 | G1015 | A945 | G873 | G809 | G742 | G660  | A621  | U555 | G478 | G406  | G323  | C271O |
| U1354 | U1284 | G1209 | U1142 | G1016 | G946 | G874 | U810 | G743 | G662  | G622  | G556 | A479 | G408  | G325  | C271P |
| G1355 | G1285 | A1210 | A1143 | G1017 | G947 | G875 | U811 | G744 | G663  | G624  | U557 | A480 | C409  | G326  | G271Q |
|       |       | U1211 |       | U1019 | G948 | U877 | C812 | A746 | C665  | U626  | G568 | G481 | G410  | G327  | G271R |
|       |       |       |       |       |      |      |      |      |       |       |      |      |       |       | G271T |



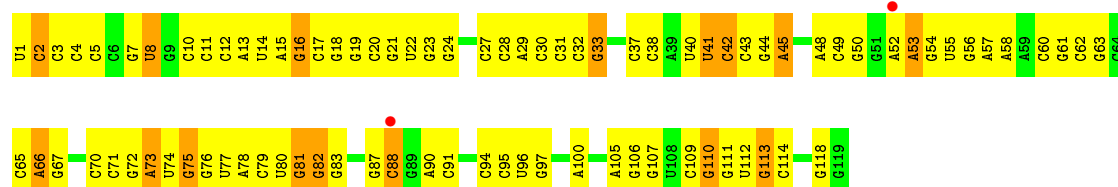




• Molecule 58: RNA (119-MER)



• Molecule 58: RNA (119-MER)



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.23Å 451.43Å 623.34Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.63 – 3.60<br>49.63 – 3.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (49.63-3.60)<br>99.8 (49.63-3.60)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.23                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.28 (at 3.57Å)                                             | Xtriage          |
| Refinement program                                                      | CNS1.2                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.215 , 0.245<br>0.221 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 30861 reflections (4.75%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 103.4                                                       | Xtriage          |
| Anisotropy                                                              | 0.072                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 102.7                                                | EDS              |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Outliers                                                                | 0 of 680802 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 297230                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 109.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MG, CCC

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   | Ab    | 0.33         | 0/1935      | 0.61        | 0/2609        |
| 1   | Bb    | 0.33         | 0/1935      | 0.62        | 0/2609        |
| 2   | Ac    | 0.31         | 0/1636      | 0.58        | 0/2205        |
| 2   | Bc    | 0.32         | 0/1636      | 0.58        | 0/2205        |
| 3   | Ad    | 0.37         | 0/1733      | 0.65        | 1/2318 (0.0%) |
| 3   | Bd    | 0.36         | 0/1733      | 0.64        | 1/2318 (0.0%) |
| 4   | Ae    | 0.35         | 0/1162      | 0.64        | 0/1564        |
| 4   | Be    | 0.37         | 0/1162      | 0.65        | 0/1564        |
| 5   | Af    | 0.34         | 0/856       | 0.64        | 0/1154        |
| 5   | Bf    | 0.37         | 0/856       | 0.65        | 0/1154        |
| 6   | Ag    | 0.32         | 0/1276      | 0.57        | 0/1709        |
| 6   | Bg    | 0.32         | 0/1276      | 0.57        | 0/1709        |
| 7   | Ah    | 0.35         | 0/1136      | 0.64        | 0/1527        |
| 7   | Bh    | 0.35         | 0/1136      | 0.64        | 0/1527        |
| 8   | Ai    | 0.33         | 0/1029      | 0.57        | 0/1379        |
| 8   | Bi    | 0.33         | 0/1029      | 0.57        | 0/1379        |
| 9   | Aj    | 0.33         | 0/807       | 0.62        | 0/1085        |
| 9   | Bj    | 0.33         | 0/807       | 0.62        | 0/1085        |
| 10  | Ak    | 0.36         | 0/900       | 0.64        | 0/1213        |
| 10  | Bk    | 0.36         | 0/900       | 0.64        | 0/1213        |
| 11  | Al    | 0.40         | 0/986       | 0.72        | 1/1320 (0.1%) |
| 11  | Bl    | 0.41         | 0/986       | 0.72        | 1/1320 (0.1%) |
| 12  | Am    | 0.30         | 0/947       | 0.56        | 0/1270        |
| 12  | Bm    | 0.30         | 0/947       | 0.61        | 0/1270        |
| 13  | An    | 0.35         | 0/501       | 0.56        | 0/664         |
| 13  | Bn    | 0.36         | 0/501       | 0.57        | 0/664         |
| 14  | Ao    | 0.33         | 0/745       | 0.59        | 0/992         |
| 14  | Bo    | 0.35         | 0/745       | 0.60        | 0/992         |
| 15  | Ap    | 0.34         | 0/716       | 0.62        | 0/963         |
| 15  | Bp    | 0.32         | 0/716       | 0.62        | 0/963         |
| 16  | Aq    | 0.38         | 0/836       | 0.67        | 0/1117        |
| 16  | Bq    | 0.36         | 0/836       | 0.66        | 0/1117        |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 17  | Ar    | 0.36         | 0/579   | 0.66        | 0/768           |
| 17  | Br    | 0.36         | 0/579   | 0.67        | 0/768           |
| 18  | As    | 0.36         | 0/642   | 0.63        | 0/865           |
| 18  | Bs    | 0.35         | 0/642   | 0.64        | 0/865           |
| 19  | At    | 0.34         | 0/765   | 0.63        | 0/1007          |
| 19  | Bt    | 0.34         | 0/765   | 0.63        | 0/1007          |
| 20  | Au    | 0.42         | 0/212   | 0.59        | 0/277           |
| 20  | Bu    | 0.40         | 0/212   | 0.59        | 0/277           |
| 21  | Ay    | 0.35         | 0/793   | 0.59        | 0/1059          |
| 21  | By    | 0.35         | 0/793   | 0.68        | 0/1059          |
| 22  | Aa    | 0.41         | 0/36190 | 0.69        | 13/56486 (0.0%) |
| 22  | Ba    | 0.42         | 0/36190 | 0.70        | 11/56486 (0.0%) |
| 23  | Ax    | 0.43         | 0/289   | 0.73        | 0/449           |
| 23  | Bx    | 0.43         | 0/289   | 0.73        | 0/449           |
| 24  | Av    | 0.43         | 0/1810  | 0.70        | 0/2821          |
| 24  | Bv    | 0.46         | 0/1810  | 0.72        | 0/2821          |
| 25  | Aw    | 0.36         | 0/1832  | 0.70        | 0/2855          |
| 25  | Bw    | 0.36         | 0/1832  | 0.71        | 0/2855          |
| 26  | AC    | 0.32         | 0/956   | 0.56        | 0/1288          |
| 26  | BC    | 0.30         | 0/956   | 0.56        | 0/1288          |
| 27  | AD    | 0.46         | 0/2154  | 0.81        | 1/2905 (0.0%)   |
| 27  | BD    | 0.48         | 0/2154  | 0.82        | 1/2905 (0.0%)   |
| 28  | AE    | 0.45         | 0/1596  | 0.80        | 1/2153 (0.0%)   |
| 28  | BE    | 0.47         | 0/1596  | 0.79        | 1/2153 (0.0%)   |
| 29  | AF    | 0.41         | 0/1658  | 0.72        | 0/2244          |
| 29  | BF    | 0.43         | 0/1658  | 0.73        | 0/2244          |
| 30  | AG    | 0.37         | 0/1499  | 0.73        | 1/2016 (0.0%)   |
| 30  | BG    | 0.39         | 0/1499  | 0.73        | 0/2016          |
| 31  | AH    | 0.39         | 0/1284  | 0.75        | 1/1739 (0.1%)   |
| 31  | BH    | 0.44         | 0/1284  | 0.78        | 1/1739 (0.1%)   |
| 32  | AI    | 0.40         | 0/1146  | 0.92        | 4/1551 (0.3%)   |
| 32  | BI    | 0.39         | 0/1146  | 0.91        | 4/1551 (0.3%)   |
| 33  | AJ    | 0.36         | 0/640   | 0.77        | 7/889 (0.8%)    |
| 33  | BJ    | 0.39         | 0/640   | 0.88        | 6/889 (0.7%)    |
| 34  | AN    | 0.39         | 0/1131  | 0.74        | 1/1525 (0.1%)   |
| 34  | BN    | 0.43         | 0/1131  | 0.75        | 1/1525 (0.1%)   |
| 35  | AO    | 0.45         | 0/943   | 0.71        | 0/1269          |
| 35  | BO    | 0.45         | 0/943   | 0.71        | 0/1269          |
| 36  | AP    | 0.46         | 0/1131  | 1.00        | 6/1504 (0.4%)   |
| 36  | BP    | 0.52         | 0/1131  | 1.03        | 6/1504 (0.4%)   |
| 37  | AQ    | 0.40         | 0/1133  | 0.65        | 0/1515          |
| 37  | BQ    | 0.40         | 0/1133  | 0.66        | 0/1515          |
| 38  | AR    | 0.43         | 0/974   | 0.79        | 1/1302 (0.1%)   |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 38  | BR    | 0.46         | 0/974           | 0.79        | 1/1302 (0.1%)     |
| 39  | AS    | 0.37         | 0/778           | 0.71        | 0/1036            |
| 39  | BS    | 0.39         | 0/778           | 0.72        | 0/1036            |
| 40  | AT    | 0.47         | 0/1137          | 0.89        | 4/1519 (0.3%)     |
| 40  | BT    | 0.47         | 0/1137          | 0.89        | 4/1519 (0.3%)     |
| 41  | AU    | 0.45         | 1/975 (0.1%)    | 0.71        | 0/1297            |
| 41  | BU    | 0.49         | 0/975           | 0.73        | 0/1297            |
| 42  | AV    | 0.40         | 0/790           | 0.77        | 0/1057            |
| 42  | BV    | 0.42         | 0/790           | 0.78        | 0/1057            |
| 43  | AW    | 0.45         | 0/907           | 0.75        | 1/1216 (0.1%)     |
| 43  | BW    | 0.47         | 0/907           | 0.76        | 1/1216 (0.1%)     |
| 44  | AX    | 0.43         | 0/739           | 0.69        | 0/993             |
| 44  | BX    | 0.47         | 0/739           | 0.72        | 0/993             |
| 45  | AY    | 0.43         | 0/788           | 0.76        | 1/1051 (0.1%)     |
| 45  | BY    | 0.48         | 0/788           | 0.78        | 1/1051 (0.1%)     |
| 46  | AZ    | 0.36         | 0/1499          | 0.68        | 0/2035            |
| 46  | BZ    | 0.37         | 0/1499          | 0.72        | 0/2035            |
| 47  | A0    | 0.39         | 0/671           | 0.65        | 0/892             |
| 47  | B0    | 0.42         | 0/671           | 0.67        | 0/892             |
| 48  | A1    | 0.39         | 0/738           | 0.76        | 1/981 (0.1%)      |
| 48  | B1    | 0.46         | 0/738           | 0.80        | 1/981 (0.1%)      |
| 49  | A2    | 0.34         | 0/600           | 0.63        | 0/793             |
| 49  | B2    | 0.44         | 0/600           | 0.75        | 0/793             |
| 50  | A3    | 0.36         | 0/472           | 0.66        | 0/634             |
| 50  | B3    | 0.41         | 0/472           | 0.67        | 0/634             |
| 51  | A4    | 0.36         | 0/460           | 0.70        | 1/621 (0.2%)      |
| 51  | B4    | 0.40         | 0/460           | 0.70        | 1/621 (0.2%)      |
| 52  | A5    | 0.48         | 0/441           | 0.81        | 0/596             |
| 52  | B5    | 0.50         | 0/441           | 0.83        | 0/596             |
| 53  | A6    | 0.43         | 0/440           | 0.81        | 0/586             |
| 53  | B6    | 0.46         | 0/440           | 0.81        | 0/586             |
| 54  | A7    | 0.41         | 0/417           | 0.65        | 0/550             |
| 54  | B7    | 0.46         | 0/417           | 0.68        | 0/550             |
| 55  | A8    | 0.52         | 0/515           | 0.90        | 0/679             |
| 55  | B8    | 0.53         | 0/515           | 0.92        | 0/679             |
| 56  | A9    | 0.34         | 0/310           | 0.60        | 0/407             |
| 56  | B9    | 0.38         | 0/310           | 0.62        | 0/407             |
| 57  | AA    | 0.50         | 1/68704 (0.0%)  | 0.74        | 40/107260 (0.0%)  |
| 57  | BA    | 0.55         | 2/68704 (0.0%)  | 0.74        | 48/107260 (0.0%)  |
| 58  | AB    | 0.41         | 0/2853          | 0.70        | 0/4451            |
| 58  | BB    | 0.44         | 0/2853          | 0.71        | 0/4451            |
| All | All   | 0.46         | 4/321584 (0.0%) | 0.72        | 176/480460 (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 |
|-----|-------|---------------------|---------------------|
| 21  | Ay    | 0                   | 1                   |
| 22  | Aa    | 0                   | 8                   |
| 22  | Ba    | 1                   | 11                  |
| 24  | Av    | 0                   | 1                   |
| 24  | Bv    | 0                   | 1                   |
| 34  | AN    | 0                   | 1                   |
| 34  | BN    | 0                   | 1                   |
| 43  | AW    | 0                   | 1                   |
| 43  | BW    | 0                   | 1                   |
| 52  | A5    | 0                   | 1                   |
| 52  | B5    | 0                   | 1                   |
| 57  | AA    | 3                   | 48                  |
| 57  | BA    | 3                   | 49                  |
| All | All   | 7                   | 125                 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 57  | BA    | 2506 | U    | N1-C2 | 5.94  | 1.43        | 1.38     |
| 57  | BA    | 783  | A    | C5-C6 | -5.52 | 1.36        | 1.41     |
| 41  | AU    | 58   | ARG  | CG-CD | 5.12  | 1.64        | 1.51     |
| 57  | AA    | 783  | A    | C5-C6 | -5.07 | 1.36        | 1.41     |

The worst 5 of 176 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 32  | AI    | 50  | ARG  | NE-CZ-NH1   | -13.91 | 113.34      | 120.30   |
| 32  | BI    | 50  | ARG  | NE-CZ-NH1   | 13.44  | 127.02      | 120.30   |
| 32  | BI    | 50  | ARG  | NE-CZ-NH2   | -13.41 | 113.60      | 120.30   |
| 32  | AI    | 50  | ARG  | NE-CZ-NH2   | 13.03  | 126.81      | 120.30   |
| 57  | BA    | 790 | C    | C2'-C3'-O3' | 10.57  | 132.76      | 109.50   |

5 of 7 chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 57  | AA    | 1799 | G    | C3'  |
| 57  | AA    | 1819 | A    | C3'  |
| 57  | AA    | 1820 | U    | C3'  |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | Ba    | 1498 | U    | C3'  |
| 57  | BA    | 1799 | G    | C3'  |

5 of 125 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 22  | Aa    | 436 | C    | Sidechain |
| 22  | Aa    | 484 | G    | Sidechain |
| 22  | Aa    | 494 | U    | Sidechain |
| 22  | Aa    | 832 | C    | Sidechain |
| 21  | Ay    | 56  | ARG  | Sidechain |

## 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   | Ab    | 1900  | 0        | 1951     | 0       | 0            |
| 1   | Bb    | 1900  | 0        | 1951     | 0       | 0            |
| 2   | Ac    | 1612  | 0        | 1677     | 0       | 0            |
| 2   | Bc    | 1612  | 0        | 1677     | 0       | 0            |
| 3   | Ad    | 1703  | 0        | 1763     | 0       | 0            |
| 3   | Bd    | 1703  | 0        | 1764     | 0       | 0            |
| 4   | Ae    | 1146  | 0        | 1207     | 0       | 0            |
| 4   | Be    | 1146  | 0        | 1207     | 0       | 0            |
| 5   | Af    | 843   | 0        | 857      | 0       | 0            |
| 5   | Bf    | 843   | 0        | 857      | 0       | 0            |
| 6   | Ag    | 1257  | 0        | 1296     | 0       | 0            |
| 6   | Bg    | 1257  | 0        | 1296     | 0       | 0            |
| 7   | Ah    | 1116  | 0        | 1177     | 0       | 0            |
| 7   | Bh    | 1116  | 0        | 1177     | 0       | 0            |
| 8   | Ai    | 1010  | 0        | 1037     | 0       | 0            |
| 8   | Bi    | 1010  | 0        | 1037     | 0       | 0            |
| 9   | Aj    | 794   | 0        | 840      | 0       | 0            |
| 9   | Bj    | 794   | 0        | 840      | 0       | 0            |
| 10  | Ak    | 885   | 0        | 904      | 0       | 0            |
| 10  | Bk    | 885   | 0        | 904      | 0       | 0            |
| 11  | Al    | 970   | 0        | 1057     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | Bl    | 970   | 0        | 1057     | 0       | 0            |
| 12  | Am    | 937   | 0        | 992      | 0       | 0            |
| 12  | Bm    | 937   | 0        | 990      | 0       | 0            |
| 13  | An    | 492   | 0        | 530      | 0       | 0            |
| 13  | Bn    | 492   | 0        | 530      | 0       | 0            |
| 14  | Ao    | 734   | 0        | 771      | 0       | 0            |
| 14  | Bo    | 734   | 0        | 771      | 0       | 0            |
| 15  | Ap    | 700   | 0        | 720      | 0       | 0            |
| 15  | Bp    | 700   | 0        | 720      | 0       | 0            |
| 16  | Aq    | 823   | 0        | 891      | 0       | 0            |
| 16  | Bq    | 823   | 0        | 891      | 0       | 0            |
| 17  | Ar    | 574   | 0        | 644      | 0       | 0            |
| 17  | Br    | 574   | 0        | 644      | 0       | 0            |
| 18  | As    | 629   | 0        | 652      | 0       | 0            |
| 18  | Bs    | 629   | 0        | 652      | 0       | 0            |
| 19  | At    | 763   | 0        | 861      | 0       | 0            |
| 19  | Bt    | 763   | 0        | 861      | 0       | 0            |
| 20  | Au    | 208   | 0        | 221      | 0       | 0            |
| 20  | Bu    | 208   | 0        | 221      | 0       | 0            |
| 21  | Ay    | 782   | 0        | 827      | 0       | 0            |
| 21  | By    | 782   | 0        | 827      | 0       | 0            |
| 22  | Aa    | 32329 | 0        | 16316    | 0       | 0            |
| 22  | Ba    | 32329 | 0        | 16317    | 0       | 0            |
| 23  | Ax    | 260   | 0        | 129      | 0       | 0            |
| 23  | Bx    | 260   | 0        | 129      | 0       | 0            |
| 24  | Av    | 1641  | 0        | 839      | 0       | 0            |
| 24  | Bv    | 1641  | 0        | 839      | 0       | 0            |
| 25  | Aw    | 1640  | 0        | 837      | 0       | 0            |
| 25  | Bw    | 1640  | 0        | 837      | 0       | 0            |
| 26  | AC    | 937   | 0        | 957      | 112     | 0            |
| 26  | BC    | 937   | 0        | 957      | 116     | 0            |
| 27  | AD    | 2104  | 0        | 2182     | 327     | 0            |
| 27  | BD    | 2104  | 0        | 2182     | 329     | 0            |
| 28  | AE    | 1563  | 0        | 1629     | 259     | 0            |
| 28  | BE    | 1563  | 0        | 1629     | 252     | 0            |
| 29  | AF    | 1623  | 0        | 1677     | 223     | 0            |
| 29  | BF    | 1623  | 0        | 1677     | 216     | 0            |
| 30  | AG    | 1474  | 0        | 1533     | 341     | 0            |
| 30  | BG    | 1474  | 0        | 1532     | 319     | 0            |
| 31  | AH    | 1259  | 0        | 1326     | 192     | 0            |
| 31  | BH    | 1259  | 0        | 1326     | 187     | 0            |
| 32  | AI    | 1131  | 0        | 1218     | 246     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | BI    | 1131  | 0        | 1218     | 264     | 0            |
| 33  | AJ    | 641   | 0        | 309      | 34      | 0            |
| 33  | BJ    | 641   | 0        | 309      | 47      | 0            |
| 34  | AN    | 1104  | 0        | 1180     | 146     | 0            |
| 34  | BN    | 1104  | 0        | 1180     | 151     | 0            |
| 35  | AO    | 933   | 0        | 996      | 98      | 0            |
| 35  | BO    | 933   | 0        | 996      | 99      | 0            |
| 36  | AP    | 1114  | 0        | 1187     | 304     | 0            |
| 36  | BP    | 1114  | 0        | 1187     | 302     | 0            |
| 37  | AQ    | 1112  | 0        | 1171     | 122     | 0            |
| 37  | BQ    | 1112  | 0        | 1171     | 124     | 0            |
| 38  | AR    | 960   | 0        | 1021     | 128     | 0            |
| 38  | BR    | 960   | 0        | 1021     | 126     | 0            |
| 39  | AS    | 770   | 0        | 832      | 139     | 0            |
| 39  | BS    | 770   | 0        | 832      | 137     | 0            |
| 40  | AT    | 1123  | 0        | 1181     | 229     | 0            |
| 40  | BT    | 1123  | 0        | 1181     | 234     | 0            |
| 41  | AU    | 958   | 0        | 1015     | 148     | 0            |
| 41  | BU    | 958   | 0        | 1015     | 145     | 0            |
| 42  | AV    | 779   | 0        | 852      | 151     | 0            |
| 42  | BV    | 779   | 0        | 852      | 153     | 0            |
| 43  | AW    | 896   | 0        | 953      | 94      | 0            |
| 43  | BW    | 896   | 0        | 953      | 89      | 0            |
| 44  | AX    | 725   | 0        | 778      | 88      | 0            |
| 44  | BX    | 725   | 0        | 778      | 91      | 0            |
| 45  | AY    | 775   | 0        | 870      | 189     | 0            |
| 45  | BY    | 775   | 0        | 870      | 197     | 0            |
| 46  | AZ    | 1467  | 0        | 1492     | 238     | 0            |
| 46  | BZ    | 1467  | 0        | 1492     | 238     | 0            |
| 47  | A0    | 662   | 0        | 688      | 79      | 0            |
| 47  | B0    | 662   | 0        | 688      | 77      | 0            |
| 48  | A1    | 731   | 0        | 808      | 98      | 0            |
| 48  | B1    | 731   | 0        | 808      | 89      | 0            |
| 49  | A2    | 598   | 0        | 653      | 96      | 0            |
| 49  | B2    | 598   | 0        | 653      | 57      | 0            |
| 50  | A3    | 467   | 0        | 523      | 40      | 0            |
| 50  | B3    | 467   | 0        | 523      | 38      | 0            |
| 51  | A4    | 450   | 0        | 449      | 91      | 0            |
| 51  | B4    | 450   | 0        | 449      | 80      | 0            |
| 52  | A5    | 427   | 0        | 445      | 83      | 0            |
| 52  | B5    | 427   | 0        | 445      | 90      | 0            |
| 53  | A6    | 433   | 0        | 461      | 115     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 53  | B6    | 433   | 0        | 461      | 117     | 0            |
| 54  | A7    | 409   | 0        | 454      | 38      | 0            |
| 54  | B7    | 409   | 0        | 454      | 38      | 0            |
| 55  | A8    | 507   | 0        | 576      | 112     | 0            |
| 55  | B8    | 507   | 0        | 576      | 120     | 0            |
| 56  | A9    | 307   | 0        | 336      | 19      | 0            |
| 56  | B9    | 307   | 0        | 336      | 25      | 0            |
| 57  | AA    | 61341 | 0        | 30925    | 2266    | 0            |
| 57  | BA    | 61341 | 0        | 30926    | 2267    | 0            |
| 58  | AB    | 2551  | 0        | 1295     | 140     | 0            |
| 58  | BB    | 2551  | 0        | 1295     | 115     | 0            |
| 59  | A4    | 1     | 0        | 0        | 0       | 0            |
| 59  | A9    | 1     | 0        | 0        | 0       | 0            |
| 59  | Ad    | 1     | 0        | 0        | 0       | 0            |
| 59  | An    | 1     | 0        | 0        | 0       | 0            |
| 59  | B4    | 1     | 0        | 0        | 0       | 0            |
| 59  | B9    | 1     | 0        | 0        | 0       | 0            |
| 59  | Bd    | 1     | 0        | 0        | 0       | 0            |
| 59  | Bn    | 1     | 0        | 0        | 0       | 0            |
| 60  | A1    | 2     | 0        | 0        | 0       | 0            |
| 60  | A5    | 1     | 0        | 0        | 0       | 0            |
| 60  | A7    | 1     | 0        | 0        | 0       | 0            |
| 60  | AA    | 367   | 0        | 0        | 0       | 0            |
| 60  | AB    | 3     | 0        | 0        | 0       | 0            |
| 60  | AD    | 2     | 0        | 0        | 0       | 0            |
| 60  | AF    | 1     | 0        | 0        | 0       | 0            |
| 60  | AQ    | 1     | 0        | 0        | 0       | 0            |
| 60  | AX    | 1     | 0        | 0        | 0       | 0            |
| 60  | Aa    | 145   | 0        | 0        | 0       | 0            |
| 60  | Ae    | 2     | 0        | 0        | 0       | 0            |
| 60  | Av    | 5     | 0        | 0        | 0       | 0            |
| 60  | Aw    | 1     | 0        | 0        | 0       | 0            |
| 60  | B0    | 2     | 0        | 0        | 0       | 0            |
| 60  | B5    | 2     | 0        | 0        | 0       | 0            |
| 60  | B7    | 2     | 0        | 0        | 0       | 0            |
| 60  | BA    | 365   | 0        | 0        | 0       | 0            |
| 60  | BB    | 3     | 0        | 0        | 0       | 0            |
| 60  | BD    | 2     | 0        | 0        | 0       | 0            |
| 60  | BF    | 1     | 0        | 0        | 0       | 0            |
| 60  | BO    | 1     | 0        | 0        | 0       | 0            |
| 60  | BX    | 1     | 0        | 0        | 0       | 0            |
| 60  | Ba    | 143   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | Bd    | 1      | 0        | 0        | 0       | 0            |
| 60  | Bl    | 1      | 0        | 0        | 0       | 0            |
| 60  | Bm    | 1      | 0        | 0        | 0       | 0            |
| 60  | Bv    | 5      | 0        | 0        | 0       | 0            |
| 60  | Bw    | 1      | 0        | 0        | 0       | 0            |
| 60  | Bx    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 297230 | 0        | 201936   | 12630   | 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 41.

The worst 5 of 12630 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:AG:106:LEU:O    | 30:AG:110:ALA:HB3 | 1.29                     | 1.28              |
| 27:AD:242:ARG:HH21 | 57:AA:1826:G:H4'  | 1.06                     | 1.17              |
| 32:AI:118:LYS:HG2  | 32:AI:119:PRO:HD2 | 1.24                     | 1.17              |
| 40:BT:28:VAL:HG13  | 40:BT:46:GLU:HA   | 1.28                     | 1.16              |
| 57:BA:1884:A:H2'   | 57:BA:1885:A:H5'' | 1.18                     | 1.16              |

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 |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 1   | Ab    | 232/256 (91%) | 149 (64%) | 48 (21%) | 35 (15%) | 0           | 5 |
| 1   | Bb    | 232/256 (91%) | 148 (64%) | 52 (22%) | 32 (14%) | 0           | 6 |
| 2   | Ac    | 204/239 (85%) | 132 (65%) | 43 (21%) | 29 (14%) | 0           | 5 |
| 2   | Bc    | 204/239 (85%) | 134 (66%) | 41 (20%) | 29 (14%) | 0           | 5 |
| 3   | Ad    | 206/209 (99%) | 131 (64%) | 52 (25%) | 23 (11%) | 0           | 9 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3   | Bd    | 206/209 (99%) | 132 (64%) | 51 (25%) | 23 (11%) | 0           | 9  |
| 4   | Ae    | 148/162 (91%) | 105 (71%) | 24 (16%) | 19 (13%) | 0           | 7  |
| 4   | Be    | 148/162 (91%) | 104 (70%) | 23 (16%) | 21 (14%) | 0           | 5  |
| 5   | Af    | 99/101 (98%)  | 67 (68%)  | 25 (25%) | 7 (7%)   | 1           | 19 |
| 5   | Bf    | 99/101 (98%)  | 66 (67%)  | 26 (26%) | 7 (7%)   | 1           | 19 |
| 6   | Ag    | 153/156 (98%) | 108 (71%) | 31 (20%) | 14 (9%)  | 1           | 13 |
| 6   | Bg    | 153/156 (98%) | 106 (69%) | 33 (22%) | 14 (9%)  | 1           | 13 |
| 7   | Ah    | 136/138 (99%) | 97 (71%)  | 32 (24%) | 7 (5%)   | 2           | 28 |
| 7   | Bh    | 136/138 (99%) | 97 (71%)  | 33 (24%) | 6 (4%)   | 3           | 32 |
| 8   | Ai    | 125/128 (98%) | 83 (66%)  | 24 (19%) | 18 (14%) | 0           | 5  |
| 8   | Bi    | 125/128 (98%) | 82 (66%)  | 25 (20%) | 18 (14%) | 0           | 5  |
| 9   | Aj    | 96/105 (91%)  | 76 (79%)  | 13 (14%) | 7 (7%)   | 1           | 18 |
| 9   | Bj    | 96/105 (91%)  | 76 (79%)  | 13 (14%) | 7 (7%)   | 1           | 18 |
| 10  | Ak    | 117/129 (91%) | 88 (75%)  | 22 (19%) | 7 (6%)   | 2           | 24 |
| 10  | Bk    | 117/129 (91%) | 87 (74%)  | 23 (20%) | 7 (6%)   | 2           | 24 |
| 11  | Al    | 122/132 (92%) | 82 (67%)  | 25 (20%) | 15 (12%) | 0           | 8  |
| 11  | Bl    | 122/132 (92%) | 82 (67%)  | 24 (20%) | 16 (13%) | 0           | 7  |
| 12  | Am    | 116/126 (92%) | 58 (50%)  | 28 (24%) | 30 (26%) | 0           | 1  |
| 12  | Bm    | 116/126 (92%) | 66 (57%)  | 25 (22%) | 25 (22%) | 0           | 1  |
| 13  | An    | 58/61 (95%)   | 38 (66%)  | 10 (17%) | 10 (17%) | 0           | 3  |
| 13  | Bn    | 58/61 (95%)   | 37 (64%)  | 11 (19%) | 10 (17%) | 0           | 3  |
| 14  | Ao    | 86/89 (97%)   | 52 (60%)  | 24 (28%) | 10 (12%) | 0           | 9  |
| 14  | Bo    | 86/89 (97%)   | 52 (60%)  | 25 (29%) | 9 (10%)  | 1           | 10 |
| 15  | Ap    | 81/88 (92%)   | 55 (68%)  | 20 (25%) | 6 (7%)   | 1           | 18 |
| 15  | Bp    | 81/88 (92%)   | 55 (68%)  | 23 (28%) | 3 (4%)   | 4           | 38 |
| 16  | Aq    | 97/105 (92%)  | 74 (76%)  | 18 (19%) | 5 (5%)   | 2           | 27 |
| 16  | Bq    | 97/105 (92%)  | 73 (75%)  | 19 (20%) | 5 (5%)   | 2           | 27 |
| 17  | Ar    | 68/88 (77%)   | 43 (63%)  | 20 (29%) | 5 (7%)   | 1           | 18 |
| 17  | Br    | 68/88 (77%)   | 42 (62%)  | 21 (31%) | 5 (7%)   | 1           | 18 |
| 18  | As    | 76/93 (82%)   | 43 (57%)  | 20 (26%) | 13 (17%) | 0           | 3  |
| 18  | Bs    | 76/93 (82%)   | 43 (57%)  | 20 (26%) | 13 (17%) | 0           | 3  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 19  | At    | 97/106 (92%)  | 60 (62%)  | 25 (26%) | 12 (12%) | 0           | 8  |
| 19  | Bt    | 97/106 (92%)  | 60 (62%)  | 25 (26%) | 12 (12%) | 0           | 8  |
| 20  | Au    | 22/27 (82%)   | 13 (59%)  | 6 (27%)  | 3 (14%)  | 0           | 6  |
| 20  | Bu    | 22/27 (82%)   | 12 (54%)  | 7 (32%)  | 3 (14%)  | 0           | 6  |
| 21  | Ay    | 92/95 (97%)   | 51 (55%)  | 24 (26%) | 17 (18%) | 0           | 3  |
| 21  | By    | 92/95 (97%)   | 58 (63%)  | 20 (22%) | 14 (15%) | 0           | 5  |
| 26  | AC    | 116/229 (51%) | 87 (75%)  | 25 (22%) | 4 (3%)   | 5           | 41 |
| 26  | BC    | 116/229 (51%) | 86 (74%)  | 26 (22%) | 4 (3%)   | 5           | 41 |
| 27  | AD    | 269/276 (98%) | 187 (70%) | 50 (19%) | 32 (12%) | 0           | 8  |
| 27  | BD    | 269/276 (98%) | 190 (71%) | 50 (19%) | 29 (11%) | 0           | 10 |
| 28  | AE    | 202/206 (98%) | 138 (68%) | 35 (17%) | 29 (14%) | 0           | 5  |
| 28  | BE    | 202/206 (98%) | 140 (69%) | 34 (17%) | 28 (14%) | 0           | 6  |
| 29  | AF    | 205/210 (98%) | 148 (72%) | 29 (14%) | 28 (14%) | 0           | 6  |
| 29  | BF    | 205/210 (98%) | 148 (72%) | 30 (15%) | 27 (13%) | 0           | 6  |
| 30  | AG    | 179/182 (98%) | 98 (55%)  | 47 (26%) | 34 (19%) | 0           | 2  |
| 30  | BG    | 179/182 (98%) | 99 (55%)  | 42 (24%) | 38 (21%) | 0           | 2  |
| 31  | AH    | 162/180 (90%) | 97 (60%)  | 36 (22%) | 29 (18%) | 0           | 3  |
| 31  | BH    | 162/180 (90%) | 97 (60%)  | 36 (22%) | 29 (18%) | 0           | 3  |
| 32  | AI    | 143/148 (97%) | 75 (52%)  | 44 (31%) | 24 (17%) | 0           | 4  |
| 32  | BI    | 143/148 (97%) | 76 (53%)  | 40 (28%) | 27 (19%) | 0           | 3  |
| 33  | AJ    | 128/173 (74%) | 46 (36%)  | 43 (34%) | 39 (30%) | 0           | 0  |
| 33  | BJ    | 128/173 (74%) | 40 (31%)  | 36 (28%) | 52 (41%) | 0           | 0  |
| 34  | AN    | 136/140 (97%) | 96 (71%)  | 23 (17%) | 17 (12%) | 0           | 8  |
| 34  | BN    | 136/140 (97%) | 98 (72%)  | 21 (15%) | 17 (12%) | 0           | 8  |
| 35  | AO    | 120/122 (98%) | 103 (86%) | 11 (9%)  | 6 (5%)   | 3           | 29 |
| 35  | BO    | 120/122 (98%) | 103 (86%) | 12 (10%) | 5 (4%)   | 3           | 33 |
| 36  | AP    | 144/150 (96%) | 75 (52%)  | 37 (26%) | 32 (22%) | 0           | 1  |
| 36  | BP    | 144/150 (96%) | 75 (52%)  | 38 (26%) | 31 (22%) | 0           | 2  |
| 37  | AQ    | 138/141 (98%) | 105 (76%) | 20 (14%) | 13 (9%)  | 1           | 12 |
| 37  | BQ    | 138/141 (98%) | 105 (76%) | 18 (13%) | 15 (11%) | 0           | 9  |
| 38  | AR    | 115/118 (98%) | 82 (71%)  | 21 (18%) | 12 (10%) | 1           | 11 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 38  | BR    | 115/118 (98%) | 83 (72%)  | 20 (17%) | 12 (10%) | 1           | 11 |
| 39  | AS    | 96/112 (86%)  | 45 (47%)  | 29 (30%) | 22 (23%) | 0           | 1  |
| 39  | BS    | 96/112 (86%)  | 45 (47%)  | 29 (30%) | 22 (23%) | 0           | 1  |
| 40  | AT    | 133/146 (91%) | 87 (65%)  | 19 (14%) | 27 (20%) | 0           | 2  |
| 40  | BT    | 133/146 (91%) | 87 (65%)  | 20 (15%) | 26 (20%) | 0           | 2  |
| 41  | AU    | 115/118 (98%) | 86 (75%)  | 23 (20%) | 6 (5%)   | 2           | 27 |
| 41  | BU    | 115/118 (98%) | 85 (74%)  | 23 (20%) | 7 (6%)   | 2           | 24 |
| 42  | AV    | 99/101 (98%)  | 66 (67%)  | 22 (22%) | 11 (11%) | 0           | 9  |
| 42  | BV    | 99/101 (98%)  | 67 (68%)  | 20 (20%) | 12 (12%) | 0           | 8  |
| 43  | AW    | 111/113 (98%) | 85 (77%)  | 16 (14%) | 10 (9%)  | 1           | 13 |
| 43  | BW    | 111/113 (98%) | 86 (78%)  | 14 (13%) | 11 (10%) | 1           | 12 |
| 44  | AX    | 90/96 (94%)   | 65 (72%)  | 22 (24%) | 3 (3%)   | 5           | 41 |
| 44  | BX    | 90/96 (94%)   | 64 (71%)  | 24 (27%) | 2 (2%)   | 8           | 51 |
| 45  | AY    | 98/110 (89%)  | 45 (46%)  | 23 (24%) | 30 (31%) | 0           | 0  |
| 45  | BY    | 98/110 (89%)  | 46 (47%)  | 21 (21%) | 31 (32%) | 0           | 0  |
| 46  | AZ    | 182/206 (88%) | 104 (57%) | 46 (25%) | 32 (18%) | 0           | 3  |
| 46  | BZ    | 182/206 (88%) | 105 (58%) | 46 (25%) | 31 (17%) | 0           | 3  |
| 47  | A0    | 82/85 (96%)   | 62 (76%)  | 15 (18%) | 5 (6%)   | 2           | 24 |
| 47  | B0    | 82/85 (96%)   | 61 (74%)  | 16 (20%) | 5 (6%)   | 2           | 24 |
| 48  | A1    | 91/98 (93%)   | 66 (72%)  | 15 (16%) | 10 (11%) | 0           | 9  |
| 48  | B1    | 91/98 (93%)   | 71 (78%)  | 11 (12%) | 9 (10%)  | 1           | 12 |
| 49  | A2    | 69/72 (96%)   | 41 (59%)  | 18 (26%) | 10 (14%) | 0           | 5  |
| 49  | B2    | 69/72 (96%)   | 47 (68%)  | 16 (23%) | 6 (9%)   | 1           | 14 |
| 50  | A3    | 57/60 (95%)   | 48 (84%)  | 7 (12%)  | 2 (4%)   | 4           | 40 |
| 50  | B3    | 57/60 (95%)   | 48 (84%)  | 7 (12%)  | 2 (4%)   | 4           | 40 |
| 51  | A4    | 55/71 (78%)   | 22 (40%)  | 20 (36%) | 13 (24%) | 0           | 1  |
| 51  | B4    | 55/71 (78%)   | 23 (42%)  | 19 (34%) | 13 (24%) | 0           | 1  |
| 52  | A5    | 53/60 (88%)   | 37 (70%)  | 8 (15%)  | 8 (15%)  | 0           | 5  |
| 52  | B5    | 53/60 (88%)   | 37 (70%)  | 8 (15%)  | 8 (15%)  | 0           | 5  |
| 53  | A6    | 48/54 (89%)   | 22 (46%)  | 13 (27%) | 13 (27%) | 0           | 0  |
| 53  | B6    | 48/54 (89%)   | 22 (46%)  | 13 (27%) | 13 (27%) | 0           | 0  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 54  | A7    | 45/49 (92%)       | 42 (93%)   | 2 (4%)     | 1 (2%)     | 8           | 51 |
| 54  | B7    | 45/49 (92%)       | 42 (93%)   | 2 (4%)     | 1 (2%)     | 8           | 51 |
| 55  | A8    | 61/65 (94%)       | 35 (57%)   | 15 (25%)   | 11 (18%)   | 0           | 3  |
| 55  | B8    | 61/65 (94%)       | 35 (57%)   | 15 (25%)   | 11 (18%)   | 0           | 3  |
| 56  | A9    | 35/37 (95%)       | 25 (71%)   | 9 (26%)    | 1 (3%)     | 6           | 44 |
| 56  | B9    | 35/37 (95%)       | 25 (71%)   | 9 (26%)    | 1 (3%)     | 6           | 44 |
| All | All   | 12016/13122 (92%) | 7873 (66%) | 2533 (21%) | 1610 (13%) | 0           | 6  |

5 of 1610 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ab    | 15  | VAL  |
| 1   | Ab    | 18  | GLY  |
| 1   | Ab    | 75  | LYS  |
| 1   | Ab    | 123 | ALA  |
| 1   | Ab    | 143 | GLU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | Ab    | 202/220 (92%) | 181 (90%) | 21 (10%) | 9           | 42 |
| 1   | Bb    | 202/220 (92%) | 181 (90%) | 21 (10%) | 9           | 42 |
| 2   | Ac    | 160/188 (85%) | 148 (92%) | 12 (8%)  | 17          | 57 |
| 2   | Bc    | 160/188 (85%) | 148 (92%) | 12 (8%)  | 17          | 57 |
| 3   | Ad    | 180/181 (99%) | 157 (87%) | 23 (13%) | 5           | 31 |
| 3   | Bd    | 180/181 (99%) | 157 (87%) | 23 (13%) | 5           | 31 |
| 4   | Ae    | 115/123 (94%) | 100 (87%) | 15 (13%) | 5           | 30 |
| 4   | Be    | 115/123 (94%) | 100 (87%) | 15 (13%) | 5           | 30 |
| 5   | Af    | 90/90 (100%)  | 82 (91%)  | 8 (9%)   | 12          | 50 |
| 5   | Bf    | 90/90 (100%)  | 81 (90%)  | 9 (10%)  | 9           | 43 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6   | Ag    | 126/127 (99%)  | 120 (95%) | 6 (5%)   | 31          | 72 |
| 6   | Bg    | 126/127 (99%)  | 120 (95%) | 6 (5%)   | 31          | 72 |
| 7   | Ah    | 119/119 (100%) | 111 (93%) | 8 (7%)   | 20          | 62 |
| 7   | Bh    | 119/119 (100%) | 110 (92%) | 9 (8%)   | 16          | 56 |
| 8   | Ai    | 98/99 (99%)    | 86 (88%)  | 12 (12%) | 6           | 32 |
| 8   | Bi    | 98/99 (99%)    | 86 (88%)  | 12 (12%) | 6           | 32 |
| 9   | Aj    | 88/92 (96%)    | 80 (91%)  | 8 (9%)   | 12          | 48 |
| 9   | Bj    | 88/92 (96%)    | 80 (91%)  | 8 (9%)   | 12          | 48 |
| 10  | Ak    | 90/99 (91%)    | 85 (94%)  | 5 (6%)   | 26          | 68 |
| 10  | Bk    | 90/99 (91%)    | 85 (94%)  | 5 (6%)   | 26          | 68 |
| 11  | Al    | 104/109 (95%)  | 94 (90%)  | 10 (10%) | 10          | 45 |
| 11  | Bl    | 104/109 (95%)  | 93 (89%)  | 11 (11%) | 8           | 40 |
| 12  | Am    | 94/101 (93%)   | 82 (87%)  | 12 (13%) | 5           | 31 |
| 12  | Bm    | 94/101 (93%)   | 83 (88%)  | 11 (12%) | 7           | 35 |
| 13  | An    | 49/50 (98%)    | 46 (94%)  | 3 (6%)   | 23          | 65 |
| 13  | Bn    | 49/50 (98%)    | 45 (92%)  | 4 (8%)   | 14          | 53 |
| 14  | Ao    | 79/80 (99%)    | 73 (92%)  | 6 (8%)   | 16          | 56 |
| 14  | Bo    | 79/80 (99%)    | 73 (92%)  | 6 (8%)   | 16          | 56 |
| 15  | Ap    | 72/74 (97%)    | 68 (94%)  | 4 (6%)   | 26          | 68 |
| 15  | Bp    | 72/74 (97%)    | 68 (94%)  | 4 (6%)   | 26          | 68 |
| 16  | Aq    | 94/97 (97%)    | 91 (97%)  | 3 (3%)   | 46          | 81 |
| 16  | Bq    | 94/97 (97%)    | 91 (97%)  | 3 (3%)   | 46          | 81 |
| 17  | Ar    | 61/77 (79%)    | 60 (98%)  | 1 (2%)   | 70          | 90 |
| 17  | Br    | 61/77 (79%)    | 60 (98%)  | 1 (2%)   | 70          | 90 |
| 18  | As    | 69/80 (86%)    | 57 (83%)  | 12 (17%) | 2           | 17 |
| 18  | Bs    | 69/80 (86%)    | 57 (83%)  | 12 (17%) | 2           | 17 |
| 19  | At    | 76/82 (93%)    | 71 (93%)  | 5 (7%)   | 21          | 63 |
| 19  | Bt    | 76/82 (93%)    | 71 (93%)  | 5 (7%)   | 21          | 63 |
| 20  | Au    | 19/22 (86%)    | 18 (95%)  | 1 (5%)   | 28          | 69 |
| 20  | Bu    | 19/22 (86%)    | 18 (95%)  | 1 (5%)   | 28          | 69 |
| 21  | Ay    | 86/87 (99%)    | 75 (87%)  | 11 (13%) | 5           | 31 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 21  | By    | 86/87 (99%)    | 77 (90%)  | 9 (10%)  | 8           | 41 |
| 26  | AC    | 99/181 (55%)   | 92 (93%)  | 7 (7%)   | 18          | 59 |
| 26  | BC    | 99/181 (55%)   | 92 (93%)  | 7 (7%)   | 18          | 59 |
| 27  | AD    | 213/218 (98%)  | 178 (84%) | 35 (16%) | 3           | 20 |
| 27  | BD    | 213/218 (98%)  | 180 (84%) | 33 (16%) | 3           | 23 |
| 28  | AE    | 165/166 (99%)  | 135 (82%) | 30 (18%) | 2           | 14 |
| 28  | BE    | 165/166 (99%)  | 133 (81%) | 32 (19%) | 2           | 12 |
| 29  | AF    | 165/166 (99%)  | 143 (87%) | 22 (13%) | 5           | 30 |
| 29  | BF    | 165/166 (99%)  | 145 (88%) | 20 (12%) | 6           | 33 |
| 30  | AG    | 155/156 (99%)  | 137 (88%) | 18 (12%) | 7           | 36 |
| 30  | BG    | 155/156 (99%)  | 128 (83%) | 27 (17%) | 2           | 17 |
| 31  | AH    | 137/148 (93%)  | 123 (90%) | 14 (10%) | 9           | 42 |
| 31  | BH    | 137/148 (93%)  | 122 (89%) | 15 (11%) | 8           | 39 |
| 32  | AI    | 122/124 (98%)  | 103 (84%) | 19 (16%) | 3           | 23 |
| 32  | BI    | 122/124 (98%)  | 103 (84%) | 19 (16%) | 3           | 23 |
| 34  | AN    | 117/119 (98%)  | 102 (87%) | 15 (13%) | 5           | 31 |
| 34  | BN    | 117/119 (98%)  | 102 (87%) | 15 (13%) | 5           | 31 |
| 35  | AO    | 100/100 (100%) | 90 (90%)  | 10 (10%) | 9           | 43 |
| 35  | BO    | 100/100 (100%) | 89 (89%)  | 11 (11%) | 8           | 39 |
| 36  | AP    | 112/116 (97%)  | 93 (83%)  | 19 (17%) | 2           | 18 |
| 36  | BP    | 112/116 (97%)  | 92 (82%)  | 20 (18%) | 2           | 15 |
| 37  | AQ    | 110/111 (99%)  | 100 (91%) | 10 (9%)  | 12          | 48 |
| 37  | BQ    | 110/111 (99%)  | 100 (91%) | 10 (9%)  | 12          | 48 |
| 38  | AR    | 100/101 (99%)  | 86 (86%)  | 14 (14%) | 4           | 28 |
| 38  | BR    | 100/101 (99%)  | 86 (86%)  | 14 (14%) | 4           | 28 |
| 39  | AS    | 77/88 (88%)    | 63 (82%)  | 14 (18%) | 2           | 14 |
| 39  | BS    | 77/88 (88%)    | 63 (82%)  | 14 (18%) | 2           | 14 |
| 40  | AT    | 118/127 (93%)  | 99 (84%)  | 19 (16%) | 3           | 21 |
| 40  | BT    | 118/127 (93%)  | 99 (84%)  | 19 (16%) | 3           | 21 |
| 41  | AU    | 92/94 (98%)    | 79 (86%)  | 13 (14%) | 4           | 28 |
| 41  | BU    | 92/94 (98%)    | 79 (86%)  | 13 (14%) | 4           | 28 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |     |
|-----|-------|------------------|------------|------------|-------------|-----|
| 42  | AV    | 82/82 (100%)     | 66 (80%)   | 16 (20%)   | 2           | 12  |
| 42  | BV    | 82/82 (100%)     | 65 (79%)   | 17 (21%)   | 1           | 10  |
| 43  | AW    | 91/92 (99%)      | 80 (88%)   | 11 (12%)   | 6           | 33  |
| 43  | BW    | 91/92 (99%)      | 81 (89%)   | 10 (11%)   | 8           | 39  |
| 44  | AX    | 74/78 (95%)      | 64 (86%)   | 10 (14%)   | 5           | 29  |
| 44  | BX    | 74/78 (95%)      | 63 (85%)   | 11 (15%)   | 4           | 25  |
| 45  | AY    | 84/91 (92%)      | 68 (81%)   | 16 (19%)   | 2           | 12  |
| 45  | BY    | 84/91 (92%)      | 68 (81%)   | 16 (19%)   | 2           | 12  |
| 46  | AZ    | 162/179 (90%)    | 141 (87%)  | 21 (13%)   | 5           | 30  |
| 46  | BZ    | 162/179 (90%)    | 134 (83%)  | 28 (17%)   | 2           | 17  |
| 47  | A0    | 66/67 (98%)      | 59 (89%)   | 7 (11%)    | 8           | 40  |
| 47  | B0    | 66/67 (98%)      | 59 (89%)   | 7 (11%)    | 8           | 40  |
| 48  | A1    | 78/83 (94%)      | 66 (85%)   | 12 (15%)   | 3           | 23  |
| 48  | B1    | 78/83 (94%)      | 62 (80%)   | 16 (20%)   | 1           | 11  |
| 49  | A2    | 66/67 (98%)      | 63 (96%)   | 3 (4%)     | 34          | 74  |
| 49  | B2    | 66/67 (98%)      | 56 (85%)   | 10 (15%)   | 3           | 24  |
| 50  | A3    | 51/52 (98%)      | 46 (90%)   | 5 (10%)    | 10          | 44  |
| 50  | B3    | 51/52 (98%)      | 46 (90%)   | 5 (10%)    | 10          | 44  |
| 51  | A4    | 51/63 (81%)      | 41 (80%)   | 10 (20%)   | 1           | 12  |
| 51  | B4    | 51/63 (81%)      | 41 (80%)   | 10 (20%)   | 1           | 12  |
| 52  | A5    | 47/52 (90%)      | 42 (89%)   | 5 (11%)    | 8           | 40  |
| 52  | B5    | 47/52 (90%)      | 42 (89%)   | 5 (11%)    | 8           | 40  |
| 53  | A6    | 49/52 (94%)      | 40 (82%)   | 9 (18%)    | 2           | 14  |
| 53  | B6    | 49/52 (94%)      | 40 (82%)   | 9 (18%)    | 2           | 14  |
| 54  | A7    | 40/42 (95%)      | 37 (92%)   | 3 (8%)     | 17          | 57  |
| 54  | B7    | 40/42 (95%)      | 37 (92%)   | 3 (8%)     | 17          | 57  |
| 55  | A8    | 53/55 (96%)      | 42 (79%)   | 11 (21%)   | 1           | 10  |
| 55  | B8    | 53/55 (96%)      | 42 (79%)   | 11 (21%)   | 1           | 10  |
| 56  | A9    | 34/34 (100%)     | 34 (100%)  | 0          | 100         | 100 |
| 56  | B9    | 34/34 (100%)     | 34 (100%)  | 0          | 100         | 100 |
| All | All   | 9962/10602 (94%) | 8764 (88%) | 1198 (12%) | 6           | 33  |

5 of 1198 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | A3    | 8   | LEU  |
| 7   | Bh    | 1   | MET  |
| 46  | BZ    | 103 | ARG  |
| 52  | A5    | 25  | LEU  |
| 2   | Bc    | 18  | TRP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | A1    | 47  | GLN  |
| 4   | Be    | 72  | GLN  |
| 44  | BX    | 41  | ASN  |
| 50  | A3    | 46  | ASN  |
| 1   | Bb    | 40  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 22  | Aa    | 1503/1504 (99%) | 211 (14%)         | 0               |
| 22  | Ba    | 1503/1504 (99%) | 210 (13%)         | 0               |
| 23  | Ax    | 11/14 (78%)     | 8 (72%)           | 0               |
| 23  | Bx    | 11/14 (78%)     | 8 (72%)           | 0               |
| 24  | Av    | 76/77 (98%)     | 15 (19%)          | 0               |
| 24  | Bv    | 76/77 (98%)     | 17 (22%)          | 0               |
| 25  | Aw    | 76/77 (98%)     | 11 (14%)          | 0               |
| 25  | Bw    | 76/77 (98%)     | 8 (10%)           | 0               |
| 57  | AA    | 2847/2848 (99%) | 521 (18%)         | 55 (1%)         |
| 57  | BA    | 2847/2848 (99%) | 517 (18%)         | 56 (1%)         |
| 58  | AB    | 118/119 (99%)   | 21 (17%)          | 1 (0%)          |
| 58  | BB    | 118/119 (99%)   | 21 (17%)          | 1 (0%)          |
| All | All   | 9262/9278 (99%) | 1568 (16%)        | 113 (1%)        |

5 of 1568 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | Aa    | 9   | G    |
| 22  | Aa    | 31  | G    |
| 22  | Aa    | 32  | A    |
| 22  | Aa    | 39  | G    |
| 22  | Aa    | 47  | C    |

5 of 113 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 57  | AA    | 2439 | A    |
| 57  | BA    | 266  | G    |
| 57  | BA    | 2311 | A    |
| 57  | AA    | 2481 | G    |
| 57  | BA    | 71   | A    |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 24  | 5MU  | Av    | 54  | 24   | 12,22,23     | 1.40 | 3 (25%)     | 14,32,35    | 4.54 | 3 (21%)     |
| 23  | CCC  | Ax    | 21  | -    | 0,2,26       | 0.00 | -           | 0,1,41      | 0.00 | -           |
| 24  | 5MU  | Bv    | 54  | 24   | 12,22,23     | 1.33 | 3 (25%)     | 14,32,35    | 4.59 | 2 (14%)     |
| 23  | CCC  | Bx    | 21  | -    | 0,2,26       | 0.00 | -           | 0,1,41      | 0.00 | -           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 24  | 5MU  | Av    | 54  | 24   | -       | 0/3/25/26 | 0/2/2/2 |
| 23  | CCC  | Ax    | 21  | -    | -       | 0/0/0/36  | 0/0/0/3 |
| 24  | 5MU  | Bv    | 54  | 24   | -       | 0/3/25/26 | 0/2/2/2 |
| 23  | CCC  | Bx    | 21  | -    | -       | 0/0/0/36  | 0/0/0/3 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 24  | Bv    | 54  | 5MU  | C6-C5 | -2.32 | 1.33        | 1.40     |
| 24  | Av    | 54  | 5MU  | C6-C5 | -2.07 | 1.34        | 1.40     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 24  | Bv    | 54  | 5MU  | C6-N1 | 2.22 | 1.38        | 1.35     |
| 24  | Av    | 54  | 5MU  | C6-N1 | 2.57 | 1.38        | 1.35     |
| 24  | Bv    | 54  | 5MU  | C4-N3 | 2.90 | 1.38        | 1.33     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 24  | Bv    | 54  | 5MU  | C5-C4-N3  | -9.16 | 114.94      | 125.14   |
| 24  | Av    | 54  | 5MU  | C5-C4-N3  | -9.09 | 115.02      | 125.14   |
| 24  | Av    | 54  | 5MU  | C5M-C5-C6 | 2.06  | 122.77      | 118.62   |
| 24  | Av    | 54  | 5MU  | C4-N3-C2  | 14.11 | 127.44      | 115.25   |
| 24  | Bv    | 54  | 5MU  | C4-N3-C2  | 14.31 | 127.62      | 115.25   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1072 ligands modelled in this entry, 1072 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | Ab    | 234/256 (91%)  | 0.13   | 8 (3%) 49 35  | 114, 153, 181, 193    | 0     |
| 1   | Bb    | 234/256 (91%)  | 0.15   | 8 (3%) 49 35  | 113, 152, 181, 193    | 0     |
| 2   | Ac    | 206/239 (86%)  | 0.33   | 12 (5%) 26 18 | 123, 150, 166, 178    | 0     |
| 2   | Bc    | 206/239 (86%)  | 0.24   | 7 (3%) 49 35  | 124, 149, 166, 179    | 0     |
| 3   | Ad    | 208/209 (99%)  | -0.05  | 0 100 100     | 97, 119, 144, 155     | 0     |
| 3   | Bd    | 208/209 (99%)  | 0.06   | 1 (0%) 91 86  | 97, 119, 145, 154     | 0     |
| 4   | Ae    | 150/162 (92%)  | 0.09   | 3 (2%) 68 54  | 88, 114, 138, 159     | 0     |
| 4   | Be    | 150/162 (92%)  | 0.11   | 0 100 100     | 84, 112, 138, 160     | 0     |
| 5   | Af    | 101/101 (100%) | -0.11  | 2 (1%) 68 54  | 91, 121, 138, 155     | 0     |
| 5   | Bf    | 101/101 (100%) | -0.28  | 0 100 100     | 91, 120, 137, 155     | 0     |
| 6   | Ag    | 155/156 (99%)  | 0.14   | 10 (6%) 22 14 | 118, 137, 171, 188    | 0     |
| 6   | Bg    | 155/156 (99%)  | 0.27   | 10 (6%) 22 14 | 118, 138, 171, 188    | 0     |
| 7   | Ah    | 138/138 (100%) | -0.03  | 1 (0%) 89 81  | 96, 117, 132, 157     | 0     |
| 7   | Bh    | 138/138 (100%) | 0.01   | 1 (0%) 89 81  | 95, 116, 131, 158     | 0     |
| 8   | Ai    | 127/128 (99%)  | 0.73   | 15 (11%) 6 5  | 120, 160, 178, 186    | 0     |
| 8   | Bi    | 127/128 (99%)  | 0.84   | 15 (11%) 6 5  | 119, 160, 178, 186    | 0     |
| 9   | Aj    | 98/105 (93%)   | 0.90   | 19 (19%) 1 1  | 126, 164, 184, 190    | 0     |
| 9   | Bj    | 98/105 (93%)   | 0.89   | 14 (14%) 4 3  | 124, 164, 184, 190    | 0     |
| 10  | Ak    | 119/129 (92%)  | 0.07   | 6 (5%) 32 22  | 89, 117, 145, 171     | 0     |
| 10  | Bk    | 119/129 (92%)  | 0.08   | 6 (5%) 32 22  | 89, 117, 145, 171     | 0     |
| 11  | Al    | 124/132 (93%)  | 0.03   | 2 (1%) 74 61  | 75, 97, 123, 161      | 0     |
| 11  | Bl    | 124/132 (93%)  | 0.11   | 2 (1%) 74 61  | 77, 97, 125, 162      | 0     |
| 12  | Am    | 118/126 (93%)  | 0.29   | 9 (7%) 17 11  | 115, 143, 157, 166    | 0     |
| 12  | Bm    | 118/126 (93%)  | 0.33   | 5 (4%) 40 28  | 115, 142, 157, 166    | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 13  | An    | 60/61 (98%)      | 0.85   | 10 (16%) 2 2  | 126, 139, 159, 162    | 0     |
| 13  | Bn    | 60/61 (98%)      | 0.23   | 0 100 100     | 127, 138, 159, 162    | 0     |
| 14  | Ao    | 88/89 (98%)      | 0.07   | 0 100 100     | 81, 110, 131, 138     | 0     |
| 14  | Bo    | 88/89 (98%)      | -0.05  | 0 100 100     | 81, 110, 132, 137     | 0     |
| 15  | Ap    | 83/88 (94%)      | 0.29   | 1 (1%) 81 69  | 93, 110, 128, 148     | 0     |
| 15  | Bp    | 83/88 (94%)      | 0.49   | 5 (6%) 25 17  | 94, 111, 130, 147     | 0     |
| 16  | Aq    | 99/105 (94%)     | -0.02  | 0 100 100     | 80, 107, 124, 132     | 0     |
| 16  | Bq    | 99/105 (94%)     | -0.10  | 0 100 100     | 80, 107, 123, 132     | 0     |
| 17  | Ar    | 70/88 (79%)      | 0.36   | 4 (5%) 27 19  | 96, 122, 142, 158     | 0     |
| 17  | Br    | 70/88 (79%)      | 0.54   | 6 (8%) 13 10  | 95, 122, 141, 157     | 0     |
| 18  | As    | 78/93 (83%)      | 0.56   | 6 (7%) 16 11  | 131, 153, 173, 181    | 0     |
| 18  | Bs    | 78/93 (83%)      | 0.49   | 6 (7%) 16 11  | 130, 153, 172, 181    | 0     |
| 19  | At    | 99/106 (93%)     | 0.14   | 1 (1%) 84 73  | 86, 114, 145, 149     | 0     |
| 19  | Bt    | 99/106 (93%)     | 0.06   | 1 (1%) 84 73  | 86, 114, 145, 149     | 0     |
| 20  | Au    | 24/27 (88%)      | 2.27   | 11 (45%) 0 0  | 108, 138, 162, 168    | 0     |
| 20  | Bu    | 24/27 (88%)      | 1.05   | 3 (12%) 5 5   | 106, 137, 162, 168    | 0     |
| 21  | Ay    | 94/95 (98%)      | 0.89   | 14 (14%) 3 3  | 118, 154, 186, 189    | 0     |
| 21  | By    | 94/95 (98%)      | 0.94   | 11 (11%) 6 5  | 110, 146, 182, 188    | 0     |
| 22  | Aa    | 1504/1504 (100%) | 0.14   | 35 (2%) 64 48 | 65, 119, 193, 208     | 0     |
| 22  | Ba    | 1504/1504 (100%) | 0.11   | 29 (1%) 70 56 | 63, 119, 193, 208     | 0     |
| 23  | Ax    | 12/14 (85%)      | 1.64   | 3 (25%) 1 1   | 108, 191, 198, 199    | 0     |
| 23  | Bx    | 12/14 (85%)      | 2.09   | 6 (50%) 0 0   | 108, 191, 198, 199    | 0     |
| 24  | Av    | 76/77 (98%)      | -0.18  | 1 (1%) 79 66  | 96, 119, 161, 163     | 0     |
| 24  | Bv    | 76/77 (98%)      | -0.17  | 1 (1%) 79 66  | 69, 107, 141, 167     | 0     |
| 25  | Aw    | 77/77 (100%)     | 0.29   | 4 (5%) 31 22  | 103, 191, 201, 203    | 0     |
| 25  | Bw    | 77/77 (100%)     | 0.18   | 3 (3%) 43 31  | 93, 188, 200, 202     | 0     |
| 26  | AC    | 120/229 (52%)    | 1.71   | 43 (35%) 0 0  | 147, 177, 190, 193    | 0     |
| 26  | BC    | 120/229 (52%)    | 1.64   | 35 (29%) 1 1  | 145, 177, 189, 194    | 0     |
| 27  | AD    | 271/276 (98%)    | -0.17  | 2 (0%) 89 81  | 48, 76, 98, 121       | 0     |
| 27  | BD    | 271/276 (98%)    | -0.20  | 1 (0%) 93 88  | 46, 75, 96, 122       | 0     |
| 28  | AE    | 204/206 (99%)    | -0.09  | 2 (0%) 84 73  | 49, 81, 127, 149      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28  | BE    | 204/206 (99%)  | -0.02  | 4 (1%) 68 54 | 49, 80, 128, 148      | 0     |
| 29  | AF    | 207/210 (98%)  | -0.15  | 3 (1%) 78 65 | 48, 89, 153, 181      | 0     |
| 29  | BF    | 207/210 (98%)  | -0.11  | 4 (1%) 70 56 | 46, 86, 154, 180      | 0     |
| 30  | AG    | 181/182 (99%)  | 0.21   | 8 (4%) 38 27 | 117, 142, 161, 186    | 0     |
| 30  | BG    | 181/182 (99%)  | 0.08   | 5 (2%) 56 42 | 99, 128, 154, 175     | 0     |
| 31  | AH    | 164/180 (91%)  | 0.91   | 29 (17%) 2 2 | 98, 127, 143, 166     | 0     |
| 31  | BH    | 164/180 (91%)  | 0.24   | 7 (4%) 39 27 | 94, 124, 141, 164     | 0     |
| 32  | AI    | 145/148 (97%)  | 1.31   | 37 (25%) 1 1 | 81, 154, 171, 176     | 0     |
| 32  | BI    | 145/148 (97%)  | 0.55   | 15 (10%) 9 6 | 82, 153, 172, 176     | 0     |
| 33  | AJ    | 130/173 (75%)  | 2.75   | 66 (50%) 0 0 | 170, 195, 202, 203    | 0     |
| 33  | BJ    | 130/173 (75%)  | 1.45   | 40 (30%) 1 1 | 147, 180, 194, 196    | 0     |
| 34  | AN    | 138/140 (98%)  | 0.00   | 1 (0%) 89 81 | 65, 91, 126, 138      | 0     |
| 34  | BN    | 138/140 (98%)  | -0.10  | 0 100 100    | 63, 88, 126, 136      | 0     |
| 35  | AO    | 122/122 (100%) | -0.28  | 0 100 100    | 59, 75, 98, 122       | 0     |
| 35  | BO    | 122/122 (100%) | -0.27  | 0 100 100    | 56, 74, 99, 120       | 0     |
| 36  | AP    | 146/150 (97%)  | 0.21   | 4 (2%) 58 43 | 51, 106, 133, 169     | 0     |
| 36  | BP    | 146/150 (97%)  | 0.20   | 3 (2%) 67 52 | 50, 104, 133, 169     | 0     |
| 37  | AQ    | 140/141 (99%)  | -0.03  | 1 (0%) 89 81 | 75, 96, 124, 147      | 0     |
| 37  | BQ    | 140/141 (99%)  | 0.00   | 1 (0%) 89 81 | 74, 94, 125, 147      | 0     |
| 38  | AR    | 117/118 (99%)  | -0.21  | 0 100 100    | 48, 80, 108, 128      | 0     |
| 38  | BR    | 117/118 (99%)  | -0.14  | 0 100 100    | 47, 79, 107, 127      | 0     |
| 39  | AS    | 98/112 (87%)   | 0.69   | 12 (12%) 5 5 | 111, 137, 154, 161    | 0     |
| 39  | BS    | 98/112 (87%)   | 0.86   | 13 (13%) 4 4 | 110, 136, 153, 162    | 0     |
| 40  | AT    | 135/146 (92%)  | -0.16  | 3 (2%) 65 50 | 66, 92, 150, 183      | 0     |
| 40  | BT    | 135/146 (92%)  | -0.02  | 3 (2%) 65 50 | 66, 92, 150, 183      | 0     |
| 41  | AU    | 117/118 (99%)  | -0.21  | 1 (0%) 85 75 | 58, 81, 117, 156      | 0     |
| 41  | BU    | 117/118 (99%)  | -0.25  | 0 100 100    | 52, 78, 116, 158      | 0     |
| 42  | AV    | 101/101 (100%) | 0.08   | 1 (0%) 84 73 | 59, 106, 125, 134     | 0     |
| 42  | BV    | 101/101 (100%) | -0.02  | 1 (0%) 84 73 | 54, 103, 125, 134     | 0     |
| 43  | AW    | 113/113 (100%) | -0.16  | 1 (0%) 85 75 | 58, 73, 106, 183      | 0     |
| 43  | BW    | 113/113 (100%) | -0.15  | 1 (0%) 85 75 | 55, 71, 105, 183      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | AX    | 92/96 (95%)       | -0.18  | 0 100 100      | 63, 86, 110, 120      | 0     |
| 44  | BX    | 92/96 (95%)       | -0.04  | 0 100 100      | 56, 84, 110, 120      | 0     |
| 45  | AY    | 100/110 (90%)     | 0.92   | 14 (14%) 4 3   | 78, 117, 153, 160     | 0     |
| 45  | BY    | 100/110 (90%)     | 0.39   | 5 (5%) 32 22   | 74, 115, 152, 158     | 0     |
| 46  | AZ    | 184/206 (89%)     | 0.18   | 11 (5%) 25 17  | 117, 141, 158, 188    | 0     |
| 46  | BZ    | 184/206 (89%)     | 0.19   | 5 (2%) 58 43   | 87, 126, 150, 173     | 0     |
| 47  | A0    | 84/85 (98%)       | 0.52   | 5 (5%) 25 17   | 81, 100, 148, 168     | 0     |
| 47  | B0    | 84/85 (98%)       | 0.47   | 6 (7%) 19 12   | 78, 100, 148, 168     | 0     |
| 48  | A1    | 93/98 (94%)       | 0.09   | 2 (2%) 65 50   | 64, 87, 127, 137      | 0     |
| 48  | B1    | 93/98 (94%)       | 0.10   | 0 100 100      | 55, 82, 119, 133      | 0     |
| 49  | A2    | 71/72 (98%)       | -0.27  | 0 100 100      | 81, 116, 134, 156     | 0     |
| 49  | B2    | 71/72 (98%)       | -0.31  | 0 100 100      | 51, 85, 123, 159      | 0     |
| 50  | A3    | 59/60 (98%)       | 0.55   | 2 (3%) 49 35   | 70, 94, 112, 162      | 0     |
| 50  | B3    | 59/60 (98%)       | 0.21   | 2 (3%) 49 35   | 62, 91, 111, 162      | 0     |
| 51  | A4    | 57/71 (80%)       | -0.05  | 0 100 100      | 150, 164, 175, 177    | 0     |
| 51  | B4    | 57/71 (80%)       | 0.03   | 3 (5%) 30 21   | 150, 164, 174, 177    | 0     |
| 52  | A5    | 55/60 (91%)       | -0.27  | 2 (3%) 46 33   | 54, 80, 113, 119      | 0     |
| 52  | B5    | 55/60 (91%)       | -0.28  | 1 (1%) 71 58   | 54, 78, 112, 121      | 0     |
| 53  | A6    | 50/54 (92%)       | 1.89   | 25 (50%) 0 0   | 121, 149, 165, 175    | 0     |
| 53  | B6    | 50/54 (92%)       | 1.92   | 26 (52%) 0 0   | 121, 149, 164, 176    | 0     |
| 54  | A7    | 47/49 (95%)       | -0.01  | 0 100 100      | 50, 64, 86, 133       | 0     |
| 54  | B7    | 47/49 (95%)       | -0.09  | 0 100 100      | 47, 60, 84, 131       | 0     |
| 55  | A8    | 63/65 (96%)       | 0.17   | 0 100 100      | 66, 83, 117, 146      | 0     |
| 55  | B8    | 63/65 (96%)       | 0.04   | 0 100 100      | 63, 83, 116, 145      | 0     |
| 56  | A9    | 37/37 (100%)      | 1.67   | 15 (40%) 0 0   | 121, 134, 149, 151    | 0     |
| 56  | B9    | 37/37 (100%)      | 2.25   | 21 (56%) 0 0   | 121, 132, 148, 152    | 0     |
| 57  | AA    | 2848/2848 (100%)  | -0.04  | 62 (2%) 65 50  | 47, 83, 185, 208      | 0     |
| 57  | BA    | 2848/2848 (100%)  | 0.07   | 44 (1%) 76 64  | 44, 80, 185, 208      | 0     |
| 58  | AB    | 119/119 (100%)    | -0.06  | 4 (3%) 49 35   | 90, 143, 176, 196     | 0     |
| 58  | BB    | 119/119 (100%)    | 0.05   | 2 (1%) 73 59   | 86, 142, 175, 197     | 0     |
| All | All   | 21500/22400 (95%) | 0.17   | 921 (4%) 39 27 | 44, 108, 181, 208     | 0     |

The worst 5 of 921 RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 22  | Ba    | 89     | C    | 13.9 |
| 32  | BI    | 88     | ILE  | 11.1 |
| 57  | BA    | 277    | C    | 11.1 |
| 22  | Aa    | 89     | C    | 10.8 |
| 57  | AA    | 654(E) | G    | 10.6 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 23  | CCC  | Bx    | 21  | 3/24  | 0.95 | 0.61 | -    | 20,20,20,20                | 0     |
| 23  | CCC  | Ax    | 21  | 3/24  | 0.88 | 0.57 | -    | 20,20,20,20                | 0     |
| 24  | 5MU  | Av    | 54  | 21/22 | 0.90 | 0.19 | -    | 130,133,148,148            | 0     |
| 24  | 5MU  | Bv    | 54  | 21/22 | 0.93 | 0.16 | -    | 114,116,124,125            | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|----------------------------|-------|
| 60  | MG   | Aa    | 1645 | 1/1   | 0.54 | 1.51 | 134.62 | 79,79,79,79                | 0     |
| 60  | MG   | AA    | 2968 | 1/1   | 0.31 | 1.47 | 77.90  | 76,76,76,76                | 0     |
| 60  | MG   | AA    | 3243 | 1/1   | 0.93 | 1.21 | 63.51  | 79,79,79,79                | 0     |
| 60  | MG   | BA    | 3254 | 1/1   | 0.57 | 0.88 | 62.24  | 66,66,66,66                | 0     |
| 60  | MG   | BA    | 3013 | 1/1   | 0.95 | 0.98 | 50.84  | 50,50,50,50                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 60  | MG   | BA    | 3131 | 1/1   | 0.89 | 0.63 | 48.79 | 96,96,96,96                | 0     |
| 60  | MG   | Aa    | 1631 | 1/1   | 0.77 | 1.14 | 47.80 | 72,72,72,72                | 0     |
| 60  | MG   | Ba    | 1630 | 1/1   | 0.77 | 0.82 | 44.69 | 76,76,76,76                | 0     |
| 60  | MG   | Ba    | 1644 | 1/1   | 0.49 | 1.03 | 37.39 | 67,67,67,67                | 0     |
| 60  | MG   | AA    | 3245 | 1/1   | 0.18 | 0.92 | 37.18 | 97,97,97,97                | 0     |
| 60  | MG   | AA    | 3097 | 1/1   | 0.80 | 0.42 | 35.72 | 43,43,43,43                | 0     |
| 60  | MG   | AA    | 3261 | 1/1   | 0.54 | 0.84 | 35.57 | 76,76,76,76                | 0     |
| 60  | MG   | Ba    | 1724 | 1/1   | 0.87 | 0.68 | 35.39 | 68,68,68,68                | 0     |
| 60  | MG   | AA    | 3197 | 1/1   | 0.96 | 0.49 | 35.26 | 22,22,22,22                | 0     |
| 60  | MG   | BA    | 3187 | 1/1   | 0.87 | 0.66 | 33.42 | 36,36,36,36                | 0     |
| 60  | MG   | Aa    | 1727 | 1/1   | 0.17 | 1.24 | 33.34 | 98,98,98,98                | 1     |
| 60  | MG   | Ba    | 1621 | 1/1   | 0.73 | 1.12 | 33.02 | 82,82,82,82                | 0     |
| 60  | MG   | AA    | 3011 | 1/1   | 0.95 | 0.61 | 30.54 | 14,14,14,14                | 0     |
| 60  | MG   | AA    | 3147 | 1/1   | 0.53 | 0.47 | 29.68 | 79,79,79,79                | 0     |
| 60  | MG   | Ba    | 1684 | 1/1   | 0.93 | 0.68 | 28.34 | 75,75,75,75                | 0     |
| 60  | MG   | BA    | 2905 | 1/1   | 0.93 | 0.53 | 26.77 | 29,29,29,29                | 0     |
| 60  | MG   | AA    | 3023 | 1/1   | 0.99 | 0.54 | 25.78 | 13,13,13,13                | 0     |
| 60  | MG   | BA    | 2995 | 1/1   | 0.94 | 0.53 | 25.31 | 14,14,14,14                | 0     |
| 60  | MG   | AA    | 3044 | 1/1   | 0.92 | 0.86 | 25.05 | 17,17,17,17                | 0     |
| 60  | MG   | Ba    | 1726 | 1/1   | 0.93 | 0.73 | 23.71 | 34,34,34,34                | 1     |
| 60  | MG   | AA    | 3069 | 1/1   | 0.94 | 0.57 | 22.62 | 68,68,68,68                | 0     |
| 60  | MG   | AA    | 2931 | 1/1   | 0.95 | 0.60 | 22.47 | 35,35,35,35                | 0     |
| 60  | MG   | Ba    | 1685 | 1/1   | 0.93 | 0.83 | 22.18 | 25,25,25,25                | 1     |
| 60  | MG   | AA    | 2980 | 1/1   | 0.82 | 0.64 | 22.16 | 69,69,69,69                | 0     |
| 60  | MG   | Aa    | 1725 | 1/1   | 0.72 | 0.63 | 21.85 | 74,74,74,74                | 0     |
| 60  | MG   | BA    | 3084 | 1/1   | 0.97 | 0.41 | 21.54 | 34,34,34,34                | 0     |
| 60  | MG   | BA    | 2912 | 1/1   | 0.97 | 0.60 | 21.09 | 37,37,37,37                | 0     |
| 60  | MG   | AA    | 3190 | 1/1   | 0.81 | 0.49 | 20.59 | 43,43,43,43                | 0     |
| 60  | MG   | BA    | 3010 | 1/1   | 0.85 | 0.50 | 20.10 | 13,13,13,13                | 0     |
| 60  | MG   | BA    | 3257 | 1/1   | 0.48 | 0.41 | 20.09 | 72,72,72,72                | 0     |
| 60  | MG   | BA    | 3150 | 1/1   | 0.66 | 0.64 | 19.55 | 76,76,76,76                | 0     |
| 60  | MG   | Ba    | 1739 | 1/1   | 0.93 | 0.51 | 18.96 | 53,53,53,53                | 0     |
| 60  | MG   | AA    | 2987 | 1/1   | 0.93 | 0.37 | 18.79 | 53,53,53,53                | 0     |
| 60  | MG   | AA    | 3099 | 1/1   | 0.85 | 0.66 | 18.74 | 57,57,57,57                | 0     |
| 60  | MG   | BA    | 2917 | 1/1   | 0.84 | 0.65 | 18.31 | 23,23,23,23                | 0     |
| 60  | MG   | BA    | 2913 | 1/1   | 0.96 | 0.43 | 18.24 | 11,11,11,11                | 0     |
| 60  | MG   | BA    | 3038 | 1/1   | 0.97 | 0.43 | 18.17 | 26,26,26,26                | 0     |
| 60  | MG   | BA    | 3055 | 1/1   | 0.98 | 0.45 | 17.86 | 7,7,7,7                    | 0     |
| 60  | MG   | BA    | 3236 | 1/1   | 0.49 | 0.54 | 17.75 | 116,116,116,116            | 0     |
| 60  | MG   | BA    | 3231 | 1/1   | 0.90 | 0.66 | 17.63 | 64,64,64,64                | 0     |
| 60  | MG   | AA    | 3259 | 1/1   | 0.74 | 0.62 | 17.35 | 78,78,78,78                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60  | MG   | BA    | 3052 | 1/1   | 0.95 | 0.48 | 17.14 | 10,10,10,10                 | 0     |
| 60  | MG   | BA    | 3035 | 1/1   | 0.94 | 0.54 | 16.62 | 52,52,52,52                 | 0     |
| 60  | MG   | BA    | 3241 | 1/1   | 0.87 | 0.52 | 16.53 | 49,49,49,49                 | 0     |
| 60  | MG   | AA    | 3179 | 1/1   | 0.83 | 0.67 | 16.23 | 56,56,56,56                 | 0     |
| 60  | MG   | AA    | 3028 | 1/1   | 0.88 | 0.64 | 16.12 | 60,60,60,60                 | 0     |
| 60  | MG   | Aa    | 1633 | 1/1   | 0.95 | 0.68 | 15.92 | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 3102 | 1/1   | 0.70 | 0.70 | 15.92 | 68,68,68,68                 | 0     |
| 60  | MG   | AA    | 3096 | 1/1   | 0.90 | 0.52 | 15.38 | 73,73,73,73                 | 0     |
| 60  | MG   | BA    | 3211 | 1/1   | 0.92 | 0.33 | 15.17 | 24,24,24,24                 | 0     |
| 60  | MG   | BA    | 3160 | 1/1   | 0.81 | 0.47 | 14.85 | 74,74,74,74                 | 0     |
| 60  | MG   | BA    | 2967 | 1/1   | 0.96 | 0.51 | 14.63 | 20,20,20,20                 | 0     |
| 60  | MG   | BA    | 2962 | 1/1   | 0.64 | 0.50 | 14.62 | 54,54,54,54                 | 0     |
| 60  | MG   | BA    | 3120 | 1/1   | 0.98 | 0.44 | 14.52 | 16,16,16,16                 | 0     |
| 60  | MG   | Ba    | 1654 | 1/1   | 0.80 | 0.37 | 14.44 | 50,50,50,50                 | 0     |
| 60  | MG   | BA    | 2980 | 1/1   | 0.90 | 0.49 | 14.09 | 9,9,9,9                     | 0     |
| 60  | MG   | AA    | 2909 | 1/1   | 0.85 | 0.46 | 14.06 | 41,41,41,41                 | 0     |
| 60  | MG   | AA    | 3072 | 1/1   | 0.86 | 0.47 | 13.71 | 122,122,122,122             | 0     |
| 60  | MG   | Aa    | 1622 | 1/1   | 0.71 | 0.98 | 13.69 | 79,79,79,79                 | 0     |
| 60  | MG   | AA    | 3177 | 1/1   | 0.96 | 0.45 | 13.64 | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3150 | 1/1   | 0.85 | 0.70 | 13.56 | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 2964 | 1/1   | 0.28 | 0.49 | 13.55 | 65,65,65,65                 | 0     |
| 60  | MG   | AA    | 2996 | 1/1   | 0.89 | 0.51 | 13.54 | 40,40,40,40                 | 0     |
| 60  | MG   | Ba    | 1691 | 1/1   | 0.88 | 0.67 | 13.40 | 58,58,58,58                 | 0     |
| 60  | MG   | AA    | 3056 | 1/1   | 0.91 | 0.45 | 13.05 | 19,19,19,19                 | 0     |
| 60  | MG   | BA    | 3101 | 1/1   | 0.67 | 0.59 | 13.02 | 52,52,52,52                 | 0     |
| 60  | MG   | BA    | 3027 | 1/1   | 0.60 | 0.44 | 12.86 | 43,43,43,43                 | 0     |
| 60  | MG   | AA    | 2928 | 1/1   | 0.71 | 0.50 | 12.74 | 110,110,110,110             | 0     |
| 60  | MG   | BA    | 3123 | 1/1   | 0.97 | 0.51 | 12.71 | 2,2,2,2                     | 0     |
| 60  | MG   | AA    | 3095 | 1/1   | 0.95 | 0.70 | 12.59 | 26,26,26,26                 | 0     |
| 60  | MG   | BA    | 3053 | 1/1   | 0.98 | 0.35 | 12.51 | 12,12,12,12                 | 0     |
| 60  | MG   | AA    | 2918 | 1/1   | 0.94 | 0.59 | 12.50 | 25,25,25,25                 | 0     |
| 60  | MG   | AA    | 3247 | 1/1   | 0.92 | 0.29 | 12.50 | 103,103,103,103             | 0     |
| 60  | MG   | AA    | 3124 | 1/1   | 0.99 | 0.40 | 12.47 | 15,15,15,15                 | 0     |
| 60  | MG   | BA    | 2968 | 1/1   | 0.95 | 0.37 | 12.20 | 69,69,69,69                 | 0     |
| 60  | MG   | AA    | 2969 | 1/1   | 0.98 | 0.28 | 12.19 | 22,22,22,22                 | 0     |
| 60  | MG   | AA    | 3126 | 1/1   | 0.44 | 0.55 | 12.09 | 47,47,47,47                 | 0     |
| 60  | MG   | BA    | 3034 | 1/1   | 0.97 | 0.39 | 11.99 | 11,11,11,11                 | 0     |
| 60  | MG   | BA    | 2979 | 1/1   | 0.89 | 0.43 | 11.89 | 55,55,55,55                 | 0     |
| 60  | MG   | BA    | 3100 | 1/1   | 0.93 | 0.42 | 11.86 | 62,62,62,62                 | 0     |
| 60  | MG   | BA    | 2930 | 1/1   | 0.98 | 0.40 | 11.72 | 28,28,28,28                 | 0     |
| 60  | MG   | BA    | 3094 | 1/1   | 0.94 | 0.63 | 11.64 | 11,11,11,11                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60  | MG   | AA    | 3025 | 1/1   | 0.84 | 0.41 | 11.60 | 26,26,26,26                 | 0     |
| 60  | MG   | Aa    | 1662 | 1/1   | 0.70 | 0.48 | 11.34 | 73,73,73,73                 | 0     |
| 60  | MG   | BA    | 3156 | 1/1   | 0.94 | 0.42 | 11.32 | 29,29,29,29                 | 0     |
| 60  | MG   | AA    | 2981 | 1/1   | 0.92 | 0.51 | 11.29 | 13,13,13,13                 | 0     |
| 60  | MG   | AA    | 2932 | 1/1   | 0.86 | 0.68 | 11.11 | 57,57,57,57                 | 0     |
| 60  | MG   | BA    | 3024 | 1/1   | 0.78 | 0.43 | 10.88 | 24,24,24,24                 | 0     |
| 60  | MG   | AA    | 2976 | 1/1   | 0.93 | 0.47 | 10.73 | 46,46,46,46                 | 0     |
| 60  | MG   | Aa    | 1729 | 1/1   | 0.93 | 0.41 | 10.64 | 30,30,30,30                 | 0     |
| 60  | MG   | BA    | 3043 | 1/1   | 0.95 | 0.52 | 10.61 | 17,17,17,17                 | 0     |
| 60  | MG   | Aa    | 1679 | 1/1   | 0.28 | 0.58 | 10.46 | 116,116,116,116             | 0     |
| 60  | MG   | Ba    | 1728 | 1/1   | 0.80 | 0.43 | 10.40 | 30,30,30,30                 | 0     |
| 60  | MG   | Ba    | 1634 | 1/1   | 0.95 | 0.38 | 10.35 | 37,37,37,37                 | 0     |
| 60  | MG   | Aa    | 1666 | 1/1   | 0.87 | 0.39 | 10.09 | 61,61,61,61                 | 0     |
| 60  | MG   | AA    | 3221 | 1/1   | 0.79 | 0.44 | 10.02 | 47,47,47,47                 | 0     |
| 60  | MG   | AA    | 2949 | 1/1   | 0.82 | 0.44 | 9.99  | 41,41,41,41                 | 0     |
| 60  | MG   | BA    | 2931 | 1/1   | 0.76 | 0.41 | 9.91  | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 2925 | 1/1   | 0.84 | 0.36 | 9.80  | 79,79,79,79                 | 0     |
| 60  | MG   | AA    | 2906 | 1/1   | 0.94 | 0.53 | 9.79  | 25,25,25,25                 | 0     |
| 60  | MG   | AA    | 3205 | 1/1   | 0.50 | 0.50 | 9.57  | 51,51,51,51                 | 0     |
| 60  | MG   | BA    | 2990 | 1/1   | 0.96 | 0.42 | 9.45  | 10,10,10,10                 | 0     |
| 60  | MG   | AA    | 3051 | 1/1   | 0.70 | 0.34 | 9.39  | 81,81,81,81                 | 0     |
| 60  | MG   | BA    | 3171 | 1/1   | 0.76 | 0.49 | 9.35  | 69,69,69,69                 | 0     |
| 60  | MG   | AA    | 3256 | 1/1   | 0.69 | 0.44 | 9.27  | 71,71,71,71                 | 0     |
| 60  | MG   | AA    | 2920 | 1/1   | 0.98 | 0.43 | 9.26  | 22,22,22,22                 | 0     |
| 60  | MG   | AA    | 3101 | 1/1   | 0.89 | 0.26 | 9.02  | 46,46,46,46                 | 0     |
| 60  | MG   | Ba    | 1742 | 1/1   | 0.94 | 0.42 | 8.92  | 92,92,92,92                 | 0     |
| 60  | MG   | BA    | 2987 | 1/1   | 0.95 | 0.35 | 8.91  | 9,9,9,9                     | 0     |
| 60  | MG   | AA    | 3133 | 1/1   | 0.55 | 0.31 | 8.90  | 48,48,48,48                 | 0     |
| 60  | MG   | A7    | 101  | 1/1   | 0.73 | 0.62 | 8.88  | 80,80,80,80                 | 0     |
| 60  | MG   | BA    | 2996 | 1/1   | 0.96 | 0.42 | 8.74  | 18,18,18,18                 | 0     |
| 60  | MG   | BA    | 2982 | 1/1   | 0.97 | 0.39 | 8.54  | 4,4,4,4                     | 0     |
| 60  | MG   | AA    | 3172 | 1/1   | 0.96 | 0.41 | 8.41  | 38,38,38,38                 | 0     |
| 60  | MG   | AA    | 3134 | 1/1   | 0.76 | 0.32 | 8.37  | 98,98,98,98                 | 0     |
| 60  | MG   | AA    | 3088 | 1/1   | 0.53 | 0.33 | 8.30  | 85,85,85,85                 | 0     |
| 60  | MG   | BA    | 3095 | 1/1   | 0.81 | 0.35 | 8.23  | 33,33,33,33                 | 0     |
| 60  | MG   | BA    | 3165 | 1/1   | 0.42 | 0.35 | 8.14  | 67,67,67,67                 | 0     |
| 60  | MG   | Aa    | 1686 | 1/1   | 0.82 | 0.30 | 8.12  | 37,37,37,37                 | 1     |
| 60  | MG   | AA    | 3138 | 1/1   | 0.95 | 0.31 | 8.12  | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 3093 | 1/1   | 0.58 | 0.48 | 8.05  | 61,61,61,61                 | 0     |
| 60  | MG   | BA    | 3172 | 1/1   | 0.94 | 0.50 | 8.05  | 50,50,50,50                 | 0     |
| 60  | MG   | AA    | 3054 | 1/1   | 0.97 | 0.40 | 8.04  | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | BA    | 2927 | 1/1   | 0.92 | 0.39 | 7.94 | 83,83,83,83                 | 0     |
| 60  | MG   | BA    | 3018 | 1/1   | 0.99 | 0.30 | 7.89 | 2,2,2,2                     | 0     |
| 60  | MG   | BA    | 3134 | 1/1   | 0.94 | 0.40 | 7.87 | 52,52,52,52                 | 0     |
| 60  | MG   | Ae    | 202  | 1/1   | 0.57 | 0.96 | 7.85 | 89,89,89,89                 | 0     |
| 60  | MG   | AA    | 3039 | 1/1   | 0.96 | 0.29 | 7.83 | 19,19,19,19                 | 0     |
| 60  | MG   | AA    | 3038 | 1/1   | 0.80 | 0.35 | 7.75 | 64,64,64,64                 | 0     |
| 60  | MG   | AA    | 3265 | 1/1   | 0.48 | 0.41 | 7.60 | 70,70,70,70                 | 0     |
| 60  | MG   | BA    | 2984 | 1/1   | 0.96 | 0.41 | 7.55 | 22,22,22,22                 | 0     |
| 60  | MG   | AA    | 2997 | 1/1   | 0.93 | 0.26 | 7.51 | 43,43,43,43                 | 0     |
| 60  | MG   | AA    | 2991 | 1/1   | 0.94 | 0.48 | 7.41 | 19,19,19,19                 | 0     |
| 60  | MG   | Ba    | 1608 | 1/1   | 0.90 | 0.48 | 7.31 | 79,79,79,79                 | 0     |
| 60  | MG   | AA    | 2921 | 1/1   | 0.96 | 0.31 | 7.25 | 50,50,50,50                 | 0     |
| 60  | MG   | BA    | 2908 | 1/1   | 0.94 | 0.39 | 7.21 | 20,20,20,20                 | 0     |
| 60  | MG   | Aa    | 1624 | 1/1   | 0.99 | 0.26 | 7.09 | 37,37,37,37                 | 0     |
| 60  | MG   | AA    | 2913 | 1/1   | 0.92 | 0.50 | 7.07 | 22,22,22,22                 | 0     |
| 60  | MG   | Bv    | 105  | 1/1   | 0.86 | 0.33 | 7.05 | 81,81,81,81                 | 1     |
| 60  | MG   | BA    | 3011 | 1/1   | 0.98 | 0.42 | 7.03 | 11,11,11,11                 | 0     |
| 60  | MG   | BA    | 2951 | 1/1   | 0.86 | 0.30 | 7.00 | 72,72,72,72                 | 0     |
| 60  | MG   | Aa    | 1744 | 1/1   | 0.90 | 0.34 | 6.94 | 87,87,87,87                 | 0     |
| 60  | MG   | BA    | 3069 | 1/1   | 0.84 | 0.33 | 6.87 | 35,35,35,35                 | 0     |
| 60  | MG   | AA    | 3019 | 1/1   | 1.00 | 0.33 | 6.78 | 26,26,26,26                 | 0     |
| 60  | MG   | Av    | 102  | 1/1   | 0.97 | 0.36 | 6.54 | 77,77,77,77                 | 0     |
| 60  | MG   | AA    | 2915 | 1/1   | 0.94 | 0.34 | 6.31 | 21,21,21,21                 | 0     |
| 60  | MG   | AA    | 2907 | 1/1   | 0.97 | 0.24 | 6.28 | 48,48,48,48                 | 0     |
| 60  | MG   | AA    | 3061 | 1/1   | 0.89 | 0.38 | 6.24 | 42,42,42,42                 | 0     |
| 60  | MG   | BA    | 2914 | 1/1   | 0.98 | 0.27 | 6.17 | 11,11,11,11                 | 0     |
| 60  | MG   | BA    | 3176 | 1/1   | 0.75 | 0.40 | 6.11 | 48,48,48,48                 | 0     |
| 60  | MG   | BA    | 2957 | 1/1   | 0.99 | 0.40 | 5.85 | 13,13,13,13                 | 0     |
| 60  | MG   | Ba    | 1671 | 1/1   | 0.91 | 0.32 | 5.84 | 87,87,87,87                 | 0     |
| 60  | MG   | AA    | 3236 | 1/1   | 0.88 | 0.37 | 5.83 | 90,90,90,90                 | 0     |
| 60  | MG   | Aa    | 1611 | 1/1   | 0.88 | 0.78 | 5.82 | 60,60,60,60                 | 0     |
| 60  | MG   | BA    | 3029 | 1/1   | 0.92 | 0.33 | 5.82 | 27,27,27,27                 | 0     |
| 60  | MG   | BA    | 3194 | 1/1   | 0.94 | 0.37 | 5.79 | 12,12,12,12                 | 0     |
| 60  | MG   | BA    | 3102 | 1/1   | 0.92 | 0.24 | 5.73 | 47,47,47,47                 | 0     |
| 60  | MG   | AA    | 2919 | 1/1   | 0.91 | 0.31 | 5.73 | 36,36,36,36                 | 0     |
| 60  | MG   | Aa    | 1635 | 1/1   | 0.92 | 0.29 | 5.71 | 39,39,39,39                 | 0     |
| 60  | MG   | AA    | 3046 | 1/1   | 0.97 | 0.40 | 5.69 | 47,47,47,47                 | 0     |
| 60  | MG   | BA    | 3091 | 1/1   | 0.95 | 0.37 | 5.60 | 32,32,32,32                 | 0     |
| 60  | MG   | B7    | 101  | 1/1   | 0.86 | 0.31 | 5.58 | 36,36,36,36                 | 0     |
| 60  | MG   | AA    | 2943 | 1/1   | 0.82 | 0.30 | 5.49 | 70,70,70,70                 | 0     |
| 60  | MG   | AA    | 3163 | 1/1   | 0.76 | 0.32 | 5.46 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3035 | 1/1   | 0.94 | 0.29 | 5.38 | 21,21,21,21                 | 0     |
| 60  | MG   | AA    | 3121 | 1/1   | 0.95 | 0.41 | 5.31 | 31,31,31,31                 | 0     |
| 60  | MG   | AA    | 3233 | 1/1   | 0.90 | 0.35 | 5.09 | 44,44,44,44                 | 0     |
| 60  | MG   | BA    | 3022 | 1/1   | 0.98 | 0.29 | 5.01 | 16,16,16,16                 | 0     |
| 60  | MG   | BA    | 3097 | 1/1   | 0.81 | 0.26 | 5.01 | 54,54,54,54                 | 0     |
| 60  | MG   | AA    | 3175 | 1/1   | 0.86 | 0.48 | 4.91 | 40,40,40,40                 | 0     |
| 60  | MG   | AA    | 2951 | 1/1   | 0.75 | 0.29 | 4.85 | 53,53,53,53                 | 0     |
| 60  | MG   | Aa    | 1735 | 1/1   | 0.81 | 0.26 | 4.74 | 68,68,68,68                 | 1     |
| 60  | MG   | Ba    | 1609 | 1/1   | 0.69 | 0.84 | 4.60 | 74,74,74,74                 | 0     |
| 60  | MG   | Aa    | 1674 | 1/1   | 0.62 | 0.32 | 4.56 | 90,90,90,90                 | 0     |
| 60  | MG   | Aa    | 1738 | 1/1   | 0.95 | 0.28 | 4.52 | 55,55,55,55                 | 0     |
| 60  | MG   | BD    | 301  | 1/1   | 0.94 | 0.32 | 4.50 | 14,14,14,14                 | 0     |
| 60  | MG   | BA    | 2965 | 1/1   | 0.79 | 0.30 | 4.50 | 58,58,58,58                 | 0     |
| 60  | MG   | BA    | 2966 | 1/1   | 0.50 | 0.30 | 4.49 | 67,67,67,67                 | 0     |
| 60  | MG   | AA    | 3158 | 1/1   | 0.89 | 0.30 | 4.32 | 46,46,46,46                 | 0     |
| 60  | MG   | AA    | 3219 | 1/1   | 0.96 | 0.48 | 4.26 | 30,30,30,30                 | 0     |
| 60  | MG   | Aa    | 1628 | 1/1   | 0.89 | 0.30 | 4.21 | 92,92,92,92                 | 0     |
| 60  | MG   | AA    | 3231 | 1/1   | 0.92 | 0.25 | 4.17 | 51,51,51,51                 | 0     |
| 60  | MG   | BA    | 3133 | 1/1   | 0.85 | 0.27 | 4.13 | 54,54,54,54                 | 0     |
| 60  | MG   | BA    | 3183 | 1/1   | 0.84 | 0.23 | 4.10 | 44,44,44,44                 | 0     |
| 60  | MG   | BA    | 3060 | 1/1   | 0.97 | 0.37 | 4.09 | 16,16,16,16                 | 0     |
| 60  | MG   | BA    | 3127 | 1/1   | 0.99 | 0.52 | 4.08 | 20,20,20,20                 | 0     |
| 60  | MG   | AA    | 2960 | 1/1   | 0.79 | 0.33 | 4.08 | 17,17,17,17                 | 0     |
| 60  | MG   | BA    | 3088 | 1/1   | 0.62 | 0.39 | 4.07 | 107,107,107,107             | 0     |
| 60  | MG   | AA    | 2953 | 1/1   | 0.96 | 0.27 | 4.04 | 96,96,96,96                 | 0     |
| 60  | MG   | AA    | 3128 | 1/1   | 0.99 | 0.49 | 3.93 | 23,23,23,23                 | 0     |
| 60  | MG   | AA    | 3195 | 1/1   | 0.97 | 0.23 | 3.87 | 30,30,30,30                 | 0     |
| 60  | MG   | BA    | 3138 | 1/1   | 0.78 | 0.23 | 3.85 | 54,54,54,54                 | 0     |
| 60  | MG   | BA    | 3147 | 1/1   | 0.81 | 0.27 | 3.85 | 56,56,56,56                 | 0     |
| 60  | MG   | AA    | 2985 | 1/1   | 0.94 | 0.43 | 3.84 | 31,31,31,31                 | 0     |
| 60  | MG   | BA    | 3037 | 1/1   | 0.88 | 0.24 | 3.81 | 35,35,35,35                 | 0     |
| 60  | MG   | AA    | 3083 | 1/1   | 0.95 | 0.26 | 3.76 | 76,76,76,76                 | 0     |
| 60  | MG   | BA    | 3028 | 1/1   | 0.96 | 0.26 | 3.73 | 24,24,24,24                 | 0     |
| 60  | MG   | AA    | 2914 | 1/1   | 0.96 | 0.30 | 3.73 | 15,15,15,15                 | 0     |
| 60  | MG   | Ba    | 1695 | 1/1   | 0.33 | 0.36 | 3.56 | 86,86,86,86                 | 0     |
| 60  | MG   | Aa    | 1678 | 1/1   | 0.65 | 0.29 | 3.50 | 93,93,93,93                 | 0     |
| 60  | MG   | Aa    | 1685 | 1/1   | 0.88 | 0.24 | 3.48 | 53,53,53,53                 | 0     |
| 60  | MG   | BA    | 3217 | 1/1   | 0.99 | 0.37 | 3.46 | 26,26,26,26                 | 0     |
| 60  | MG   | AA    | 3194 | 1/1   | 0.97 | 0.28 | 3.44 | 26,26,26,26                 | 0     |
| 60  | MG   | BA    | 3045 | 1/1   | 0.97 | 0.27 | 3.20 | 16,16,16,16                 | 0     |
| 60  | MG   | BA    | 2920 | 1/1   | 0.97 | 0.24 | 3.20 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | Ba    | 1731 | 1/1   | 0.96 | 0.30 | 3.10 | 20,20,20,20                 | 0     |
| 60  | MG   | AA    | 2929 | 1/1   | 0.93 | 0.28 | 3.09 | 29,29,29,29                 | 0     |
| 60  | MG   | Ba    | 1668 | 1/1   | 0.92 | 0.33 | 3.05 | 49,49,49,49                 | 0     |
| 60  | MG   | AA    | 3012 | 1/1   | 0.95 | 0.23 | 3.00 | 22,22,22,22                 | 0     |
| 60  | MG   | BA    | 3191 | 1/1   | 0.97 | 0.23 | 2.96 | 23,23,23,23                 | 0     |
| 60  | MG   | Aa    | 1613 | 1/1   | 0.90 | 0.34 | 2.91 | 100,100,100,100             | 0     |
| 60  | MG   | AA    | 3070 | 1/1   | 0.92 | 0.23 | 2.84 | 54,54,54,54                 | 0     |
| 60  | MG   | BA    | 2928 | 1/1   | 0.90 | 0.23 | 2.83 | 17,17,17,17                 | 0     |
| 60  | MG   | AA    | 2965 | 1/1   | 0.92 | 0.24 | 2.71 | 69,69,69,69                 | 0     |
| 60  | MG   | Aa    | 1642 | 1/1   | 0.90 | 0.26 | 2.62 | 95,95,95,95                 | 0     |
| 60  | MG   | BA    | 3070 | 1/1   | 0.90 | 0.30 | 2.58 | 83,83,83,83                 | 0     |
| 60  | MG   | BA    | 3105 | 1/1   | 0.93 | 0.32 | 2.44 | 40,40,40,40                 | 0     |
| 60  | MG   | Aa    | 1670 | 1/1   | 0.92 | 0.23 | 2.35 | 43,43,43,43                 | 0     |
| 60  | MG   | AA    | 3029 | 1/1   | 0.96 | 0.22 | 2.18 | 37,37,37,37                 | 0     |
| 60  | MG   | BA    | 3234 | 1/1   | 0.68 | 0.26 | 2.11 | 74,74,74,74                 | 0     |
| 60  | MG   | AA    | 2988 | 1/1   | 0.97 | 0.28 | 2.00 | 33,33,33,33                 | 0     |
| 60  | MG   | Aa    | 1732 | 1/1   | 0.85 | 0.29 | 1.98 | 49,49,49,49                 | 0     |
| 60  | MG   | Ba    | 1718 | 1/1   | 0.84 | 0.31 | 1.94 | 107,107,107,107             | 0     |
| 60  | MG   | BA    | 3090 | 1/1   | 0.96 | 0.23 | 1.83 | 32,32,32,32                 | 0     |
| 60  | MG   | AA    | 3094 | 1/1   | 0.87 | 0.33 | 1.79 | 67,67,67,67                 | 0     |
| 60  | MG   | Aa    | 1654 | 1/1   | 0.90 | 0.17 | 1.77 | 56,56,56,56                 | 0     |
| 60  | MG   | AA    | 3091 | 1/1   | 0.95 | 0.23 | 1.70 | 27,27,27,27                 | 0     |
| 60  | MG   | AA    | 3085 | 1/1   | 0.98 | 0.23 | 1.63 | 47,47,47,47                 | 0     |
| 60  | MG   | AA    | 3123 | 1/1   | 0.97 | 0.30 | 1.58 | 18,18,18,18                 | 0     |
| 60  | MG   | Ba    | 1736 | 1/1   | 0.83 | 0.32 | 1.56 | 59,59,59,59                 | 0     |
| 60  | MG   | BA    | 2923 | 1/1   | 0.99 | 0.24 | 1.53 | 29,29,29,29                 | 0     |
| 60  | MG   | AA    | 3182 | 1/1   | 0.90 | 0.40 | 1.30 | 40,40,40,40                 | 0     |
| 60  | MG   | BA    | 3179 | 1/1   | 0.68 | 0.37 | 1.24 | 24,24,24,24                 | 0     |
| 60  | MG   | BA    | 2910 | 1/1   | 0.93 | 0.22 | 1.23 | 2,2,2,2                     | 0     |
| 60  | MG   | AA    | 3002 | 1/1   | 0.83 | 0.17 | 1.23 | 58,58,58,58                 | 0     |
| 60  | MG   | AA    | 2922 | 1/1   | 0.95 | 0.22 | 1.20 | 48,48,48,48                 | 0     |
| 60  | MG   | Ba    | 1648 | 1/1   | 0.92 | 0.25 | 1.15 | 32,32,32,32                 | 0     |
| 60  | MG   | Aa    | 1657 | 1/1   | 0.92 | 0.36 | 1.13 | 71,71,71,71                 | 0     |
| 60  | MG   | BA    | 3169 | 1/1   | 0.94 | 0.22 | 1.10 | 25,25,25,25                 | 0     |
| 60  | MG   | AD    | 301  | 1/1   | 0.96 | 0.33 | 1.06 | 21,21,21,21                 | 0     |
| 60  | MG   | BA    | 3063 | 1/1   | 0.98 | 0.21 | 1.06 | 26,26,26,26                 | 0     |
| 60  | MG   | Aa    | 1668 | 1/1   | 0.98 | 0.25 | 1.06 | 40,40,40,40                 | 0     |
| 60  | MG   | BA    | 3020 | 1/1   | 0.96 | 0.21 | 1.04 | 84,84,84,84                 | 0     |
| 60  | MG   | Bv    | 102  | 1/1   | 0.97 | 0.27 | 1.03 | 37,37,37,37                 | 0     |
| 60  | MG   | BA    | 3015 | 1/1   | 0.95 | 0.20 | 0.88 | 18,18,18,18                 | 0     |
| 60  | MG   | BA    | 3086 | 1/1   | 0.80 | 0.19 | 0.79 | 48,48,48,48                 | 0     |
| 60  | MG   | Ba    | 1693 | 1/1   | 0.91 | 0.18 | 0.75 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60  | MG   | AD    | 302  | 1/1   | 0.86 | 0.34 | 0.74  | 21,21,21,21                 | 0     |
| 60  | MG   | BA    | 2939 | 1/1   | 0.98 | 0.24 | 0.72  | 71,71,71,71                 | 0     |
| 60  | MG   | Aa    | 1740 | 1/1   | 0.94 | 0.24 | 0.71  | 42,42,42,42                 | 0     |
| 60  | MG   | AA    | 3032 | 1/1   | 0.98 | 0.21 | 0.69  | 33,33,33,33                 | 0     |
| 60  | MG   | Ba    | 1672 | 1/1   | 0.78 | 0.29 | 0.65  | 95,95,95,95                 | 0     |
| 60  | MG   | AA    | 3184 | 1/1   | 0.94 | 0.19 | 0.61  | 44,44,44,44                 | 0     |
| 60  | MG   | Aa    | 1616 | 1/1   | 0.88 | 0.25 | 0.59  | 64,64,64,64                 | 0     |
| 59  | ZN   | Ad    | 301  | 1/1   | 0.99 | 0.29 | 0.57  | 76,76,76,76                 | 0     |
| 60  | MG   | BA    | 2950 | 1/1   | 0.97 | 0.20 | 0.55  | 37,37,37,37                 | 0     |
| 60  | MG   | BA    | 2921 | 1/1   | 0.98 | 0.21 | 0.54  | 31,31,31,31                 | 0     |
| 60  | MG   | B0    | 101  | 1/1   | 0.70 | 0.48 | 0.51  | 71,71,71,71                 | 0     |
| 60  | MG   | AA    | 2912 | 1/1   | 0.97 | 0.20 | 0.50  | 26,26,26,26                 | 0     |
| 60  | MG   | BA    | 2918 | 1/1   | 0.87 | 0.18 | 0.44  | 29,29,29,29                 | 0     |
| 60  | MG   | BA    | 3230 | 1/1   | 0.83 | 0.21 | 0.44  | 45,45,45,45                 | 0     |
| 60  | MG   | BA    | 2978 | 1/1   | 0.94 | 0.16 | 0.40  | 56,56,56,56                 | 0     |
| 59  | ZN   | Bd    | 302  | 1/1   | 0.99 | 0.29 | 0.33  | 80,80,80,80                 | 0     |
| 60  | MG   | Ba    | 1623 | 1/1   | 0.95 | 0.18 | 0.26  | 34,34,34,34                 | 0     |
| 60  | MG   | AA    | 3063 | 1/1   | 0.93 | 0.22 | 0.05  | 53,53,53,53                 | 0     |
| 60  | MG   | BA    | 3050 | 1/1   | 0.87 | 0.20 | 0.03  | 29,29,29,29                 | 0     |
| 60  | MG   | BD    | 302  | 1/1   | 0.98 | 0.24 | -0.04 | 18,18,18,18                 | 0     |
| 60  | MG   | AA    | 3049 | 1/1   | 0.97 | 0.20 | -0.05 | 54,54,54,54                 | 0     |
| 60  | MG   | BA    | 3122 | 1/1   | 0.96 | 0.24 | -0.06 | 24,24,24,24                 | 0     |
| 60  | MG   | Aa    | 1721 | 1/1   | 0.87 | 0.23 | -0.35 | 68,68,68,68                 | 0     |
| 60  | MG   | BA    | 3001 | 1/1   | 0.93 | 0.15 | -0.36 | 37,37,37,37                 | 0     |
| 60  | MG   | Aa    | 1673 | 1/1   | 0.89 | 0.19 | -0.36 | 60,60,60,60                 | 0     |
| 60  | MG   | Aa    | 1609 | 1/1   | 0.95 | 0.20 | -0.38 | 64,64,64,64                 | 0     |
| 60  | MG   | Ba    | 1612 | 1/1   | 0.90 | 0.14 | -0.42 | 82,82,82,82                 | 0     |
| 60  | MG   | AF    | 301  | 1/1   | 0.66 | 0.22 | -0.43 | 74,74,74,74                 | 0     |
| 60  | MG   | Aa    | 1649 | 1/1   | 0.90 | 0.23 | -0.46 | 32,32,32,32                 | 0     |
| 60  | MG   | BA    | 3031 | 1/1   | 0.97 | 0.18 | -0.49 | 14,14,14,14                 | 0     |
| 60  | MG   | Ba    | 1611 | 1/1   | 0.92 | 0.19 | -0.50 | 97,97,97,97                 | 0     |
| 60  | MG   | AA    | 3062 | 1/1   | 0.97 | 0.21 | -0.53 | 26,26,26,26                 | 0     |
| 60  | MG   | AA    | 3030 | 1/1   | 0.87 | 0.17 | -0.55 | 28,28,28,28                 | 0     |
| 60  | MG   | Bm    | 201  | 1/1   | 0.75 | 0.28 | -0.57 | 118,118,118,118             | 0     |
| 60  | MG   | BA    | 2942 | 1/1   | 0.72 | 0.15 | -0.59 | 42,42,42,42                 | 0     |
| 60  | MG   | AA    | 3050 | 1/1   | 0.98 | 0.17 | -0.61 | 96,96,96,96                 | 0     |
| 60  | MG   | Aa    | 1688 | 1/1   | 0.52 | 0.23 | -0.70 | 63,63,63,63                 | 1     |
| 60  | MG   | AA    | 3213 | 1/1   | 0.94 | 0.19 | -0.71 | 33,33,33,33                 | 0     |
| 60  | MG   | BA    | 2986 | 1/1   | 0.95 | 0.17 | -0.74 | 63,63,63,63                 | 0     |
| 60  | MG   | Ba    | 1694 | 1/1   | 0.89 | 0.17 | -0.84 | 83,83,83,83                 | 0     |
| 60  | MG   | Ba    | 1673 | 1/1   | 0.95 | 0.20 | -0.85 | 39,39,39,39                 | 0     |
| 60  | MG   | Ba    | 1674 | 1/1   | 0.84 | 0.15 | -0.85 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60  | MG   | Aa    | 1620 | 1/1   | 0.94 | 0.17 | -0.86 | 73,73,73,73                 | 0     |
| 60  | MG   | Ba    | 1687 | 1/1   | 0.83 | 0.18 | -0.86 | 50,50,50,50                 | 1     |
| 60  | MG   | BA    | 2988 | 1/1   | 0.98 | 0.18 | -0.89 | 34,34,34,34                 | 0     |
| 60  | MG   | AA    | 2971 | 1/1   | 0.85 | 0.12 | -0.95 | 52,52,52,52                 | 0     |
| 60  | MG   | Aa    | 1694 | 1/1   | 0.97 | 0.16 | -0.98 | 89,89,89,89                 | 0     |
| 60  | MG   | Aa    | 1614 | 1/1   | 0.74 | 0.11 | -1.03 | 69,69,69,69                 | 0     |
| 60  | MG   | Ba    | 1670 | 1/1   | 0.92 | 0.18 | -1.08 | 58,58,58,58                 | 0     |
| 60  | MG   | AA    | 3171 | 1/1   | 0.88 | 0.15 | -1.13 | 57,57,57,57                 | 0     |
| 60  | MG   | BA    | 3195 | 1/1   | 0.89 | 0.17 | -1.23 | 37,37,37,37                 | 0     |
| 60  | MG   | AA    | 3232 | 1/1   | 0.92 | 0.19 | -1.24 | 64,64,64,64                 | 0     |
| 59  | ZN   | An    | 101  | 1/1   | 0.98 | 0.13 | -1.25 | 153,153,153,153             | 0     |
| 59  | ZN   | Bn    | 101  | 1/1   | 0.97 | 0.14 | -1.30 | 137,137,137,137             | 0     |
| 60  | MG   | AA    | 2979 | 1/1   | 0.93 | 0.12 | -1.37 | 51,51,51,51                 | 0     |
| 59  | ZN   | A4    | 101  | 1/1   | 0.83 | 0.08 | -1.54 | 186,186,186,186             | 0     |
| 60  | MG   | AA    | 2911 | 1/1   | 0.97 | 0.15 | -1.58 | 20,20,20,20                 | 0     |
| 60  | MG   | BA    | 2911 | 1/1   | 0.99 | 0.16 | -1.65 | 21,21,21,21                 | 0     |
| 60  | MG   | BF    | 301  | 1/1   | 0.90 | 0.14 | -1.67 | 40,40,40,40                 | 0     |
| 60  | MG   | BA    | 2919 | 1/1   | 0.97 | 0.19 | -1.68 | 13,13,13,13                 | 0     |
| 60  | MG   | BA    | 3017 | 1/1   | 0.95 | 0.19 | -1.76 | 38,38,38,38                 | 0     |
| 60  | MG   | BA    | 3203 | 1/1   | 0.95 | 0.13 | -1.79 | 95,95,95,95                 | 0     |
| 60  | MG   | BA    | 3132 | 1/1   | 0.70 | 0.15 | -1.81 | 43,43,43,43                 | 0     |
| 60  | MG   | Ba    | 1680 | 1/1   | 0.93 | 0.12 | -1.83 | 63,63,63,63                 | 0     |
| 60  | MG   | BA    | 3168 | 1/1   | 0.85 | 0.14 | -1.91 | 53,53,53,53                 | 0     |
| 59  | ZN   | A9    | 101  | 1/1   | 0.97 | 0.07 | -1.95 | 138,138,138,138             | 0     |
| 60  | MG   | BA    | 3181 | 1/1   | 0.64 | 0.14 | -2.03 | 61,61,61,61                 | 0     |
| 60  | MG   | BA    | 3096 | 1/1   | 0.94 | 0.12 | -2.06 | 49,49,49,49                 | 0     |
| 60  | MG   | AA    | 3106 | 1/1   | 0.96 | 0.15 | -2.12 | 65,65,65,65                 | 0     |
| 60  | MG   | AA    | 3103 | 1/1   | 0.90 | 0.09 | -2.17 | 35,35,35,35                 | 0     |
| 60  | MG   | AA    | 3186 | 1/1   | 0.90 | 0.11 | -2.20 | 77,77,77,77                 | 0     |
| 60  | MG   | Ba    | 1677 | 1/1   | 0.96 | 0.11 | -2.21 | 138,138,138,138             | 0     |
| 60  | MG   | Ba    | 1606 | 1/1   | 0.98 | 0.16 | -2.26 | 50,50,50,50                 | 0     |
| 60  | MG   | Aa    | 1677 | 1/1   | 0.91 | 0.12 | -2.29 | 69,69,69,69                 | 0     |
| 60  | MG   | BA    | 2959 | 1/1   | 0.85 | 0.12 | -2.32 | 37,37,37,37                 | 0     |
| 60  | MG   | AA    | 3016 | 1/1   | 0.98 | 0.13 | -2.41 | 31,31,31,31                 | 0     |
| 60  | MG   | AA    | 2940 | 1/1   | 0.96 | 0.11 | -2.54 | 34,34,34,34                 | 0     |
| 59  | ZN   | B4    | 101  | 1/1   | 0.87 | 0.08 | -2.64 | 201,201,201,201             | 0     |
| 60  | MG   | Aa    | 1733 | 1/1   | 0.97 | 0.12 | -2.72 | 60,60,60,60                 | 0     |
| 60  | MG   | BA    | 3192 | 1/1   | 0.96 | 0.14 | -2.76 | 34,34,34,34                 | 0     |
| 60  | MG   | Aa    | 1653 | 1/1   | 0.95 | 0.12 | -2.79 | 59,59,59,59                 | 0     |
| 60  | MG   | AA    | 3064 | 1/1   | 0.98 | 0.16 | -3.11 | 29,29,29,29                 | 0     |
| 60  | MG   | AA    | 2924 | 1/1   | 0.99 | 0.11 | -3.30 | 32,32,32,32                 | 0     |
| 60  | MG   | AA    | 2962 | 1/1   | 0.96 | 0.07 | -3.48 | 19,19,19,19                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 60  | MG   | BA    | 2929 | 1/1   | 0.89 | 0.12 | -3.61  | 10,10,10,10                 | 0     |
| 60  | MG   | AA    | 3174 | 1/1   | 0.96 | 0.13 | -3.64  | 72,72,72,72                 | 0     |
| 59  | ZN   | B9    | 101  | 1/1   | 0.99 | 0.07 | -3.93  | 116,116,116,116             | 0     |
| 60  | MG   | AA    | 2989 | 1/1   | 0.98 | 0.10 | -3.96  | 33,33,33,33                 | 0     |
| 60  | MG   | BA    | 3210 | 1/1   | 0.99 | 0.14 | -3.99  | 22,22,22,22                 | 0     |
| 60  | MG   | Ba    | 1619 | 1/1   | 0.96 | 0.07 | -4.19  | 44,44,44,44                 | 0     |
| 60  | MG   | BA    | 2969 | 1/1   | 0.87 | 0.10 | -4.25  | 35,35,35,35                 | 0     |
| 60  | MG   | Aa    | 1608 | 1/1   | 0.99 | 0.15 | -4.38  | 39,39,39,39                 | 0     |
| 60  | MG   | Aa    | 1737 | 1/1   | 0.97 | 0.14 | -4.52  | 119,119,119,119             | 0     |
| 60  | MG   | Ba    | 1633 | 1/1   | 0.98 | 0.09 | -5.22  | 39,39,39,39                 | 0     |
| 60  | MG   | Aa    | 1634 | 1/1   | 0.99 | 0.07 | -5.43  | 47,47,47,47                 | 0     |
| 60  | MG   | Aa    | 1671 | 1/1   | 0.94 | 0.14 | -5.56  | 49,49,49,49                 | 0     |
| 60  | MG   | Aa    | 1695 | 1/1   | 0.96 | 0.08 | -6.11  | 78,78,78,78                 | 0     |
| 60  | MG   | Aa    | 1681 | 1/1   | 0.97 | 0.08 | -6.67  | 76,76,76,76                 | 0     |
| 60  | MG   | Ba    | 1652 | 1/1   | 0.97 | 0.09 | -8.86  | 69,69,69,69                 | 0     |
| 60  | MG   | Ba    | 1732 | 1/1   | 0.98 | 0.11 | -11.19 | 70,70,70,70                 | 0     |
| 60  | MG   | BA    | 3056 | 1/1   | 0.92 | 0.21 | -      | 92,92,92,92                 | 0     |
| 60  | MG   | BA    | 3200 | 1/1   | 0.90 | 0.26 | -      | 33,33,33,33                 | 0     |
| 60  | MG   | AA    | 3250 | 1/1   | 0.95 | 0.59 | -      | 40,40,40,40                 | 0     |
| 60  | MG   | Ba    | 1702 | 1/1   | 0.85 | 1.11 | -      | 97,97,97,97                 | 0     |
| 60  | MG   | BA    | 2993 | 1/1   | 0.96 | 0.39 | -      | 12,12,12,12                 | 0     |
| 60  | MG   | AA    | 3013 | 1/1   | 0.72 | 0.96 | -      | 78,78,78,78                 | 0     |
| 60  | MG   | Ba    | 1717 | 1/1   | 0.79 | 1.16 | -      | 71,71,71,71                 | 0     |
| 60  | MG   | AA    | 3037 | 1/1   | 0.95 | 0.39 | -      | 27,27,27,27                 | 0     |
| 60  | MG   | Ba    | 1729 | 1/1   | 0.77 | 1.25 | -      | 66,66,66,66                 | 0     |
| 60  | MG   | Ba    | 1716 | 1/1   | 0.68 | 0.41 | -      | 63,63,63,63                 | 0     |
| 60  | MG   | AA    | 3107 | 1/1   | 0.93 | 0.29 | -      | 47,47,47,47                 | 0     |
| 60  | MG   | AA    | 2916 | 1/1   | 0.98 | 0.41 | -      | 25,25,25,25                 | 0     |
| 60  | MG   | Ba    | 1605 | 1/1   | 0.89 | 0.73 | -      | 73,73,73,73                 | 0     |
| 60  | MG   | Ba    | 1676 | 1/1   | 0.61 | 0.28 | -      | 137,137,137,137             | 1     |
| 60  | MG   | Ba    | 1699 | 1/1   | 0.46 | 1.12 | -      | 88,88,88,88                 | 0     |
| 60  | MG   | Bl    | 201  | 1/1   | 0.80 | 0.66 | -      | 5,5,5,5                     | 1     |
| 60  | MG   | Aa    | 1698 | 1/1   | 0.91 | 1.04 | -      | 98,98,98,98                 | 1     |
| 60  | MG   | Ba    | 1666 | 1/1   | 0.89 | 0.80 | -      | 73,73,73,73                 | 0     |
| 60  | MG   | AA    | 2995 | 1/1   | 0.95 | 0.62 | -      | 18,18,18,18                 | 0     |
| 60  | MG   | BA    | 2935 | 1/1   | 0.97 | 0.58 | -      | 25,25,25,25                 | 0     |
| 60  | MG   | BA    | 3044 | 1/1   | 0.97 | 0.44 | -      | 21,21,21,21                 | 0     |
| 60  | MG   | AA    | 3251 | 1/1   | 0.89 | 0.71 | -      | 84,84,84,84                 | 0     |
| 60  | MG   | Aa    | 1709 | 1/1   | 0.92 | 0.12 | -      | 148,148,148,148             | 0     |
| 60  | MG   | Ba    | 1629 | 1/1   | 0.97 | 0.14 | -      | 36,36,36,36                 | 0     |
| 60  | MG   | BA    | 2926 | 1/1   | 0.96 | 0.50 | -      | 24,24,24,24                 | 0     |
| 60  | MG   | BA    | 3039 | 1/1   | 0.98 | 0.28 | -      | 15,15,15,15                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | BA    | 3051 | 1/1   | 0.95 | 0.39 | -    | 16,16,16,16                 | 0     |
| 60  | MG   | Ba    | 1667 | 1/1   | 0.85 | 0.49 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | AA    | 3206 | 1/1   | 0.47 | 0.34 | -    | 115,115,115,115             | 0     |
| 60  | MG   | AA    | 2958 | 1/1   | 0.91 | 0.22 | -    | 47,47,47,47                 | 0     |
| 60  | MG   | BA    | 3007 | 1/1   | 0.70 | 0.41 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | Ba    | 1722 | 1/1   | 0.81 | 0.33 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | AA    | 3189 | 1/1   | 0.97 | 0.35 | -    | 107,107,107,107             | 0     |
| 60  | MG   | AQ    | 201  | 1/1   | 0.78 | 1.97 | -    | 94,94,94,94                 | 0     |
| 60  | MG   | Aa    | 1615 | 1/1   | 0.76 | 1.01 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | Ba    | 1686 | 1/1   | 0.86 | 0.30 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | Ba    | 1641 | 1/1   | 0.96 | 0.67 | -    | 94,94,94,94                 | 0     |
| 60  | MG   | AA    | 3113 | 1/1   | 0.91 | 0.56 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | Aa    | 1731 | 1/1   | 0.89 | 0.42 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | BA    | 3003 | 1/1   | 0.99 | 0.31 | -    | 22,22,22,22                 | 0     |
| 60  | MG   | Ba    | 1737 | 1/1   | 0.74 | 0.56 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | Aa    | 1717 | 1/1   | 0.73 | 0.39 | -    | 66,66,66,66                 | 0     |
| 60  | MG   | BA    | 3216 | 1/1   | 0.75 | 0.56 | -    | 117,117,117,117             | 0     |
| 60  | MG   | BA    | 3049 | 1/1   | 0.96 | 0.35 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | BA    | 2973 | 1/1   | 0.77 | 0.41 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | BA    | 3174 | 1/1   | 0.88 | 0.25 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | BA    | 3110 | 1/1   | 0.93 | 0.36 | -    | 23,23,23,23                 | 0     |
| 60  | MG   | BO    | 201  | 1/1   | 0.85 | 0.53 | -    | 122,122,122,122             | 0     |
| 60  | MG   | AA    | 3223 | 1/1   | 0.60 | 0.54 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | AA    | 2986 | 1/1   | 0.87 | 0.74 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | BA    | 3214 | 1/1   | 0.81 | 0.63 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | Aa    | 1625 | 1/1   | 0.91 | 0.80 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | Aa    | 1713 | 1/1   | 0.90 | 1.27 | -    | 98,98,98,98                 | 0     |
| 60  | MG   | Ba    | 1616 | 1/1   | 0.84 | 0.29 | -    | 29,29,29,29                 | 1     |
| 60  | MG   | AA    | 3117 | 1/1   | 0.31 | 0.52 | -    | 148,148,148,148             | 0     |
| 60  | MG   | Aa    | 1730 | 1/1   | 0.03 | 1.12 | -    | 77,77,77,77                 | 0     |
| 60  | MG   | BA    | 3012 | 1/1   | 0.60 | 0.85 | -    | 61,61,61,61                 | 0     |
| 60  | MG   | Aa    | 1711 | 1/1   | 0.83 | 0.43 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | AA    | 3191 | 1/1   | 0.96 | 0.19 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | BA    | 3066 | 1/1   | 0.81 | 0.72 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | AA    | 3074 | 1/1   | 0.89 | 0.39 | -    | 33,33,33,33                 | 0     |
| 60  | MG   | AA    | 3162 | 1/1   | 0.92 | 0.35 | -    | 94,94,94,94                 | 0     |
| 60  | MG   | AA    | 3067 | 1/1   | 0.88 | 0.59 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | BA    | 3263 | 1/1   | 0.51 | 0.27 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | BA    | 2903 | 1/1   | 0.96 | 0.10 | -    | 99,99,99,99                 | 0     |
| 60  | MG   | BA    | 3040 | 1/1   | 0.97 | 0.21 | -    | 17,17,17,17                 | 0     |
| 60  | MG   | BA    | 3225 | 1/1   | 0.88 | 0.57 | -    | 38,38,38,38                 | 0     |
| 60  | MG   | BA    | 3092 | 1/1   | 0.91 | 0.27 | -    | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3218 | 1/1   | 0.80 | 0.81 | -    | 98,98,98,98                 | 0     |
| 60  | MG   | Aa    | 1726 | 1/1   | 0.90 | 0.72 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | BA    | 3083 | 1/1   | 0.86 | 0.54 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | BA    | 3113 | 1/1   | 0.96 | 0.43 | -    | 24,24,24,24                 | 1     |
| 60  | MG   | AA    | 3055 | 1/1   | 0.94 | 0.43 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | AA    | 3022 | 1/1   | 0.98 | 0.47 | -    | 22,22,22,22                 | 0     |
| 60  | MG   | BA    | 3114 | 1/1   | 0.90 | 0.27 | -    | 8,8,8,8                     | 0     |
| 60  | MG   | AA    | 3203 | 1/1   | 0.79 | 0.23 | -    | 66,66,66,66                 | 0     |
| 60  | MG   | BA    | 3158 | 1/1   | 0.81 | 0.32 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | Ba    | 1720 | 1/1   | 0.77 | 0.38 | -    | 91,91,91,91                 | 0     |
| 60  | MG   | Ba    | 1697 | 1/1   | 0.74 | 1.00 | -    | 93,93,93,93                 | 1     |
| 60  | MG   | AA    | 3266 | 1/1   | 0.83 | 0.30 | -    | 87,87,87,87                 | 0     |
| 60  | MG   | Ba    | 1721 | 1/1   | 0.53 | 0.77 | -    | 92,92,92,92                 | 0     |
| 60  | MG   | BA    | 3235 | 1/1   | 0.75 | 0.64 | -    | 51,51,51,51                 | 0     |
| 60  | MG   | BA    | 2943 | 1/1   | 0.85 | 0.30 | -    | 35,35,35,35                 | 0     |
| 60  | MG   | Aa    | 1745 | 1/1   | 0.96 | 0.39 | -    | 48,48,48,48                 | 0     |
| 60  | MG   | BA    | 3185 | 1/1   | 0.96 | 0.44 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | Aa    | 1693 | 1/1   | 0.73 | 0.56 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | BA    | 2941 | 1/1   | 0.90 | 0.27 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | BA    | 3157 | 1/1   | 0.99 | 0.12 | -    | 85,85,85,85                 | 0     |
| 60  | MG   | Ba    | 1647 | 1/1   | 0.80 | 0.60 | -    | 117,117,117,117             | 0     |
| 60  | MG   | Ba    | 1624 | 1/1   | 0.75 | 1.05 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | AA    | 2933 | 1/1   | 0.95 | 0.59 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | Ba    | 1657 | 1/1   | 0.92 | 0.43 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | BA    | 3177 | 1/1   | 0.95 | 0.23 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | BA    | 2992 | 1/1   | 0.96 | 0.20 | -    | 33,33,33,33                 | 0     |
| 60  | MG   | AA    | 3090 | 1/1   | 0.97 | 0.46 | -    | 59,59,59,59                 | 0     |
| 60  | MG   | BA    | 3228 | 1/1   | 0.76 | 1.00 | -    | 94,94,94,94                 | 0     |
| 60  | MG   | Aa    | 1610 | 1/1   | 0.73 | 0.78 | -    | 115,115,115,115             | 0     |
| 60  | MG   | AA    | 3157 | 1/1   | 0.87 | 0.92 | -    | 66,66,66,66                 | 0     |
| 60  | MG   | Bv    | 101  | 1/1   | 0.71 | 0.58 | -    | 52,52,52,52                 | 1     |
| 60  | MG   | Av    | 104  | 1/1   | 0.86 | 0.77 | -    | 50,50,50,50                 | 1     |
| 60  | MG   | AA    | 3119 | 1/1   | 0.71 | 0.91 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | AA    | 3084 | 1/1   | 0.71 | 0.57 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | AA    | 2904 | 1/1   | 0.95 | 0.29 | -    | 131,131,131,131             | 0     |
| 60  | MG   | BA    | 3106 | 1/1   | 0.97 | 0.40 | -    | 41,41,41,41                 | 0     |
| 60  | MG   | AB    | 201  | 1/1   | 0.85 | 0.41 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | Ba    | 1710 | 1/1   | 0.84 | 0.36 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | BA    | 3116 | 1/1   | 0.83 | 0.45 | -    | 91,91,91,91                 | 0     |
| 60  | MG   | AA    | 3159 | 1/1   | 0.95 | 0.20 | -    | 114,114,114,114             | 0     |
| 60  | MG   | AA    | 3220 | 1/1   | 0.50 | 0.57 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | BA    | 2909 | 1/1   | 0.92 | 0.48 | -    | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3183 | 1/1   | 0.92 | 0.38 | -    | 69,69,69,69                 | 0     |
| 60  | MG   | Ba    | 1683 | 1/1   | 0.67 | 0.54 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | AA    | 3115 | 1/1   | 0.94 | 0.31 | -    | 19,19,19,19                 | 0     |
| 60  | MG   | Ba    | 1639 | 1/1   | 0.81 | 0.52 | -    | 58,58,58,58                 | 0     |
| 60  | MG   | BA    | 3112 | 1/1   | 0.94 | 0.19 | -    | 69,69,69,69                 | 0     |
| 60  | MG   | AA    | 2973 | 1/1   | 0.76 | 0.39 | -    | 79,79,79,79                 | 0     |
| 60  | MG   | Aa    | 1639 | 1/1   | 0.68 | 0.38 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | AA    | 3066 | 1/1   | 0.96 | 0.48 | -    | 27,27,27,27                 | 0     |
| 60  | MG   | Ba    | 1679 | 1/1   | 0.65 | 0.73 | -    | 92,92,92,92                 | 0     |
| 60  | MG   | AA    | 3217 | 1/1   | 0.95 | 0.29 | -    | 85,85,85,85                 | 0     |
| 60  | MG   | AA    | 3093 | 1/1   | 0.96 | 0.23 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 2946 | 1/1   | 0.95 | 0.20 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | AA    | 3075 | 1/1   | 0.42 | 0.90 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | Ba    | 1741 | 1/1   | 0.88 | 0.25 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | AA    | 2957 | 1/1   | 0.48 | 0.48 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | Aa    | 1665 | 1/1   | 0.78 | 2.75 | -    | 120,120,120,120             | 0     |
| 60  | MG   | BA    | 3042 | 1/1   | 0.94 | 0.19 | -    | 30,30,30,30                 | 0     |
| 60  | MG   | Bw    | 101  | 1/1   | 0.61 | 0.13 | -    | 132,132,132,132             | 1     |
| 60  | MG   | AA    | 3036 | 1/1   | 0.96 | 1.26 | -    | 100,100,100,100             | 0     |
| 60  | MG   | BA    | 2960 | 1/1   | 0.73 | 0.13 | -    | 101,101,101,101             | 0     |
| 60  | MG   | AA    | 3001 | 1/1   | 0.91 | 0.61 | -    | 26,26,26,26                 | 0     |
| 60  | MG   | AA    | 3257 | 1/1   | 0.95 | 0.30 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | BA    | 3206 | 1/1   | 0.53 | 0.52 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | AA    | 3263 | 1/1   | 0.27 | 0.85 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | BA    | 3261 | 1/1   | 0.54 | 0.64 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | BA    | 3207 | 1/1   | 0.81 | 0.36 | -    | 118,118,118,118             | 0     |
| 60  | MG   | BA    | 3077 | 1/1   | 0.92 | 0.28 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | Ba    | 1692 | 1/1   | 0.61 | 0.56 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | AA    | 3249 | 1/1   | 0.97 | 0.13 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | AA    | 3089 | 1/1   | 0.68 | 0.16 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | Aa    | 1680 | 1/1   | 0.62 | 0.56 | -    | 107,107,107,107             | 0     |
| 60  | MG   | AA    | 3161 | 1/1   | 0.93 | 0.48 | -    | 61,61,61,61                 | 0     |
| 60  | MG   | AA    | 3255 | 1/1   | 0.78 | 0.38 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | BA    | 3170 | 1/1   | 0.88 | 0.25 | -    | 13,13,13,13                 | 0     |
| 60  | MG   | AA    | 3224 | 1/1   | 0.94 | 0.83 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | Aa    | 1629 | 1/1   | 0.85 | 0.44 | -    | 59,59,59,59                 | 0     |
| 60  | MG   | AA    | 3137 | 1/1   | 0.68 | 0.85 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | BA    | 3229 | 1/1   | 0.93 | 0.21 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | BA    | 3125 | 1/1   | 0.94 | 0.44 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | Aa    | 1603 | 1/1   | 0.99 | 0.13 | -    | 68,68,68,68                 | 1     |
| 60  | MG   | BA    | 3212 | 1/1   | 0.94 | 1.44 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | AA    | 3237 | 1/1   | 0.88 | 0.33 | -    | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | Aa    | 1701 | 1/1   | 0.83 | 0.40 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | AA    | 2901 | 1/1   | 0.80 | 0.40 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | AA    | 3185 | 1/1   | 0.90 | 0.37 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | BA    | 3201 | 1/1   | 0.93 | 0.56 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | BA    | 3129 | 1/1   | 0.68 | 0.45 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | BA    | 3008 | 1/1   | 0.99 | 0.43 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | Ba    | 1688 | 1/1   | 0.97 | 0.19 | -    | 120,120,120,120             | 1     |
| 60  | MG   | Ba    | 1622 | 1/1   | 0.89 | 0.23 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | BA    | 3115 | 1/1   | 0.89 | 0.55 | -    | 21,21,21,21                 | 0     |
| 60  | MG   | BA    | 3048 | 1/1   | 0.85 | 0.28 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | Aa    | 1638 | 1/1   | 0.82 | 0.36 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | BA    | 3202 | 1/1   | 0.91 | 0.19 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | AA    | 2930 | 1/1   | 0.87 | 0.07 | -    | 15,15,15,15                 | 0     |
| 60  | MG   | AA    | 3131 | 1/1   | 0.87 | 0.49 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | AA    | 3033 | 1/1   | 0.99 | 0.32 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | BA    | 3059 | 1/1   | 0.89 | 0.18 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | Ba    | 1703 | 1/1   | 0.91 | 0.44 | -    | 25,25,25,25                 | 1     |
| 60  | MG   | AA    | 3031 | 1/1   | 0.94 | 0.54 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | AA    | 2947 | 1/1   | 0.92 | 0.32 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | Ba    | 1618 | 1/1   | 0.97 | 0.37 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | BA    | 3030 | 1/1   | 0.97 | 0.51 | -    | 26,26,26,26                 | 0     |
| 60  | MG   | Ba    | 1632 | 1/1   | 0.90 | 0.78 | -    | 41,41,41,41                 | 0     |
| 60  | MG   | BA    | 3065 | 1/1   | 0.97 | 0.27 | -    | 13,13,13,13                 | 0     |
| 60  | MG   | BA    | 3218 | 1/1   | 0.69 | 0.82 | -    | 80,80,80,80                 | 0     |
| 60  | MG   | Aa    | 1655 | 1/1   | 0.88 | 0.96 | -    | 87,87,87,87                 | 0     |
| 60  | MG   | Aa    | 1650 | 1/1   | 0.69 | 0.78 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | BA    | 3005 | 1/1   | 0.94 | 0.34 | -    | 21,21,21,21                 | 0     |
| 60  | MG   | BA    | 3074 | 1/1   | 0.65 | 0.73 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | BA    | 3109 | 1/1   | 0.84 | 1.22 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | AB    | 203  | 1/1   | 0.71 | 0.68 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 2976 | 1/1   | 0.82 | 0.37 | -    | 104,104,104,104             | 0     |
| 60  | MG   | AA    | 3079 | 1/1   | 0.93 | 0.58 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | AA    | 3193 | 1/1   | 0.95 | 0.26 | -    | 20,20,20,20                 | 0     |
| 60  | MG   | Ae    | 201  | 1/1   | 0.82 | 0.92 | -    | 108,108,108,108             | 0     |
| 60  | MG   | AA    | 3226 | 1/1   | 0.73 | 0.38 | -    | 95,95,95,95                 | 0     |
| 60  | MG   | AA    | 3015 | 1/1   | 0.94 | 0.24 | -    | 14,14,14,14                 | 0     |
| 60  | MG   | AA    | 3252 | 1/1   | 0.78 | 1.27 | -    | 80,80,80,80                 | 0     |
| 60  | MG   | BA    | 3025 | 1/1   | 0.98 | 0.19 | -    | 12,12,12,12                 | 0     |
| 60  | MG   | Ba    | 1675 | 1/1   | 0.86 | 0.97 | -    | 58,58,58,58                 | 0     |
| 60  | MG   | BA    | 3076 | 1/1   | 0.95 | 0.39 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | BA    | 2944 | 1/1   | 0.99 | 0.14 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 3059 | 1/1   | 0.82 | 0.77 | -    | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | Aa    | 1715 | 1/1   | 0.88 | 0.16 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | Ba    | 1614 | 1/1   | 0.94 | 0.44 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | BA    | 2989 | 1/1   | 0.97 | 0.60 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | AA    | 3058 | 1/1   | 0.97 | 0.26 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | AA    | 3253 | 1/1   | 0.93 | 0.24 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | AA    | 2982 | 1/1   | 0.94 | 1.17 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | Aa    | 1669 | 1/1   | 0.83 | 0.68 | -    | 122,122,122,122             | 0     |
| 60  | MG   | Ba    | 1704 | 1/1   | 0.77 | 0.47 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 2978 | 1/1   | 0.79 | 0.64 | -    | 124,124,124,124             | 0     |
| 60  | MG   | Aa    | 1656 | 1/1   | 0.64 | 0.44 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | BA    | 3073 | 1/1   | 0.93 | 0.32 | -    | 30,30,30,30                 | 0     |
| 60  | MG   | BA    | 3188 | 1/1   | 0.95 | 0.07 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | BA    | 3186 | 1/1   | 0.90 | 0.66 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | AA    | 3021 | 1/1   | 0.92 | 0.24 | -    | 96,96,96,96                 | 0     |
| 60  | MG   | Aa    | 1707 | 1/1   | 0.91 | 0.48 | -    | 79,79,79,79                 | 0     |
| 60  | MG   | AA    | 2938 | 1/1   | 0.99 | 0.12 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | BA    | 2972 | 1/1   | 0.96 | 0.61 | -    | 30,30,30,30                 | 0     |
| 60  | MG   | BA    | 3208 | 1/1   | 0.91 | 0.28 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | AA    | 3122 | 1/1   | 0.85 | 0.42 | -    | 39,39,39,39                 | 0     |
| 60  | MG   | Aa    | 1676 | 1/1   | 0.73 | 0.82 | -    | 90,90,90,90                 | 1     |
| 60  | MG   | AA    | 2974 | 1/1   | 0.96 | 0.76 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | AA    | 3118 | 1/1   | 0.91 | 0.50 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | Ba    | 1615 | 1/1   | 0.83 | 0.15 | -    | 81,81,81,81                 | 0     |
| 60  | MG   | AA    | 3042 | 1/1   | 0.98 | 0.47 | -    | 27,27,27,27                 | 0     |
| 60  | MG   | Aa    | 1623 | 1/1   | 0.95 | 0.32 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | AA    | 3188 | 1/1   | 0.97 | 0.30 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | AA    | 3155 | 1/1   | 0.72 | 0.16 | -    | 92,92,92,92                 | 1     |
| 60  | MG   | BA    | 3223 | 1/1   | 0.90 | 0.18 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | Aa    | 1640 | 1/1   | 0.91 | 0.36 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | Aa    | 1667 | 1/1   | 0.88 | 0.69 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | BA    | 3199 | 1/1   | 0.86 | 0.23 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | Ba    | 1738 | 1/1   | 0.65 | 0.94 | -    | 106,106,106,106             | 0     |
| 60  | MG   | Ba    | 1709 | 1/1   | 0.96 | 0.35 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | AA    | 3153 | 1/1   | 0.69 | 0.35 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | BA    | 3021 | 1/1   | 0.91 | 0.32 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | BA    | 2933 | 1/1   | 0.92 | 0.38 | -    | 18,18,18,18                 | 1     |
| 60  | MG   | AA    | 3007 | 1/1   | 0.98 | 0.13 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | BA    | 2953 | 1/1   | 0.97 | 0.21 | -    | 25,25,25,25                 | 0     |
| 60  | MG   | BA    | 3006 | 1/1   | 0.98 | 0.37 | -    | 21,21,21,21                 | 0     |
| 60  | MG   | AA    | 2975 | 1/1   | 0.96 | 0.42 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | AA    | 2934 | 1/1   | 0.96 | 0.25 | -    | 32,32,32,32                 | 1     |
| 60  | MG   | BA    | 3265 | 1/1   | 0.50 | 0.51 | -    | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 2927 | 1/1   | 0.93 | 0.48 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | AA    | 3200 | 1/1   | 0.72 | 0.75 | -    | 72,72,72,72                 | 1     |
| 60  | MG   | B5    | 101  | 1/1   | 0.91 | 0.38 | -    | 27,27,27,27                 | 0     |
| 60  | MG   | AA    | 3240 | 1/1   | 0.67 | 0.77 | -    | 106,106,106,106             | 0     |
| 60  | MG   | Ba    | 1640 | 1/1   | 0.77 | 0.84 | -    | 80,80,80,80                 | 0     |
| 60  | MG   | BA    | 3111 | 1/1   | 0.64 | 0.41 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | Aa    | 1605 | 1/1   | 0.97 | 0.11 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | AA    | 3060 | 1/1   | 0.94 | 0.24 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | BA    | 3232 | 1/1   | 0.95 | 0.22 | -    | 77,77,77,77                 | 0     |
| 60  | MG   | BA    | 3164 | 1/1   | 0.93 | 0.51 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | BA    | 2956 | 1/1   | 0.72 | 0.15 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | BA    | 3082 | 1/1   | 0.91 | 0.17 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | BA    | 3198 | 1/1   | 0.77 | 1.32 | -    | 91,91,91,91                 | 0     |
| 60  | MG   | AA    | 3215 | 1/1   | 0.98 | 0.14 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | AA    | 3160 | 1/1   | 0.91 | 0.51 | -    | 99,99,99,99                 | 0     |
| 60  | MG   | BA    | 3149 | 1/1   | 0.75 | 0.42 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | AA    | 3198 | 1/1   | 0.95 | 0.46 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | Ba    | 1662 | 1/1   | 0.81 | 0.27 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | BA    | 3117 | 1/1   | 0.95 | 0.62 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | Aa    | 1691 | 1/1   | 0.93 | 0.33 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | BA    | 3085 | 1/1   | 0.82 | 0.20 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | BA    | 3000 | 1/1   | 0.93 | 0.44 | -    | 16,16,16,16                 | 0     |
| 60  | MG   | BA    | 3209 | 1/1   | 0.81 | 0.43 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | Ba    | 1740 | 1/1   | 0.70 | 0.28 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | BA    | 3242 | 1/1   | 0.75 | 0.84 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | AA    | 3241 | 1/1   | 0.70 | 0.51 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | BA    | 2916 | 1/1   | 0.96 | 0.68 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 3100 | 1/1   | 0.85 | 0.92 | -    | 97,97,97,97                 | 0     |
| 60  | MG   | AA    | 3229 | 1/1   | 0.78 | 0.53 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | AA    | 3145 | 1/1   | 0.89 | 0.65 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | Ba    | 1637 | 1/1   | 0.76 | 0.60 | -    | 80,80,80,80                 | 0     |
| 60  | MG   | BA    | 2994 | 1/1   | 0.91 | 0.56 | -    | 14,14,14,14                 | 0     |
| 60  | MG   | BA    | 3249 | 1/1   | 0.83 | 0.85 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | Ba    | 1715 | 1/1   | 0.52 | 0.27 | -    | 94,94,94,94                 | 0     |
| 60  | MG   | BA    | 3153 | 1/1   | 0.73 | 0.63 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | AA    | 3076 | 1/1   | 0.90 | 0.23 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | BA    | 3130 | 1/1   | 0.74 | 0.41 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | BA    | 3252 | 1/1   | 0.77 | 0.18 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | BA    | 3145 | 1/1   | 0.94 | 0.83 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | BA    | 3262 | 1/1   | 0.75 | 0.32 | -    | 39,39,39,39                 | 0     |
| 60  | MG   | BA    | 3081 | 1/1   | 0.87 | 0.16 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | AA    | 3008 | 1/1   | 0.69 | 0.37 | -    | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | Ba    | 1604 | 1/1   | 0.67 | 0.58 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | AA    | 2917 | 1/1   | 0.66 | 0.49 | -    | 112,112,112,112             | 0     |
| 60  | MG   | BA    | 3144 | 1/1   | 0.69 | 1.04 | -    | 59,59,59,59                 | 0     |
| 60  | MG   | AA    | 3068 | 1/1   | 0.97 | 0.27 | -    | 19,19,19,19                 | 0     |
| 60  | MG   | Ba    | 1730 | 1/1   | 0.93 | 0.24 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | BA    | 2936 | 1/1   | 0.79 | 0.22 | -    | 35,35,35,35                 | 0     |
| 60  | MG   | AA    | 2944 | 1/1   | 0.73 | 0.51 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | Ba    | 1725 | 1/1   | 0.95 | 0.86 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | Aa    | 1716 | 1/1   | 0.88 | 0.12 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | AA    | 3196 | 1/1   | 0.87 | 0.67 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | Aa    | 1659 | 1/1   | 0.80 | 0.40 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | BA    | 3009 | 1/1   | 0.98 | 0.32 | -    | 3,3,3,3                     | 0     |
| 60  | MG   | Ba    | 1698 | 1/1   | 0.55 | 0.85 | -    | 89,89,89,89                 | 1     |
| 60  | MG   | BA    | 3098 | 1/1   | 0.57 | 0.81 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | BA    | 3016 | 1/1   | 0.93 | 0.25 | -    | 11,11,11,11                 | 0     |
| 60  | MG   | BA    | 3036 | 1/1   | 0.99 | 0.41 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | Ba    | 1663 | 1/1   | 0.33 | 0.80 | -    | 85,85,85,85                 | 0     |
| 60  | MG   | Aa    | 1699 | 1/1   | 0.58 | 0.60 | -    | 84,84,84,84                 | 1     |
| 60  | MG   | AA    | 2956 | 1/1   | 0.95 | 0.21 | -    | 61,61,61,61                 | 0     |
| 60  | MG   | AA    | 3246 | 1/1   | 0.68 | 0.27 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | BA    | 3250 | 1/1   | 0.89 | 1.26 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | Aa    | 1697 | 1/1   | 0.93 | 0.66 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | Ba    | 1664 | 1/1   | 0.76 | 0.77 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | BA    | 2932 | 1/1   | 0.93 | 0.39 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | AA    | 3057 | 1/1   | 0.98 | 0.10 | -    | 92,92,92,92                 | 0     |
| 60  | MG   | BA    | 3046 | 1/1   | 0.88 | 0.35 | -    | 28,28,28,28                 | 0     |
| 60  | MG   | Aa    | 1607 | 1/1   | 0.93 | 0.65 | -    | 69,69,69,69                 | 0     |
| 60  | MG   | BA    | 3057 | 1/1   | 0.96 | 0.26 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | BA    | 3078 | 1/1   | 0.94 | 0.58 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | BA    | 2970 | 1/1   | 0.98 | 0.42 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | AA    | 3144 | 1/1   | 0.85 | 1.08 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | A1    | 101  | 1/1   | 0.93 | 0.28 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | Aa    | 1687 | 1/1   | 0.68 | 0.15 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | BA    | 3196 | 1/1   | 0.92 | 0.31 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | BA    | 3162 | 1/1   | 0.85 | 0.34 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3214 | 1/1   | 0.89 | 0.79 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | Aa    | 1661 | 1/1   | 0.92 | 0.22 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | Aa    | 1658 | 1/1   | 0.89 | 0.57 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | AA    | 2937 | 1/1   | 0.98 | 0.16 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | Ba    | 1712 | 1/1   | 0.36 | 0.83 | -    | 79,79,79,79                 | 0     |
| 60  | MG   | AA    | 3154 | 1/1   | 0.46 | 0.20 | -    | 142,142,142,142             | 0     |
| 60  | MG   | AA    | 3077 | 1/1   | 0.90 | 0.47 | -    | 99,99,99,99                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3143 | 1/1   | 0.96 | 0.38 | -    | 29,29,29,29                 | 0     |
| 60  | MG   | Aa    | 1720 | 1/1   | 0.84 | 1.05 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | BA    | 3224 | 1/1   | 0.93 | 0.41 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 3227 | 1/1   | 0.99 | 0.31 | -    | 39,39,39,39                 | 0     |
| 60  | MG   | BA    | 3163 | 1/1   | 0.90 | 0.74 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | BA    | 3220 | 1/1   | 0.69 | 0.79 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | BA    | 3184 | 1/1   | 0.96 | 0.14 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | Av    | 103  | 1/1   | 0.97 | 0.06 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | BA    | 3071 | 1/1   | 0.82 | 0.49 | -    | 39,39,39,39                 | 0     |
| 60  | MG   | Aa    | 1619 | 1/1   | 0.97 | 0.46 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | Ba    | 1659 | 1/1   | 0.52 | 0.33 | -    | 79,79,79,79                 | 0     |
| 60  | MG   | Aa    | 1632 | 1/1   | 0.87 | 0.41 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | Ba    | 1651 | 1/1   | 0.81 | 1.00 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | AA    | 3024 | 1/1   | 0.93 | 0.36 | -    | 25,25,25,25                 | 0     |
| 60  | MG   | AA    | 3151 | 1/1   | 0.83 | 0.48 | -    | 85,85,85,85                 | 0     |
| 60  | MG   | AA    | 3202 | 1/1   | 0.96 | 0.33 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3187 | 1/1   | 0.96 | 0.39 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | BA    | 3237 | 1/1   | 0.93 | 0.25 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | Aa    | 1723 | 1/1   | 0.79 | 0.40 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | Aa    | 1612 | 1/1   | 0.89 | 0.19 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | Ba    | 1669 | 1/1   | 0.39 | 0.60 | -    | 94,94,94,94                 | 0     |
| 60  | MG   | BA    | 2945 | 1/1   | 0.85 | 0.32 | -    | 112,112,112,112             | 0     |
| 60  | MG   | AA    | 3264 | 1/1   | 0.92 | 0.97 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | AA    | 3027 | 1/1   | 0.88 | 0.21 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | AA    | 3010 | 1/1   | 0.98 | 0.48 | -    | 10,10,10,10                 | 0     |
| 60  | MG   | BA    | 3079 | 1/1   | 0.89 | 0.24 | -    | 82,82,82,82                 | 0     |
| 60  | MG   | AA    | 3140 | 1/1   | 0.94 | 0.49 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | BA    | 2991 | 1/1   | 0.89 | 0.55 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | AA    | 3165 | 1/1   | 0.88 | 0.37 | -    | 97,97,97,97                 | 0     |
| 60  | MG   | BA    | 3253 | 1/1   | 0.88 | 0.67 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | AA    | 3082 | 1/1   | 0.74 | 0.43 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | Ba    | 1642 | 1/1   | 0.84 | 0.46 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | B7    | 102  | 1/1   | 0.91 | 0.66 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3120 | 1/1   | 0.96 | 0.15 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | AA    | 3080 | 1/1   | 0.93 | 0.54 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | AA    | 3207 | 1/1   | 0.93 | 0.50 | -    | 59,59,59,59                 | 0     |
| 60  | MG   | AA    | 2935 | 1/1   | 0.84 | 0.64 | -    | 69,69,69,69                 | 0     |
| 60  | MG   | BA    | 3004 | 1/1   | 0.96 | 0.14 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | BA    | 2961 | 1/1   | 0.93 | 0.28 | -    | 28,28,28,28                 | 0     |
| 60  | MG   | BB    | 201  | 1/1   | 0.84 | 0.49 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | AA    | 3199 | 1/1   | 0.98 | 0.43 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | BA    | 3087 | 1/1   | 0.87 | 0.59 | -    | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3235 | 1/1   | 0.76 | 0.58 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | AA    | 3166 | 1/1   | 0.79 | 0.35 | -    | 48,48,48,48                 | 0     |
| 60  | MG   | AA    | 3176 | 1/1   | 0.75 | 1.25 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | AA    | 3267 | 1/1   | 0.92 | 0.88 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | AA    | 3105 | 1/1   | 0.93 | 0.17 | -    | 47,47,47,47                 | 0     |
| 60  | MG   | AA    | 2950 | 1/1   | 0.94 | 0.24 | -    | 51,51,51,51                 | 0     |
| 60  | MG   | Aa    | 1683 | 1/1   | 0.94 | 0.12 | -    | 66,66,66,66                 | 0     |
| 60  | MG   | AA    | 3173 | 1/1   | 0.90 | 0.32 | -    | 14,14,14,14                 | 0     |
| 60  | MG   | AA    | 2992 | 1/1   | 0.95 | 0.44 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | BA    | 3032 | 1/1   | 0.89 | 0.41 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | AA    | 2926 | 1/1   | 0.96 | 0.36 | -    | 26,26,26,26                 | 0     |
| 60  | MG   | Ba    | 1650 | 1/1   | 0.93 | 0.52 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | BA    | 2924 | 1/1   | 0.73 | 0.32 | -    | 93,93,93,93                 | 0     |
| 60  | MG   | AA    | 2993 | 1/1   | 0.86 | 0.28 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 3155 | 1/1   | 0.98 | 0.33 | -    | 59,59,59,59                 | 0     |
| 60  | MG   | BA    | 2907 | 1/1   | 0.97 | 0.51 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | BA    | 3175 | 1/1   | 0.85 | 0.72 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3238 | 1/1   | 0.64 | 0.75 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | AA    | 2967 | 1/1   | 0.91 | 1.41 | -    | 69,69,69,69                 | 0     |
| 60  | MG   | BA    | 3142 | 1/1   | 0.93 | 0.84 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | BA    | 2952 | 1/1   | 0.84 | 0.41 | -    | 102,102,102,102             | 0     |
| 60  | MG   | BA    | 3248 | 1/1   | 0.95 | 0.83 | -    | 47,47,47,47                 | 0     |
| 60  | MG   | Ba    | 1653 | 1/1   | 0.83 | 0.38 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | BA    | 3140 | 1/1   | 0.95 | 0.33 | -    | 25,25,25,25                 | 0     |
| 60  | MG   | BA    | 3061 | 1/1   | 0.99 | 0.14 | -    | 35,35,35,35                 | 0     |
| 60  | MG   | BA    | 3137 | 1/1   | 0.82 | 0.88 | -    | 80,80,80,80                 | 0     |
| 60  | MG   | BA    | 2922 | 1/1   | 0.97 | 0.29 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | BA    | 2902 | 1/1   | 0.94 | 0.32 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | AA    | 3132 | 1/1   | 0.67 | 0.99 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | BA    | 3246 | 1/1   | 0.79 | 0.31 | -    | 89,89,89,89                 | 0     |
| 60  | MG   | BA    | 2983 | 1/1   | 0.99 | 0.16 | -    | 21,21,21,21                 | 0     |
| 60  | MG   | AA    | 3052 | 1/1   | 0.93 | 0.29 | -    | 18,18,18,18                 | 0     |
| 60  | MG   | Aa    | 1696 | 1/1   | 0.90 | 0.22 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | AA    | 3212 | 1/1   | 0.88 | 0.65 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | AA    | 2939 | 1/1   | 0.85 | 0.87 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | Aa    | 1602 | 1/1   | 0.74 | 0.28 | -    | 126,126,126,126             | 0     |
| 60  | MG   | Ba    | 1620 | 1/1   | 0.75 | 0.21 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | AA    | 3201 | 1/1   | 0.74 | 1.19 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | AA    | 3211 | 1/1   | 0.98 | 0.17 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | BA    | 3245 | 1/1   | 0.85 | 0.27 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | BA    | 2975 | 1/1   | 0.90 | 0.60 | -    | 105,105,105,105             | 0     |
| 60  | MG   | BA    | 3189 | 1/1   | 0.72 | 0.70 | -    | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3170 | 1/1   | 0.88 | 0.42 | -    | 47,47,47,47                 | 0     |
| 60  | MG   | AA    | 3003 | 1/1   | 0.95 | 0.28 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | Ba    | 1705 | 1/1   | 0.60 | 0.34 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | Ba    | 1707 | 1/1   | 0.45 | 0.46 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | Aa    | 1712 | 1/1   | 0.44 | 1.12 | -    | 117,117,117,117             | 0     |
| 60  | MG   | Ba    | 1690 | 1/1   | 0.86 | 0.37 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 2998 | 1/1   | 0.99 | 0.23 | -    | 14,14,14,14                 | 0     |
| 60  | MG   | Aa    | 1618 | 1/1   | 0.94 | 0.35 | -    | 28,28,28,28                 | 0     |
| 60  | MG   | AA    | 3156 | 1/1   | 0.97 | 0.36 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | BA    | 3264 | 1/1   | 0.77 | 0.89 | -    | 89,89,89,89                 | 0     |
| 60  | MG   | AA    | 3204 | 1/1   | 0.76 | 0.67 | -    | 51,51,51,51                 | 0     |
| 60  | MG   | Ba    | 1708 | 1/1   | 0.71 | 0.20 | -    | 132,132,132,132             | 0     |
| 60  | MG   | BA    | 2925 | 1/1   | 0.95 | 0.45 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | AA    | 3071 | 1/1   | 0.85 | 0.41 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | Ba    | 1602 | 1/1   | 0.85 | 0.28 | -    | 93,93,93,93                 | 0     |
| 60  | MG   | Ba    | 1655 | 1/1   | 0.98 | 0.60 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | Aa    | 1710 | 1/1   | 0.96 | 0.25 | -    | 29,29,29,29                 | 0     |
| 60  | MG   | BA    | 3107 | 1/1   | 0.98 | 0.38 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | Aa    | 1689 | 1/1   | 0.88 | 0.25 | -    | 65,65,65,65                 | 1     |
| 60  | MG   | AA    | 3073 | 1/1   | 0.88 | 0.89 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | BA    | 3023 | 1/1   | 0.97 | 0.40 | -    | 21,21,21,21                 | 0     |
| 60  | MG   | AA    | 2999 | 1/1   | 0.95 | 0.29 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | Aa    | 1637 | 1/1   | 0.78 | 0.36 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | BA    | 3205 | 1/1   | 0.78 | 0.42 | -    | 92,92,92,92                 | 0     |
| 60  | MG   | BA    | 3121 | 1/1   | 0.86 | 1.31 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | AA    | 3169 | 1/1   | 0.94 | 0.07 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | BA    | 2904 | 1/1   | 0.98 | 0.35 | -    | 1,1,1,1                     | 0     |
| 60  | MG   | AA    | 3142 | 1/1   | 0.84 | 0.40 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | AA    | 2902 | 1/1   | 0.95 | 0.18 | -    | 167,167,167,167             | 0     |
| 60  | MG   | Aa    | 1641 | 1/1   | 0.87 | 0.35 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | A5    | 101  | 1/1   | 0.92 | 0.48 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | BA    | 3128 | 1/1   | 0.96 | 0.39 | -    | 26,26,26,26                 | 0     |
| 60  | MG   | AA    | 3086 | 1/1   | 0.92 | 0.12 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | Ba    | 1626 | 1/1   | 0.96 | 0.31 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 2985 | 1/1   | 0.84 | 0.32 | -    | 26,26,26,26                 | 0     |
| 60  | MG   | AA    | 3014 | 1/1   | 0.89 | 0.85 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | Ba    | 1646 | 1/1   | 0.84 | 0.26 | -    | 128,128,128,128             | 0     |
| 60  | MG   | BA    | 3135 | 1/1   | 0.92 | 1.30 | -    | 96,96,96,96                 | 0     |
| 60  | MG   | BA    | 3159 | 1/1   | 0.98 | 0.23 | -    | 52,52,52,52                 | 0     |
| 60  | MG   | AA    | 2955 | 1/1   | 0.96 | 0.41 | -    | 48,48,48,48                 | 0     |
| 60  | MG   | BA    | 2949 | 1/1   | 0.98 | 0.31 | -    | 42,42,42,42                 | 0     |
| 60  | MG   | Aa    | 1739 | 1/1   | 0.94 | 0.49 | -    | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | Aa    | 1684 | 1/1   | 0.82 | 1.01 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | AA    | 2941 | 1/1   | 0.76 | 0.76 | -    | 92,92,92,92                 | 0     |
| 60  | MG   | Ba    | 1735 | 1/1   | 0.71 | 0.21 | -    | 122,122,122,122             | 0     |
| 60  | MG   | Ba    | 1714 | 1/1   | 0.75 | 0.10 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | BA    | 3197 | 1/1   | 0.97 | 0.17 | -    | 103,103,103,103             | 1     |
| 60  | MG   | Ba    | 1706 | 1/1   | 0.69 | 0.74 | -    | 104,104,104,104             | 0     |
| 60  | MG   | Ba    | 1658 | 1/1   | 0.62 | 0.32 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | BA    | 3180 | 1/1   | 0.95 | 0.86 | -    | 105,105,105,105             | 0     |
| 60  | MG   | Ba    | 1631 | 1/1   | 0.80 | 0.55 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | BA    | 3238 | 1/1   | 0.55 | 0.95 | -    | 113,113,113,113             | 0     |
| 60  | MG   | AA    | 3000 | 1/1   | 0.82 | 0.62 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | BA    | 2915 | 1/1   | 0.95 | 0.53 | -    | 20,20,20,20                 | 0     |
| 60  | MG   | Aa    | 1652 | 1/1   | 0.80 | 0.83 | -    | 58,58,58,58                 | 0     |
| 60  | MG   | BA    | 2974 | 1/1   | 0.87 | 0.42 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | BA    | 2963 | 1/1   | 0.96 | 0.23 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | AA    | 2966 | 1/1   | 0.98 | 0.56 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | Ba    | 1665 | 1/1   | 0.74 | 0.74 | -    | 144,144,144,144             | 0     |
| 60  | MG   | AA    | 3254 | 1/1   | 0.91 | 0.49 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | Aa    | 1714 | 1/1   | 0.92 | 0.17 | -    | 47,47,47,47                 | 0     |
| 60  | MG   | BA    | 2940 | 1/1   | 0.93 | 0.25 | -    | 82,82,82,82                 | 0     |
| 60  | MG   | Ba    | 1601 | 1/1   | 0.73 | 0.48 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | AA    | 3141 | 1/1   | 0.81 | 1.13 | -    | 86,86,86,86                 | 0     |
| 60  | MG   | Aa    | 1627 | 1/1   | 0.96 | 0.19 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | BA    | 3148 | 1/1   | 0.82 | 0.44 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | BA    | 3080 | 1/1   | 0.76 | 0.34 | -    | 58,58,58,58                 | 0     |
| 60  | MG   | AA    | 3146 | 1/1   | 0.62 | 0.75 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | BA    | 2947 | 1/1   | 0.64 | 0.33 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | AA    | 3045 | 1/1   | 0.98 | 0.49 | -    | 22,22,22,22                 | 0     |
| 60  | MG   | BA    | 3118 | 1/1   | 0.65 | 0.47 | -    | 70,70,70,70                 | 0     |
| 60  | MG   | BA    | 3041 | 1/1   | 0.96 | 0.42 | -    | 15,15,15,15                 | 0     |
| 60  | MG   | BA    | 3026 | 1/1   | 0.93 | 0.20 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | Aa    | 1742 | 1/1   | 0.33 | 0.55 | -    | 106,106,106,106             | 0     |
| 60  | MG   | BA    | 3167 | 1/1   | 0.93 | 0.77 | -    | 59,59,59,59                 | 0     |
| 60  | MG   | Aa    | 1736 | 1/1   | 0.88 | 0.27 | -    | 117,117,117,117             | 0     |
| 60  | MG   | BA    | 3068 | 1/1   | 0.86 | 0.52 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | Ba    | 1689 | 1/1   | 0.69 | 0.42 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3168 | 1/1   | 0.82 | 0.27 | -    | 82,82,82,82                 | 0     |
| 60  | MG   | BA    | 2977 | 1/1   | 0.74 | 0.40 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | AA    | 3164 | 1/1   | 0.97 | 0.64 | -    | 69,69,69,69                 | 0     |
| 60  | MG   | BB    | 203  | 1/1   | 0.72 | 0.55 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | Av    | 101  | 1/1   | 0.91 | 0.74 | -    | 90,90,90,90                 | 1     |
| 60  | MG   | Aa    | 1734 | 1/1   | 0.95 | 0.58 | -    | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | Av    | 105  | 1/1   | 0.81 | 0.33 | -    | 92,92,92,92                 | 1     |
| 60  | MG   | Ba    | 1628 | 1/1   | 0.85 | 0.34 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | BA    | 3143 | 1/1   | 0.89 | 1.02 | -    | 95,95,95,95                 | 0     |
| 60  | MG   | BA    | 3067 | 1/1   | 0.96 | 0.29 | -    | 28,28,28,28                 | 0     |
| 60  | MG   | AA    | 2923 | 1/1   | 0.97 | 0.54 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | AA    | 3148 | 1/1   | 0.68 | 0.27 | -    | 77,77,77,77                 | 0     |
| 60  | MG   | AA    | 3178 | 1/1   | 0.79 | 0.33 | -    | 35,35,35,35                 | 0     |
| 60  | MG   | AA    | 2942 | 1/1   | 0.93 | 0.34 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | BA    | 3247 | 1/1   | 0.83 | 0.36 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | AA    | 3110 | 1/1   | 0.71 | 1.25 | -    | 91,91,91,91                 | 0     |
| 60  | MG   | BA    | 2964 | 1/1   | 0.94 | 0.39 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | BA    | 2981 | 1/1   | 0.73 | 1.34 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | Ba    | 1723 | 1/1   | 0.98 | 0.14 | -    | 103,103,103,103             | 0     |
| 60  | MG   | AA    | 2994 | 1/1   | 0.84 | 0.58 | -    | 30,30,30,30                 | 0     |
| 60  | MG   | BA    | 3256 | 1/1   | 0.97 | 0.50 | -    | 39,39,39,39                 | 0     |
| 60  | MG   | Ba    | 1660 | 1/1   | 0.87 | 0.73 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | Aa    | 1703 | 1/1   | 0.34 | 0.93 | -    | 94,94,94,94                 | 0     |
| 60  | MG   | AA    | 3260 | 1/1   | 0.19 | 0.75 | -    | 80,80,80,80                 | 0     |
| 60  | MG   | BA    | 3119 | 1/1   | 0.82 | 0.33 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | Ba    | 1713 | 1/1   | 0.70 | 0.61 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | AA    | 2970 | 1/1   | 0.88 | 0.20 | -    | 53,53,53,53                 | 0     |
| 60  | MG   | AA    | 3017 | 1/1   | 0.91 | 0.32 | -    | 18,18,18,18                 | 0     |
| 60  | MG   | Bv    | 103  | 1/1   | 0.79 | 0.30 | -    | 93,93,93,93                 | 0     |
| 60  | MG   | BA    | 3259 | 1/1   | 0.84 | 0.25 | -    | 86,86,86,86                 | 0     |
| 60  | MG   | BA    | 2997 | 1/1   | 0.97 | 0.22 | -    | 22,22,22,22                 | 0     |
| 60  | MG   | AA    | 2908 | 1/1   | 0.95 | 0.40 | -    | 25,25,25,25                 | 0     |
| 60  | MG   | BA    | 3014 | 1/1   | 0.97 | 0.26 | -    | 1,1,1,1                     | 0     |
| 60  | MG   | Ba    | 1678 | 1/1   | 0.92 | 0.49 | -    | 51,51,51,51                 | 0     |
| 60  | MG   | Aa    | 1644 | 1/1   | 0.92 | 0.29 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 3124 | 1/1   | 0.96 | 0.29 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | Ba    | 1696 | 1/1   | 0.72 | 0.64 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | Ba    | 1734 | 1/1   | 0.94 | 0.25 | -    | 84,84,84,84                 | 1     |
| 60  | MG   | BB    | 202  | 1/1   | 0.84 | 0.33 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | Aa    | 1643 | 1/1   | 0.76 | 1.21 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | AA    | 2903 | 1/1   | 0.83 | 0.59 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | Aa    | 1601 | 1/1   | 0.38 | 0.90 | -    | 123,123,123,123             | 0     |
| 60  | MG   | Aa    | 1702 | 1/1   | 0.90 | 0.41 | -    | 91,91,91,91                 | 0     |
| 60  | MG   | BA    | 3152 | 1/1   | 0.77 | 0.34 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | AA    | 3129 | 1/1   | 0.98 | 0.37 | -    | 29,29,29,29                 | 0     |
| 60  | MG   | BA    | 3204 | 1/1   | 0.59 | 0.53 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | Aa    | 1604 | 1/1   | 0.96 | 0.13 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | Aa    | 1651 | 1/1   | 0.83 | 0.66 | -    | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | Aa    | 1617 | 1/1   | 0.86 | 0.36 | -    | 49,49,49,49                 | 1     |
| 60  | MG   | Aa    | 1660 | 1/1   | 0.89 | 0.47 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | AA    | 2972 | 1/1   | 0.83 | 0.25 | -    | 43,43,43,43                 | 0     |
| 60  | MG   | Aa    | 1682 | 1/1   | 0.91 | 0.59 | -    | 59,59,59,59                 | 0     |
| 60  | MG   | AA    | 2945 | 1/1   | 0.97 | 0.12 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | BA    | 3072 | 1/1   | 0.66 | 0.90 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | BA    | 2934 | 1/1   | 0.80 | 0.68 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | Ba    | 1636 | 1/1   | 0.92 | 0.20 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | BA    | 3161 | 1/1   | 0.88 | 0.41 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | BA    | 3033 | 1/1   | 0.65 | 0.58 | -    | 61,61,61,61                 | 0     |
| 60  | MG   | Aa    | 1708 | 1/1   | 0.71 | 0.55 | -    | 81,81,81,81                 | 0     |
| 60  | MG   | Ba    | 1682 | 1/1   | 0.97 | 0.10 | -    | 66,66,66,66                 | 0     |
| 60  | MG   | Ba    | 1627 | 1/1   | 0.98 | 0.56 | -    | 74,74,74,74                 | 0     |
| 60  | MG   | AA    | 3234 | 1/1   | 0.91 | 0.20 | -    | 79,79,79,79                 | 0     |
| 60  | MG   | BA    | 3240 | 1/1   | 0.86 | 0.99 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | Bd    | 301  | 1/1   | 0.84 | 0.86 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | BA    | 3103 | 1/1   | 0.87 | 0.27 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | Ba    | 1610 | 1/1   | 0.73 | 0.20 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | BA    | 3178 | 1/1   | 0.49 | 0.39 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | Ba    | 1727 | 1/1   | 0.92 | 0.49 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | AX    | 101  | 1/1   | 0.84 | 0.85 | -    | 55,55,55,55                 | 1     |
| 60  | MG   | AA    | 3228 | 1/1   | 0.82 | 0.64 | -    | 51,51,51,51                 | 0     |
| 60  | MG   | AA    | 3239 | 1/1   | 0.95 | 0.34 | -    | 77,77,77,77                 | 0     |
| 60  | MG   | AA    | 3040 | 1/1   | 0.94 | 0.14 | -    | 21,21,21,21                 | 0     |
| 60  | MG   | BA    | 2999 | 1/1   | 0.93 | 0.41 | -    | 26,26,26,26                 | 0     |
| 60  | MG   | Aa    | 1621 | 1/1   | 0.74 | 0.30 | -    | 89,89,89,89                 | 0     |
| 60  | MG   | BA    | 3104 | 1/1   | 0.92 | 0.20 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | AA    | 3104 | 1/1   | 0.79 | 0.33 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 3047 | 1/1   | 0.93 | 0.27 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | AA    | 2952 | 1/1   | 0.74 | 0.44 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | AA    | 3210 | 1/1   | 0.62 | 0.17 | -    | 115,115,115,115             | 0     |
| 60  | MG   | AA    | 3180 | 1/1   | 0.95 | 0.22 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | Aa    | 1647 | 1/1   | 0.87 | 0.21 | -    | 138,138,138,138             | 0     |
| 60  | MG   | AA    | 3081 | 1/1   | 0.96 | 0.34 | -    | 99,99,99,99                 | 0     |
| 60  | MG   | BA    | 3193 | 1/1   | 0.95 | 0.44 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | Aa    | 1626 | 1/1   | 0.92 | 0.12 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | AA    | 3136 | 1/1   | 0.82 | 0.64 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | BA    | 3151 | 1/1   | 0.60 | 0.99 | -    | 119,119,119,119             | 0     |
| 60  | MG   | Aa    | 1692 | 1/1   | 0.89 | 0.63 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | AA    | 3053 | 1/1   | 0.97 | 0.64 | -    | 42,42,42,42                 | 0     |
| 60  | MG   | AA    | 3135 | 1/1   | 0.90 | 0.59 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | BA    | 3227 | 1/1   | 0.94 | 0.64 | -    | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3108 | 1/1   | 0.98 | 0.13 | -    | 38,38,38,38                 | 0     |
| 60  | MG   | BA    | 3243 | 1/1   | 0.81 | 1.07 | -    | 111,111,111,111             | 0     |
| 60  | MG   | AA    | 3087 | 1/1   | 0.90 | 0.37 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | BA    | 3173 | 1/1   | 0.70 | 0.96 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | Aa    | 1646 | 1/1   | 0.62 | 0.90 | -    | 102,102,102,102             | 0     |
| 60  | MG   | Aa    | 1724 | 1/1   | 0.93 | 0.17 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | Aa    | 1705 | 1/1   | 0.69 | 0.51 | -    | 71,71,71,71                 | 0     |
| 60  | MG   | BA    | 3213 | 1/1   | 0.97 | 0.17 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | Aa    | 1728 | 1/1   | 0.96 | 0.55 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | BA    | 3058 | 1/1   | 0.82 | 0.49 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | Ba    | 1625 | 1/1   | 0.95 | 0.20 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | Aa    | 1690 | 1/1   | 0.79 | 0.21 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | BA    | 3233 | 1/1   | 0.72 | 0.42 | -    | 97,97,97,97                 | 0     |
| 60  | MG   | BA    | 3222 | 1/1   | 0.70 | 0.52 | -    | 61,61,61,61                 | 0     |
| 60  | MG   | BA    | 2954 | 1/1   | 0.95 | 0.22 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3111 | 1/1   | 0.93 | 0.66 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | Ba    | 1743 | 1/1   | 0.92 | 0.55 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3262 | 1/1   | 0.02 | 1.11 | -    | 81,81,81,81                 | 0     |
| 60  | MG   | Aa    | 1719 | 1/1   | 0.81 | 0.39 | -    | 101,101,101,101             | 0     |
| 60  | MG   | Ba    | 1635 | 1/1   | 0.65 | 0.61 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | Ba    | 1656 | 1/1   | 0.79 | 0.51 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | AA    | 3222 | 1/1   | 0.93 | 0.64 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | BA    | 3126 | 1/1   | 0.82 | 0.37 | -    | 122,122,122,122             | 0     |
| 60  | MG   | AA    | 2963 | 1/1   | 0.80 | 0.81 | -    | 46,46,46,46                 | 0     |
| 60  | MG   | AA    | 3225 | 1/1   | 0.91 | 0.18 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | BA    | 3019 | 1/1   | 0.96 | 0.35 | -    | 30,30,30,30                 | 0     |
| 60  | MG   | BA    | 3182 | 1/1   | 0.89 | 0.32 | -    | 63,63,63,63                 | 0     |
| 60  | MG   | Ba    | 1607 | 1/1   | 0.97 | 0.18 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | AA    | 3098 | 1/1   | 0.56 | 0.58 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | AA    | 3065 | 1/1   | 0.51 | 0.74 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | Ba    | 1700 | 1/1   | 0.69 | 0.50 | -    | 58,58,58,58                 | 0     |
| 60  | MG   | AA    | 3248 | 1/1   | 0.67 | 0.70 | -    | 106,106,106,106             | 0     |
| 60  | MG   | AA    | 2990 | 1/1   | 0.85 | 0.60 | -    | 34,34,34,34                 | 0     |
| 60  | MG   | AA    | 3216 | 1/1   | 0.70 | 0.47 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | AA    | 2954 | 1/1   | 0.55 | 0.53 | -    | 112,112,112,112             | 0     |
| 60  | MG   | AA    | 3192 | 1/1   | 0.88 | 1.12 | -    | 101,101,101,101             | 0     |
| 60  | MG   | AA    | 3020 | 1/1   | 0.88 | 0.29 | -    | 39,39,39,39                 | 0     |
| 60  | MG   | BA    | 2948 | 1/1   | 0.65 | 0.50 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | BA    | 2971 | 1/1   | 0.78 | 0.93 | -    | 66,66,66,66                 | 0     |
| 60  | MG   | AA    | 3018 | 1/1   | 0.94 | 0.49 | -    | 48,48,48,48                 | 0     |
| 60  | MG   | AA    | 3181 | 1/1   | 0.59 | 0.46 | -    | 61,61,61,61                 | 0     |
| 60  | MG   | Aa    | 1718 | 1/1   | 0.95 | 1.02 | -    | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | BA    | 3221 | 1/1   | 0.64 | 0.44 | -    | 106,106,106,106             | 0     |
| 60  | MG   | Aa    | 1704 | 1/1   | 0.70 | 0.42 | -    | 29,29,29,29                 | 1     |
| 60  | MG   | Aa    | 1743 | 1/1   | 0.68 | 0.60 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | BA    | 3255 | 1/1   | 0.96 | 0.34 | -    | 81,81,81,81                 | 0     |
| 60  | MG   | Aa    | 1741 | 1/1   | 0.59 | 1.45 | -    | 79,79,79,79                 | 0     |
| 60  | MG   | AA    | 2910 | 1/1   | 0.93 | 0.54 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | BA    | 3226 | 1/1   | 0.92 | 0.35 | -    | 75,75,75,75                 | 0     |
| 60  | MG   | AA    | 3242 | 1/1   | 0.86 | 0.89 | -    | 85,85,85,85                 | 0     |
| 60  | MG   | AA    | 3009 | 1/1   | 0.99 | 0.45 | -    | 31,31,31,31                 | 0     |
| 60  | MG   | Ba    | 1733 | 1/1   | 0.22 | 0.39 | -    | 86,86,86,86                 | 0     |
| 60  | MG   | BA    | 3166 | 1/1   | 0.91 | 0.13 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | AA    | 2948 | 1/1   | 0.93 | 0.25 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | AA    | 3152 | 1/1   | 0.78 | 0.83 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | BA    | 3190 | 1/1   | 0.98 | 0.29 | -    | 13,13,13,13                 | 0     |
| 60  | MG   | BA    | 3146 | 1/1   | 0.59 | 0.85 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | Aa    | 1636 | 1/1   | 0.45 | 1.40 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | AA    | 2946 | 1/1   | 0.98 | 0.10 | -    | 101,101,101,101             | 0     |
| 60  | MG   | AA    | 2959 | 1/1   | 0.65 | 0.44 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | AB    | 202  | 1/1   | 0.74 | 0.40 | -    | 62,62,62,62                 | 0     |
| 60  | MG   | Aa    | 1672 | 1/1   | 0.65 | 0.33 | -    | 87,87,87,87                 | 0     |
| 60  | MG   | Ba    | 1649 | 1/1   | 0.86 | 0.36 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | Ba    | 1638 | 1/1   | 0.84 | 0.24 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | BA    | 2955 | 1/1   | 0.73 | 0.26 | -    | 49,49,49,49                 | 0     |
| 60  | MG   | Ba    | 1681 | 1/1   | 0.45 | 0.84 | -    | 122,122,122,122             | 0     |
| 60  | MG   | Aa    | 1700 | 1/1   | 0.57 | 2.14 | -    | 114,114,114,114             | 0     |
| 60  | MG   | A1    | 102  | 1/1   | 0.97 | 0.42 | -    | 116,116,116,116             | 0     |
| 60  | MG   | BA    | 3089 | 1/1   | 0.97 | 0.20 | -    | 56,56,56,56                 | 0     |
| 60  | MG   | BA    | 3239 | 1/1   | 0.67 | 0.27 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | Bv    | 104  | 1/1   | 0.70 | 1.01 | -    | 75,75,75,75                 | 1     |
| 60  | MG   | AA    | 3078 | 1/1   | 0.97 | 0.14 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | AA    | 3139 | 1/1   | 0.89 | 0.40 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | Ba    | 1603 | 1/1   | 0.94 | 0.10 | -    | 64,64,64,64                 | 0     |
| 60  | MG   | BA    | 3244 | 1/1   | 0.68 | 0.23 | -    | 91,91,91,91                 | 0     |
| 60  | MG   | AA    | 3112 | 1/1   | 0.92 | 0.34 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | Ba    | 1643 | 1/1   | 0.76 | 0.37 | -    | 108,108,108,108             | 0     |
| 60  | MG   | AA    | 3109 | 1/1   | 0.88 | 0.31 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | BA    | 3215 | 1/1   | 0.95 | 0.39 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | AA    | 3209 | 1/1   | 0.83 | 0.66 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | AA    | 2998 | 1/1   | 0.97 | 0.28 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | BA    | 3141 | 1/1   | 0.89 | 0.55 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | Aa    | 1606 | 1/1   | 0.89 | 0.82 | -    | 66,66,66,66                 | 0     |
| 60  | MG   | Ba    | 1661 | 1/1   | 0.93 | 0.29 | -    | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3047 | 1/1   | 0.95 | 0.51 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | BA    | 2901 | 1/1   | 0.85 | 0.21 | -    | 138,138,138,138             | 0     |
| 60  | MG   | BA    | 3099 | 1/1   | 0.85 | 0.77 | -    | 90,90,90,90                 | 0     |
| 60  | MG   | AA    | 3258 | 1/1   | 0.87 | 0.54 | -    | 38,38,38,38                 | 0     |
| 60  | MG   | AA    | 2977 | 1/1   | 0.97 | 0.84 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | BA    | 2958 | 1/1   | 0.75 | 1.59 | -    | 88,88,88,88                 | 0     |
| 60  | MG   | Ba    | 1617 | 1/1   | 0.95 | 0.25 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | AA    | 3149 | 1/1   | 0.90 | 0.85 | -    | 100,100,100,100             | 0     |
| 60  | MG   | Aa    | 1675 | 1/1   | 0.47 | 0.87 | -    | 72,72,72,72                 | 0     |
| 60  | MG   | AA    | 3041 | 1/1   | 0.99 | 0.18 | -    | 21,21,21,21                 | 0     |
| 60  | MG   | B0    | 102  | 1/1   | 0.92 | 0.21 | -    | 47,47,47,47                 | 0     |
| 60  | MG   | AA    | 3125 | 1/1   | 0.98 | 0.66 | -    | 42,42,42,42                 | 0     |
| 60  | MG   | BA    | 3002 | 1/1   | 0.99 | 0.25 | -    | 41,41,41,41                 | 0     |
| 60  | MG   | AA    | 3005 | 1/1   | 0.96 | 0.23 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | AA    | 3034 | 1/1   | 0.68 | 0.60 | -    | 55,55,55,55                 | 0     |
| 60  | MG   | BA    | 2938 | 1/1   | 0.53 | 1.22 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | BA    | 3260 | 1/1   | 0.91 | 1.12 | -    | 80,80,80,80                 | 0     |
| 60  | MG   | Ba    | 1711 | 1/1   | 0.68 | 0.35 | -    | 123,123,123,123             | 0     |
| 60  | MG   | AA    | 3004 | 1/1   | 0.96 | 0.23 | -    | 39,39,39,39                 | 0     |
| 60  | MG   | AA    | 2961 | 1/1   | 0.92 | 0.49 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | BA    | 3136 | 1/1   | 0.60 | 0.74 | -    | 106,106,106,106             | 0     |
| 60  | MG   | AA    | 3043 | 1/1   | 0.98 | 0.19 | -    | 37,37,37,37                 | 0     |
| 60  | MG   | AA    | 3127 | 1/1   | 0.90 | 0.46 | -    | 89,89,89,89                 | 0     |
| 60  | MG   | Aa    | 1630 | 1/1   | 0.99 | 0.11 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | AA    | 3116 | 1/1   | 0.69 | 0.40 | -    | 35,35,35,35                 | 0     |
| 60  | MG   | Aa    | 1663 | 1/1   | 0.31 | 0.54 | -    | 112,112,112,112             | 0     |
| 60  | MG   | Ba    | 1719 | 1/1   | 0.72 | 0.68 | -    | 57,57,57,57                 | 0     |
| 60  | MG   | Bx    | 101  | 1/1   | 0.56 | 0.28 | -    | 83,83,83,83                 | 0     |
| 60  | MG   | BA    | 2906 | 1/1   | 0.97 | 0.22 | -    | 26,26,26,26                 | 0     |
| 60  | MG   | AA    | 2984 | 1/1   | 0.98 | 0.21 | -    | 45,45,45,45                 | 0     |
| 60  | MG   | BA    | 2937 | 1/1   | 0.91 | 0.26 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | BA    | 3108 | 1/1   | 0.98 | 0.13 | -    | 50,50,50,50                 | 0     |
| 60  | MG   | Ba    | 1701 | 1/1   | 0.97 | 0.47 | -    | 60,60,60,60                 | 0     |
| 60  | MG   | AA    | 2983 | 1/1   | 0.90 | 0.28 | -    | 27,27,27,27                 | 0     |
| 60  | MG   | BA    | 3075 | 1/1   | 0.94 | 0.29 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | AA    | 3167 | 1/1   | 0.95 | 0.48 | -    | 73,73,73,73                 | 0     |
| 60  | MG   | AA    | 3026 | 1/1   | 0.86 | 0.23 | -    | 35,35,35,35                 | 0     |
| 60  | MG   | BA    | 3054 | 1/1   | 0.92 | 0.40 | -    | 36,36,36,36                 | 0     |
| 60  | MG   | Aa    | 1664 | 1/1   | 0.81 | 0.58 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | BA    | 3064 | 1/1   | 0.88 | 0.29 | -    | 44,44,44,44                 | 0     |
| 60  | MG   | AA    | 3208 | 1/1   | 0.87 | 0.76 | -    | 86,86,86,86                 | 0     |
| 60  | MG   | Aa    | 1648 | 1/1   | 0.12 | 0.59 | -    | 121,121,121,121             | 0     |

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*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60  | MG   | AA    | 3006 | 1/1   | 0.91 | 0.28 | -    | 32,32,32,32                 | 0     |
| 60  | MG   | BA    | 3251 | 1/1   | 0.82 | 0.29 | -    | 65,65,65,65                 | 0     |
| 60  | MG   | AA    | 3244 | 1/1   | 0.79 | 0.99 | -    | 67,67,67,67                 | 0     |
| 60  | MG   | Aw    | 101  | 1/1   | 0.78 | 0.44 | -    | 83,83,83,83                 | 1     |
| 60  | MG   | BA    | 3219 | 1/1   | 0.83 | 0.46 | -    | 40,40,40,40                 | 0     |
| 60  | MG   | Ba    | 1613 | 1/1   | 0.94 | 0.85 | -    | 38,38,38,38                 | 0     |
| 60  | MG   | BX    | 101  | 1/1   | 0.94 | 0.60 | -    | 31,31,31,31                 | 1     |
| 60  | MG   | B5    | 102  | 1/1   | 0.83 | 0.60 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | AA    | 3230 | 1/1   | 0.85 | 0.99 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | AA    | 2936 | 1/1   | 0.96 | 0.53 | -    | 5,5,5,5                     | 0     |
| 60  | MG   | Aa    | 1706 | 1/1   | 0.77 | 0.58 | -    | 54,54,54,54                 | 0     |
| 60  | MG   | Ba    | 1645 | 1/1   | 0.79 | 1.00 | -    | 101,101,101,101             | 0     |
| 60  | MG   | BA    | 3154 | 1/1   | 0.85 | 0.21 | -    | 73,73,73,73                 | 1     |
| 60  | MG   | BA    | 3139 | 1/1   | 0.98 | 0.14 | -    | 15,15,15,15                 | 0     |
| 60  | MG   | AA    | 3130 | 1/1   | 0.76 | 0.63 | -    | 76,76,76,76                 | 0     |
| 60  | MG   | Aa    | 1722 | 1/1   | 0.55 | 0.36 | -    | 78,78,78,78                 | 0     |
| 60  | MG   | AA    | 3048 | 1/1   | 0.79 | 0.42 | -    | 68,68,68,68                 | 0     |
| 60  | MG   | BA    | 3258 | 1/1   | 0.49 | 0.36 | -    | 84,84,84,84                 | 0     |
| 60  | MG   | AA    | 3092 | 1/1   | 0.87 | 0.23 | -    | 51,51,51,51                 | 0     |
| 60  | MG   | AA    | 3114 | 1/1   | 0.90 | 0.39 | -    | 18,18,18,18                 | 1     |
| 60  | MG   | AA    | 2905 | 1/1   | 0.93 | 0.36 | -    | 15,15,15,15                 | 0     |
| 60  | MG   | BA    | 3062 | 1/1   | 0.95 | 0.25 | -    | 36,36,36,36                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.