



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 27, 2017 – 08:25 PM EDT

PDB ID : 4L71  
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-A on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : unknown  
Resolution : 3.90 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:

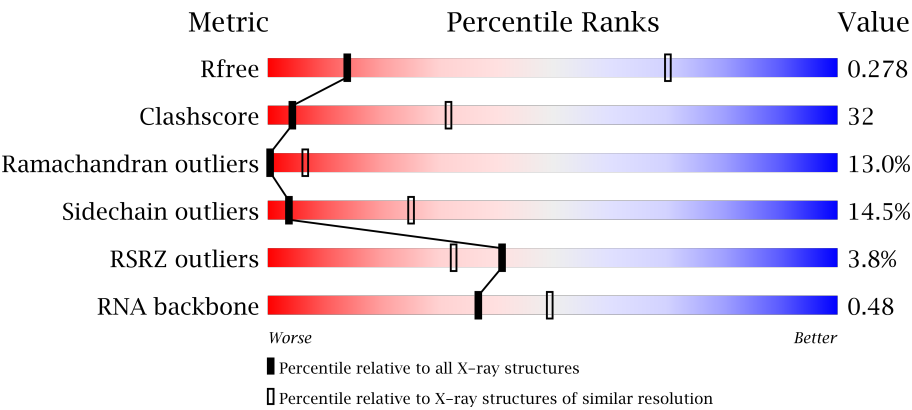
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1007 (4.20-3.60)                                      |
| Clashscore            | 112137                      | 1103 (4.20-3.60)                                      |
| Ramachandran outliers | 110173                      | 1062 (4.20-3.60)                                      |
| Sidechain outliers    | 110143                      | 1053 (4.20-3.60)                                      |
| RSRZ outliers         | 101464                      | 1020 (4.20-3.60)                                      |
| RNA backbone          | 2435                        | 1018 (4.84-2.90)                                      |

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   | QA    | 1522   | <div><div>2%</div><div><div></div><div>45%</div><div>42%</div><div>11%</div><div>..</div></div></div> |
| 1   | XA    | 1522   | <div><div>0%</div><div><div></div><div>43%</div><div>42%</div><div>12%</div><div>..</div></div></div> |
| 2   | QB    | 256    | <div><div>6%</div><div><div></div><div>17%</div><div>59%</div><div>16%</div><div>7%</div></div></div> |
| 2   | XB    | 256    | <div><div>4%</div><div><div></div><div>17%</div><div>59%</div><div>16%</div><div>7%</div></div></div> |

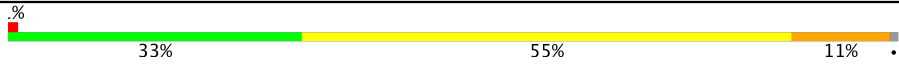
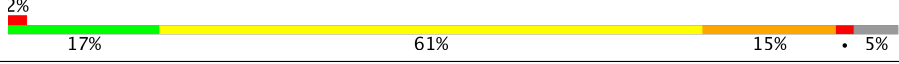
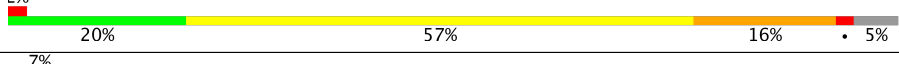
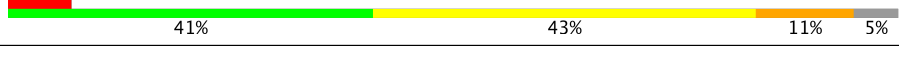
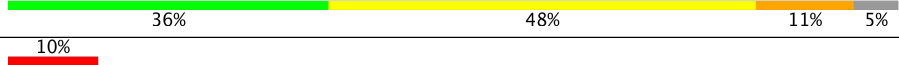
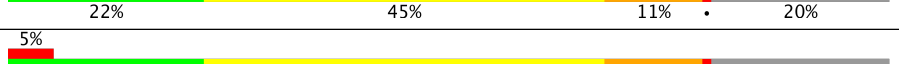
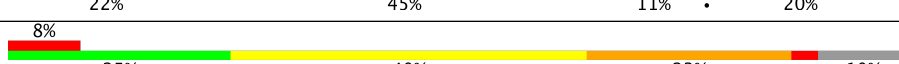
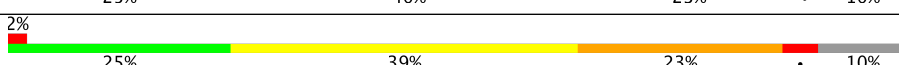
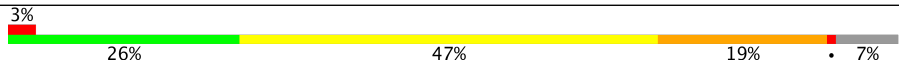
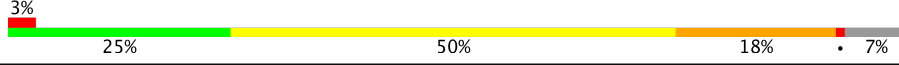
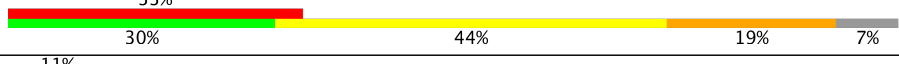
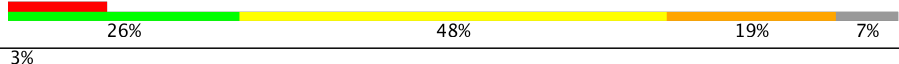
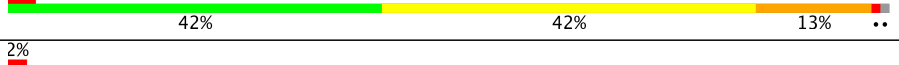

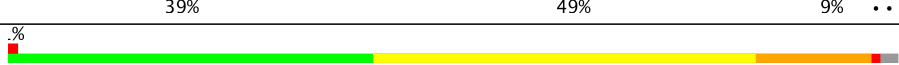
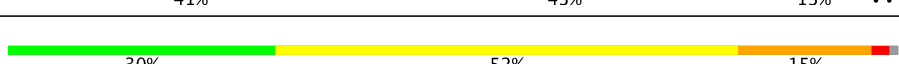
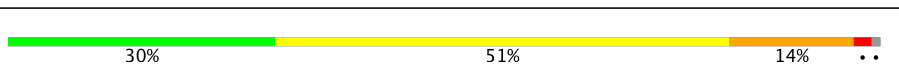
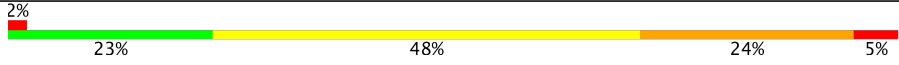
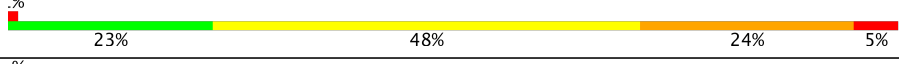


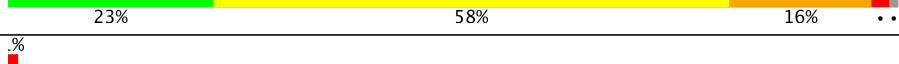
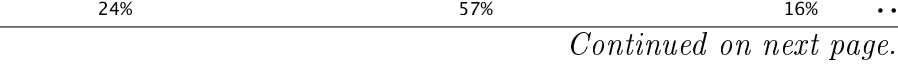


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | QC    | 239    |                  |
| 3   | XC    | 239    |                  |
| 4   | QD    | 209    |                  |
| 4   | XD    | 209    |   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

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | XO    | 89     |    |
| 16  | QP    | 88     |    |
| 16  | XP    | 88     |    |
| 17  | QQ    | 105    |    |
| 17  | XQ    | 105    |    |
| 18  | QR    | 88     |    |
| 18  | XR    | 88     |    |
| 19  | QS    | 93     |    |
| 19  | XS    | 93     |    |
| 20  | QT    | 106    |    |
| 20  | XT    | 106    |   |
| 21  | QU    | 27     |  |
| 21  | XU    | 27     |  |
| 22  | RA    | 2916   |  |
| 22  | YA    | 2916   |  |
| 23  | RB    | 122    |  |
| 23  | YB    | 122    |  |
| 24  | RD    | 276    |  |
| 24  | YD    | 276    |  |
| 25  | RE    | 206    |  |
| 25  | YE    | 206    |  |
| 26  | RF    | 210    |  |
| 26  | YF    | 210    |  |
| 27  | RG    | 182    |  |
| 27  | YG    | 182    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | RH    | 180    |                  |
| 28  | YH    | 180    |                  |
| 29  | RI    | 148    |                  |
| 29  | YI    | 148    |                  |
| 30  | RN    | 140    |                  |
| 30  | YN    | 140    |                  |
| 31  | RO    | 122    |                  |
| 31  | YO    | 122    |                  |
| 32  | RP    | 150    |                  |
| 32  | YP    | 150    |                  |
| 33  | RQ    | 141    |                  |
| 33  | YQ    | 141    |                  |
| 34  | RR    | 118    |                  |
| 34  | YR    | 118    |                  |
| 35  | RS    | 112    |                  |
| 35  | YS    | 112    |                  |
| 36  | RT    | 146    |                  |
| 36  | YT    | 146    |                  |
| 37  | RU    | 118    |                  |
| 37  | YU    | 118    |                  |
| 38  | RV    | 101    |                  |
| 38  | YV    | 101    |                  |
| 39  | RW    | 113    |                  |
| 39  | YW    | 113    |                  |
| 40  | RX    | 96     |                  |

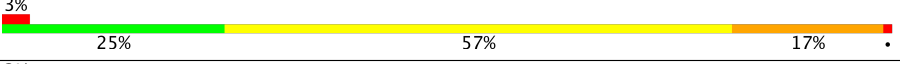


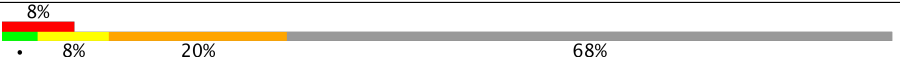
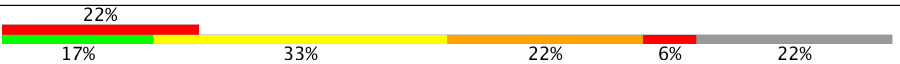
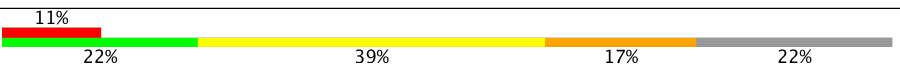
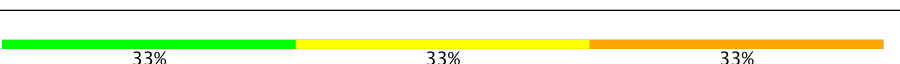
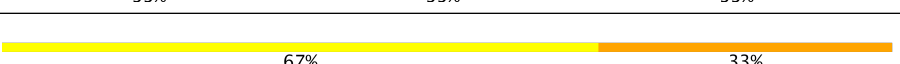
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | YX    | 96     |                  |
| 41  | RY    | 110    |                  |
| 41  | YY    | 110    |                  |
| 42  | RZ    | 206    |                  |
| 42  | YZ    | 206    |                  |
| 43  | R0    | 85     |                  |
| 43  | Y0    | 85     |                  |
| 44  | R1    | 98     |                  |
| 44  | Y1    | 98     |                  |
| 45  | R2    | 72     |                  |
| 45  | Y2    | 72     |                  |
| 46  | R3    | 60     |                  |
| 46  | Y3    | 60     |                  |
| 47  | R4    | 71     |                  |
| 47  | Y4    | 71     |                  |
| 48  | R5    | 60     |                  |
| 48  | Y5    | 60     |                  |
| 49  | R6    | 54     |                  |
| 49  | Y6    | 54     |                  |
| 50  | R7    | 49     |                  |
| 50  | Y7    | 49     |                  |
| 51  | R8    | 65     |                  |
| 51  | Y8    | 65     |                  |
| 52  | R9    | 37     |                  |
| 52  | Y9    | 37     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 53  | QV    | 77     |  |
| 53  | XV    | 77     |  |
| 54  | QX    | 25     |  |
| 54  | XX    | 25     |  |
| 55  | QY    | 18     |  |
| 55  | XY    | 18     |  |
| 56  | Z6    | 3      |  |
| 56  | Z8    | 3      |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | QA    | 1604 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1610 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1612 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1613 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1617 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1631 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1639 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1645 | -         | -        | -       | X                |
| 57  | MG   | QA    | 1646 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3003 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3005 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3007 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3009 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3013 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3018 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3020 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3022 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3023 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3025 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3027 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3033 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3034 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3035 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | RA    | 3036 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3037 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3038 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3042 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3044 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3051 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3052 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3054 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3056 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3057 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3060 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3061 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3062 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3064 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3065 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3066 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3074 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3077 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3079 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3081 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3083 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3086 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3087 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3088 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3089 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3093 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3096 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3099 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3100 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3101 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3107 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3109 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3118 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3122 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3123 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3124 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3126 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3127 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3132 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3138 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3149 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3152 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | RA    | 3153 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3157 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3164 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3172 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3173 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3177 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3181 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3184 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3185 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3186 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3201 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3211 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3219 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3222 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3223 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3226 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3240 | -         | -        | -       | X                |
| 57  | MG   | RA    | 3242 | -         | -        | -       | X                |
| 57  | MG   | RP    | 201  | -         | -        | -       | X                |
| 57  | MG   | XA    | 1603 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1604 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1607 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1608 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1610 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1611 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1612 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1615 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1618 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1619 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1623 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1625 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1634 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1635 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1644 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1645 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1646 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1650 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1656 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1664 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1668 | -         | -        | -       | X                |
| 57  | MG   | XA    | 1672 | -         | -        | -       | X                |
| 57  | MG   | XV    | 101  | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | YA    | 3002 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3006 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3009 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3011 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3014 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3015 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3017 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3019 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3023 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3024 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3025 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3026 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3031 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3032 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3033 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3034 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3037 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3038 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3041 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3042 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3044 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3045 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3048 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3049 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3050 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3053 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3056 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3057 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3067 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3071 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3072 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3073 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3077 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3078 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3079 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3085 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3088 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3092 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3093 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3097 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3098 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3099 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | YA    | 3106 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3107 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3111 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3113 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3114 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3116 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3118 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3134 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3135 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3140 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3142 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3151 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3152 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3156 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3157 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3162 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3163 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3165 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3169 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3173 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3176 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3178 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3179 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3180 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3182 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3184 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3191 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3193 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3195 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3196 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3202 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3203 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3205 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3206 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3209 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3213 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3215 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3216 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3217 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3226 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3241 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3254 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | YA    | 3257 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3259 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3260 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3261 | -         | -        | -       | X                |
| 57  | MG   | YA    | 3262 | -         | -        | -       | X                |
| 57  | MG   | YB    | 203  | -         | -        | -       | X                |
| 57  | MG   | YX    | 101  | -         | -        | -       | X                |
| 58  | PAR  | QA    | 1666 | -         | -        | -       | X                |
| 58  | PAR  | XA    | 1673 | -         | -        | -       | X                |
| 59  | ZN   | R9    | 101  | -         | -        | -       | X                |
| 59  | ZN   | Y9    | 101  | -         | -        | -       | X                |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291950 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22  | RA    | 2882     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62071 | 27627 | 11611 | 19952 | 2881 |         |         |       |
| 22  | YA    | 2883     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62091 | 27636 | 11613 | 19960 | 2882 |         |         |       |

- Molecule 23 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23  | RB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |
| 23  | YB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24  | RD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |
| 24  | YD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | RE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 25  | YE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | RF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | YF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | RG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 27  | YG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | RH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |
| 28  | YH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | RI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |
| 29  | YI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | RN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 30  | YN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | RO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 31  | YO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | RP    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 32  | YP    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | RQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 33  | YQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | RR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 34  | YR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 35  | RS    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |
| 35  | YS    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | RT    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 36  | YT    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | RU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 37  | YU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | RV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 38  | YV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | RW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |
| 39  | YW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40  | RX    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |
| 40  | YX    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | RY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |
| 41  | YY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | RZ    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1461  | 933 | 260 | 265 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | YZ    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1461  | 933 | 260 | 265 | 3 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | R0    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 401 | 138 | 108 | 1 |         |         |       |
| 43  | Y0    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 401 | 138 | 108 | 1 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | R1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |
| 44  | Y1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | R2    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |
| 45  | Y2    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 46  | R3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 46  | Y3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | R4    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |         |       |
| 47  | Y4    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | R5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 48  | Y5    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 451   | 283 | 89 | 74 | 5 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 50  | R7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |
| 50  | Y7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51  | R8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |
| 51  | Y8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | R9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 52  | Y9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 53 is a RNA chain called P-site tRNA fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 53  | QV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1644  | 732 | 297 | 538 | 77 |         |         |       |
| 53  | XV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1644  | 732 | 297 | 538 | 77 |         |         |       |

- Molecule 54 is a RNA chain called A-site ASL SufA6.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 54  | QX    | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 169   | 76 | 31 | 54 | 8 |         |         |       |
| 54  | XX    | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 169   | 76 | 31 | 54 | 8 |         |         |       |

- Molecule 55 is a RNA chain called messenger RNA.

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

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

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

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | QA    | 65       | Total | Mg  | 0       | 0       |
|     |       |          | 65    | 65  |         |         |
| 57  | RP    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 57  | QX    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | YA    | 265      | Total | Mg  | 0       | 0       |
|     |       |          | 265   | 265 |         |         |
| 57  | QM    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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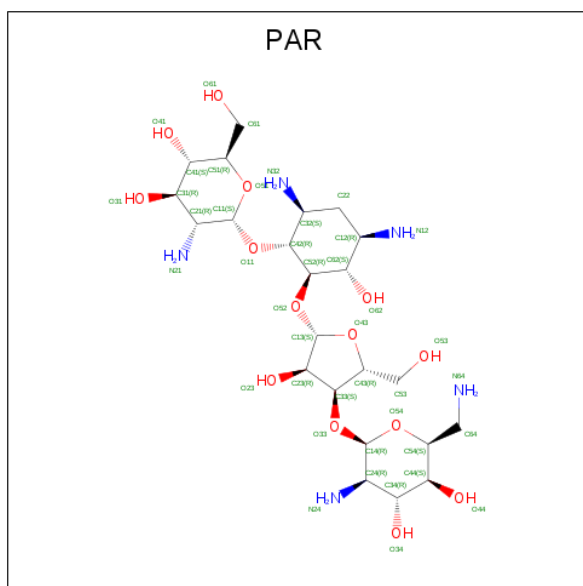
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | XX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | XA    | 72       | Total<br>72  | Mg<br>72  | 0       | 0       |
| 57  | RU    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | QH    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | YQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | R8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | YX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | Y7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | QF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | R5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RA    | 244      | Total<br>244 | Mg<br>244 | 0       | 0       |
| 57  | YP    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | Y5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | RE    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | YB    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | XV    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | RB    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | RF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | XM    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57  | YE    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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



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

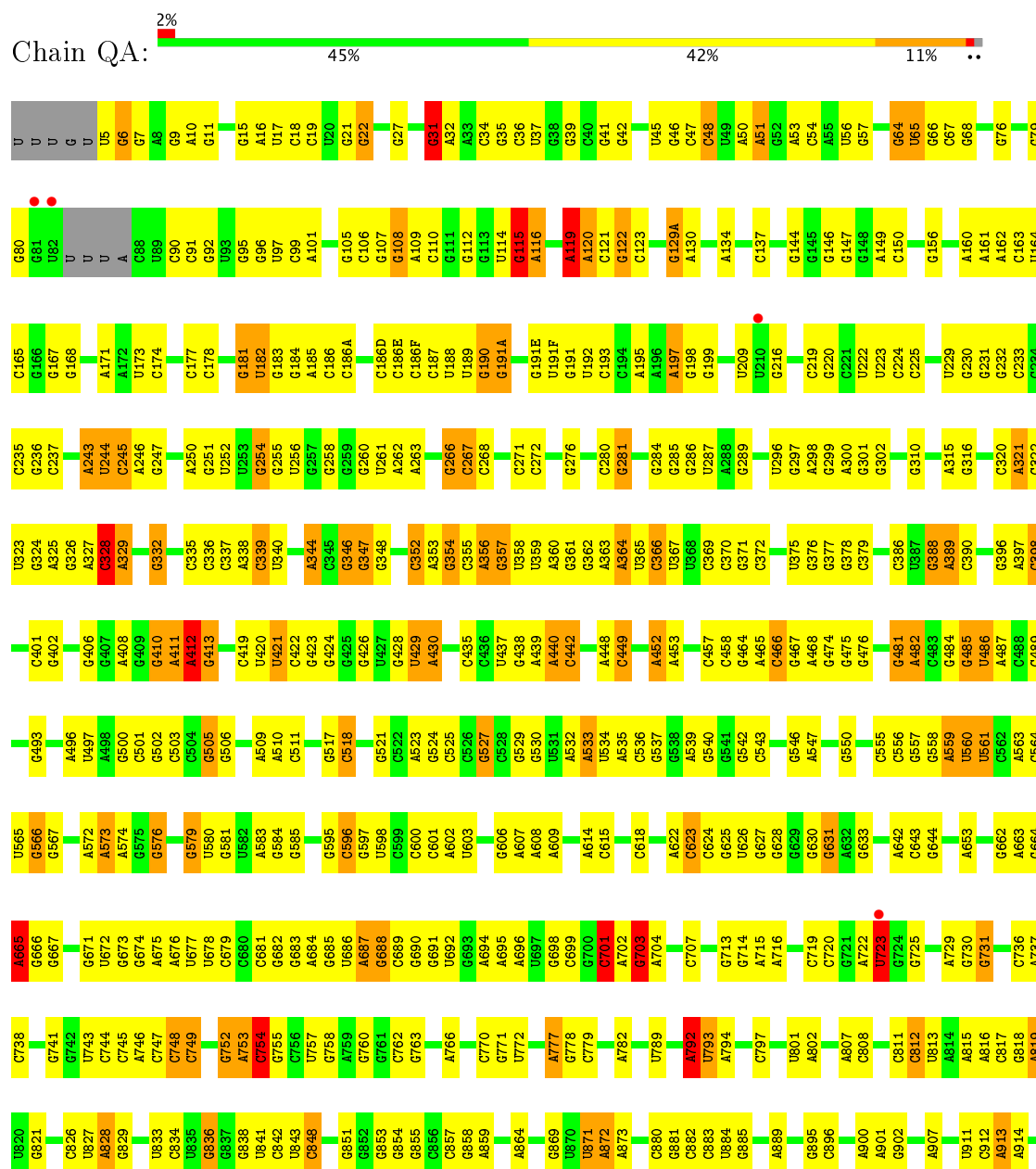
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | Y9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | QN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | XN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | QD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | XD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | R9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

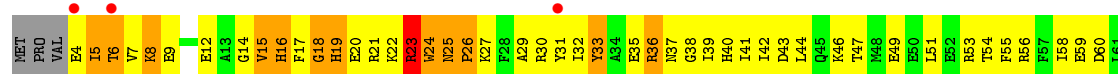
### 3 Residue-property plots

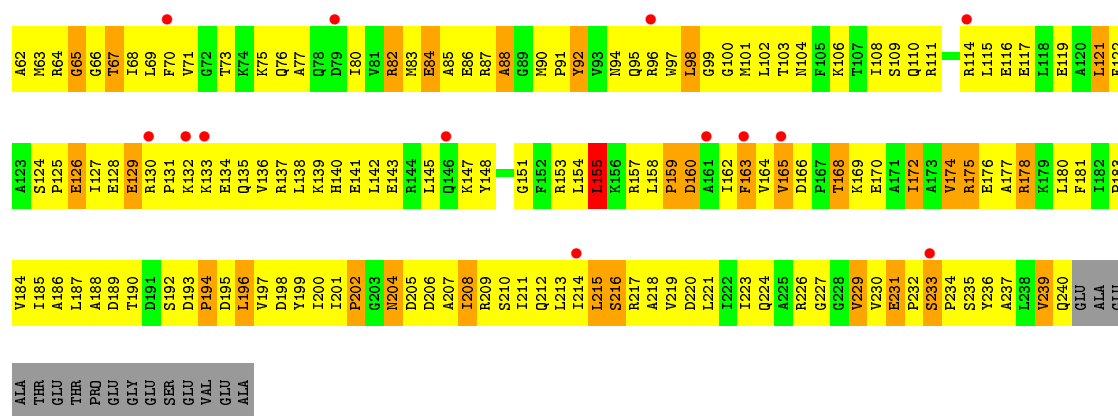
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S Ribosomal RNA

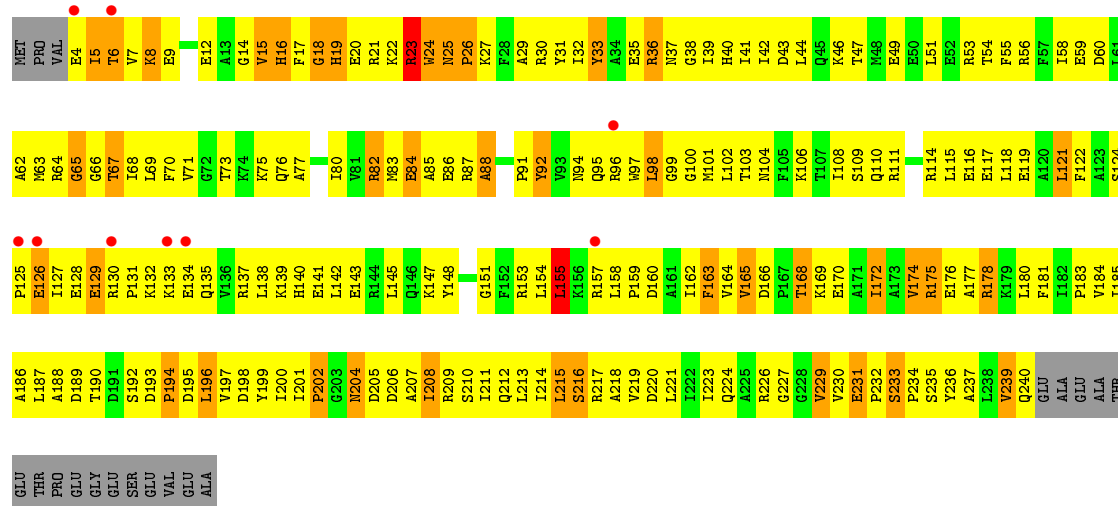




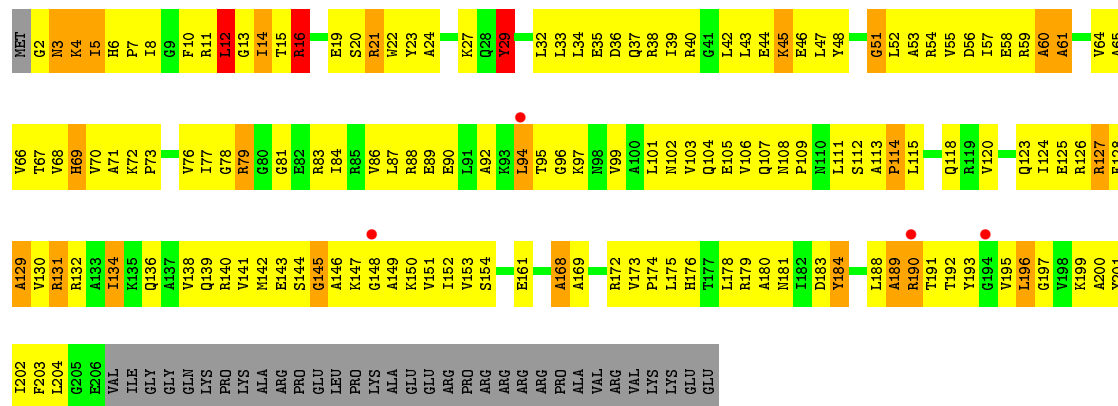




• Molecule 2: 30S ribosomal protein S2



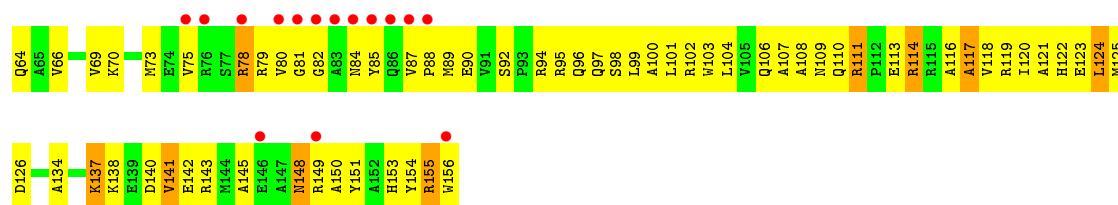
• Molecule 3: 30S ribosomal protein S3



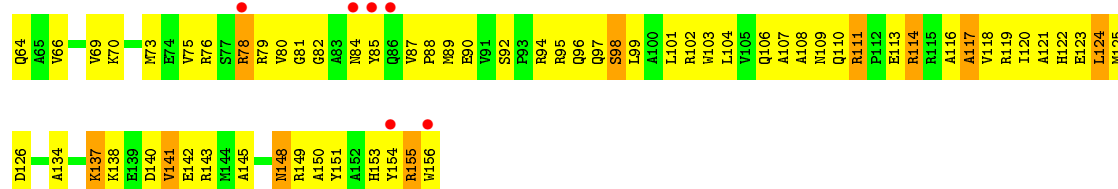
• Molecule 3: 30S ribosomal protein S3



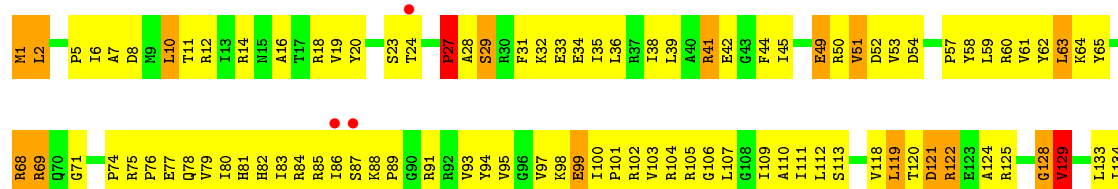




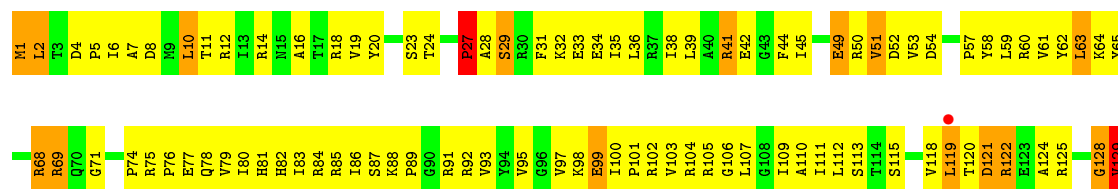
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

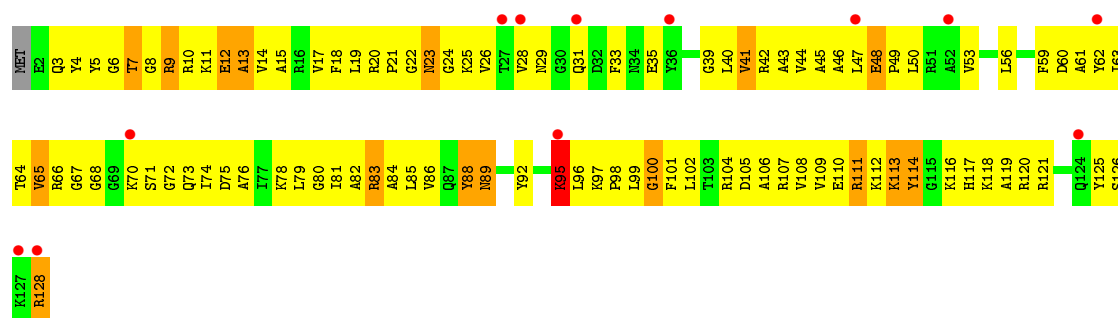


• Molecule 8: 30S ribosomal protein S8

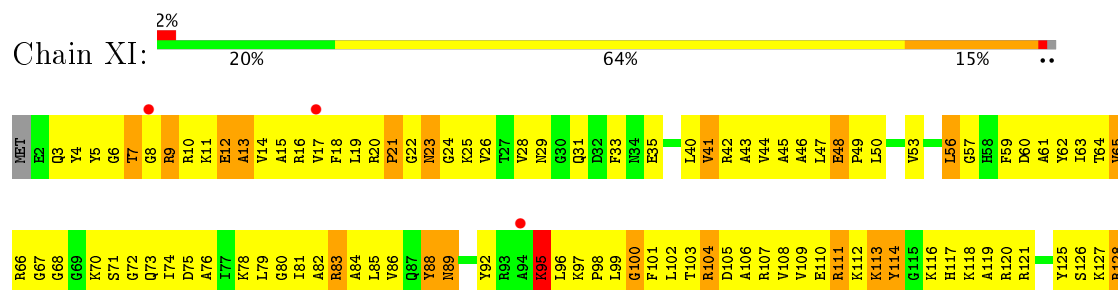


• Molecule 9: 30S ribosomal protein S9

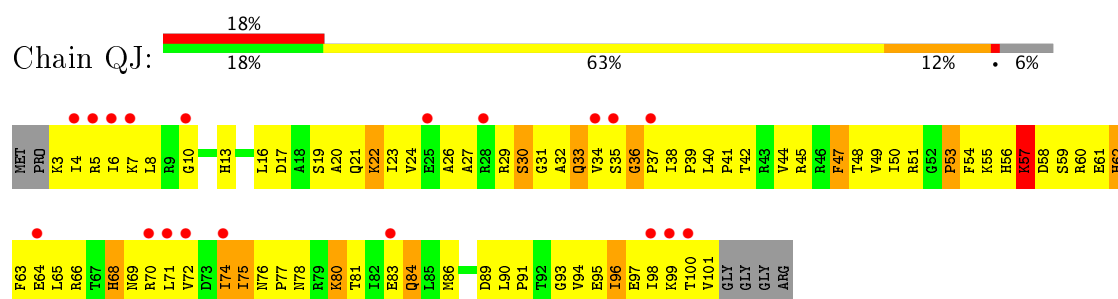




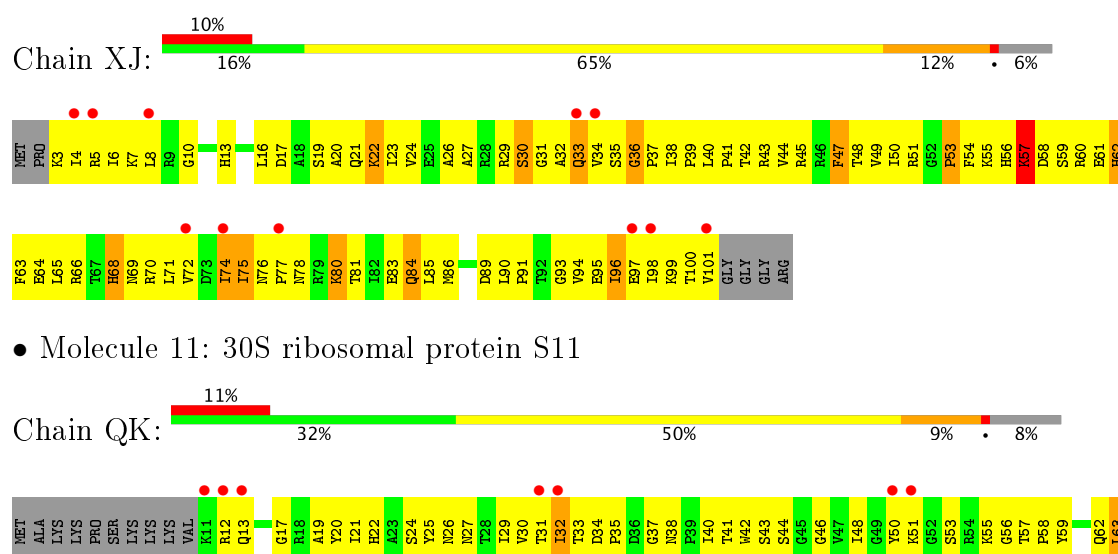
• Molecule 9: 30S ribosomal protein S9

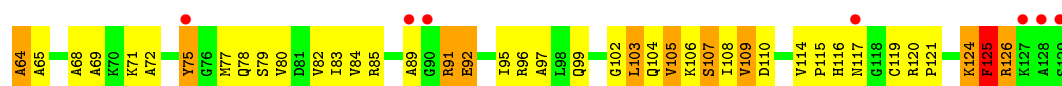


• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11





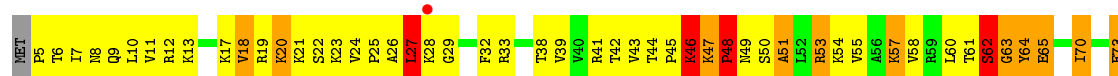
- Molecule 11: 30S ribosomal protein S11



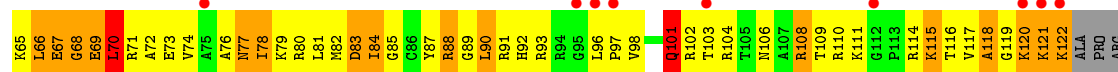
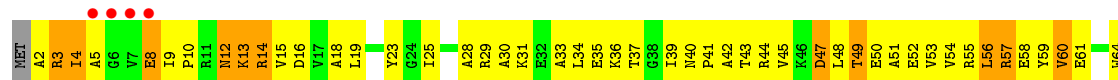
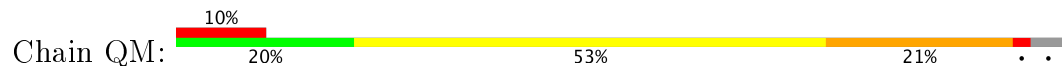
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

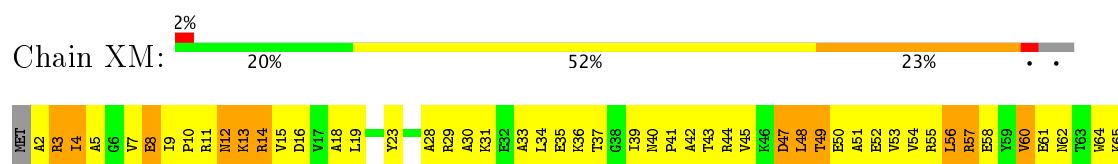


- Molecule 13: 30S ribosomal protein S13

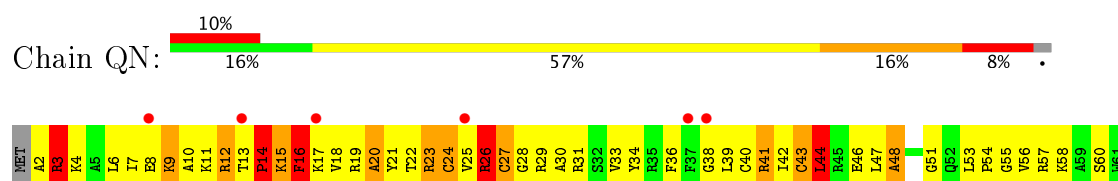


LYS

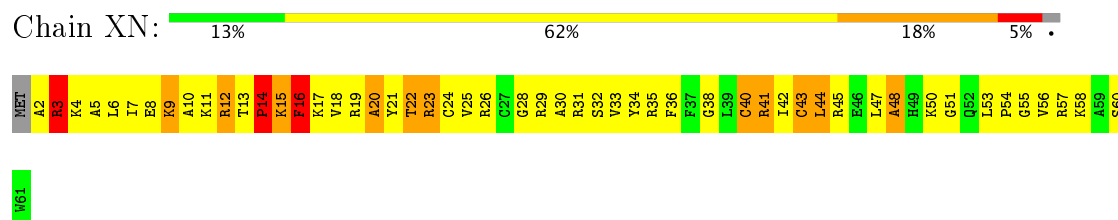
- Molecule 13: 30S ribosomal protein S13



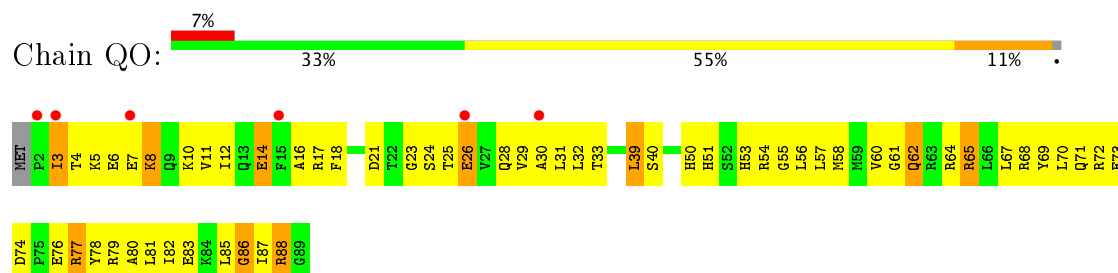
- Molecule 14: 30S ribosomal protein S14 type Z



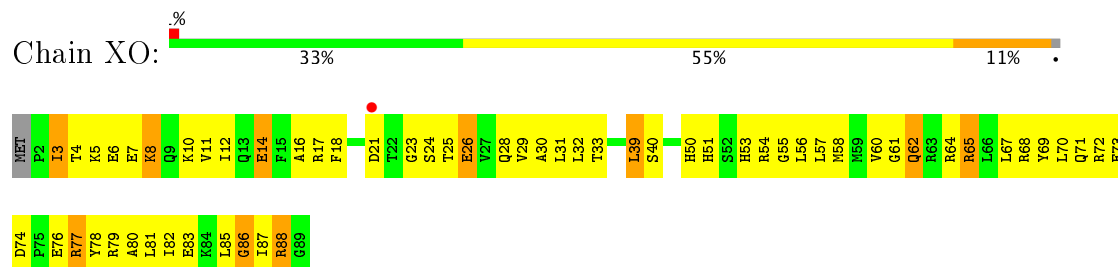
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

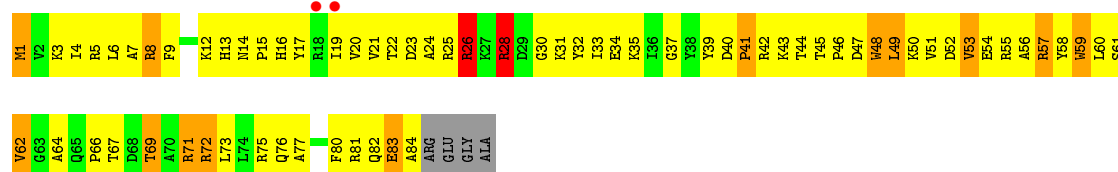


- Molecule 15: 30S ribosomal protein S15

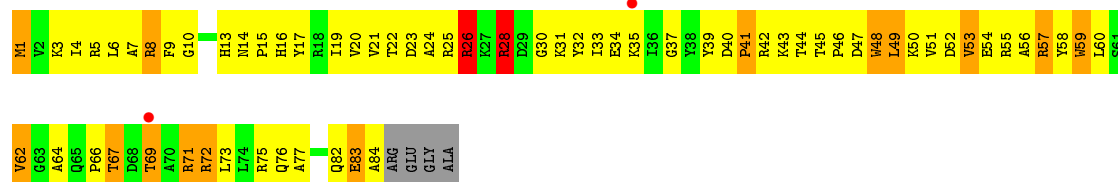


- Molecule 16: 30S ribosomal protein S16

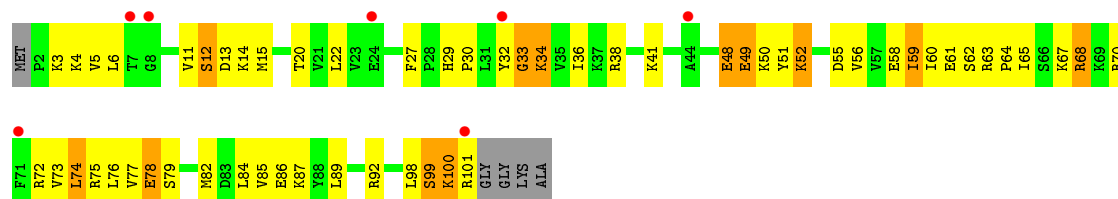
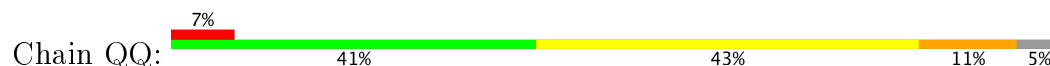




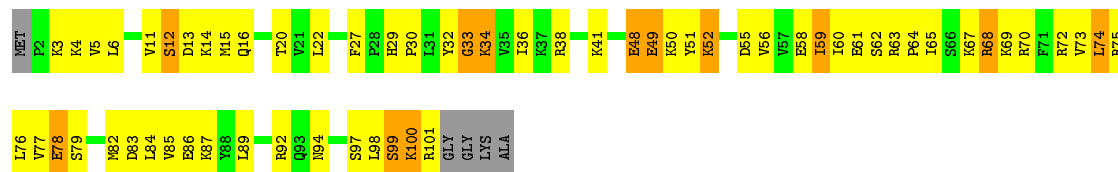
- Molecule 16: 30S ribosomal protein S16



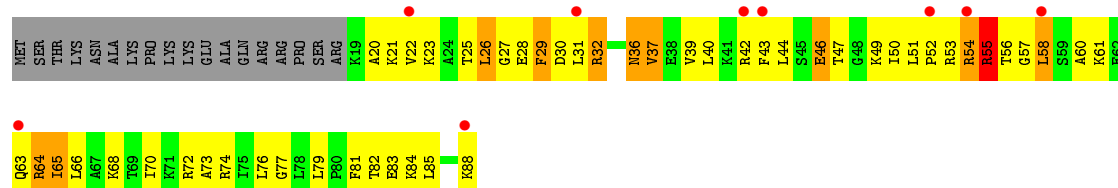
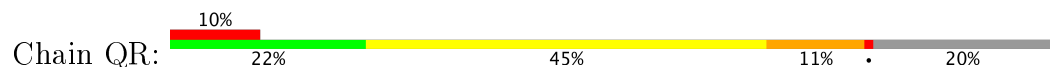
- Molecule 17: 30S ribosomal protein S17



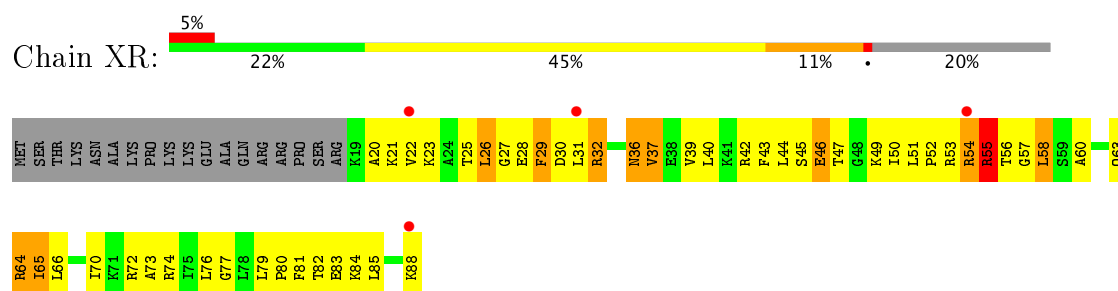
- Molecule 17: 30S ribosomal protein S17



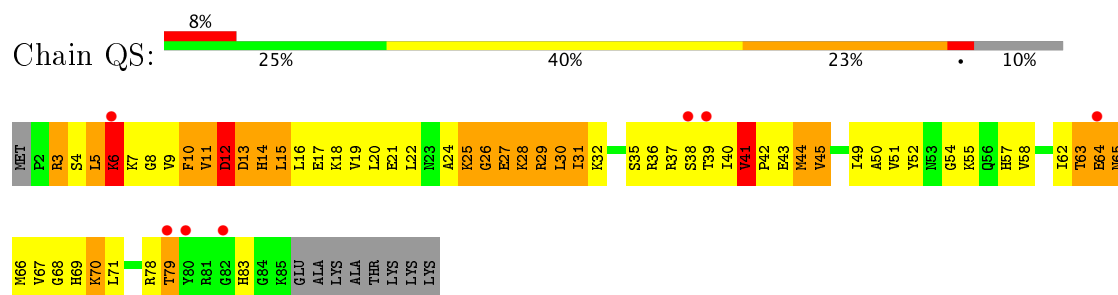
- Molecule 18: 30S ribosomal protein S18



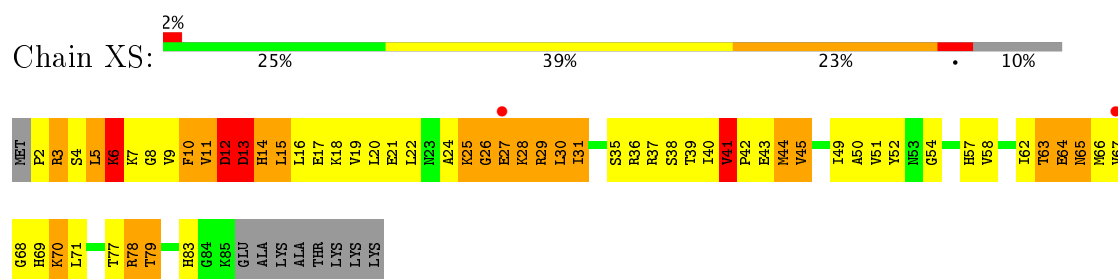
- Molecule 18: 30S ribosomal protein S18



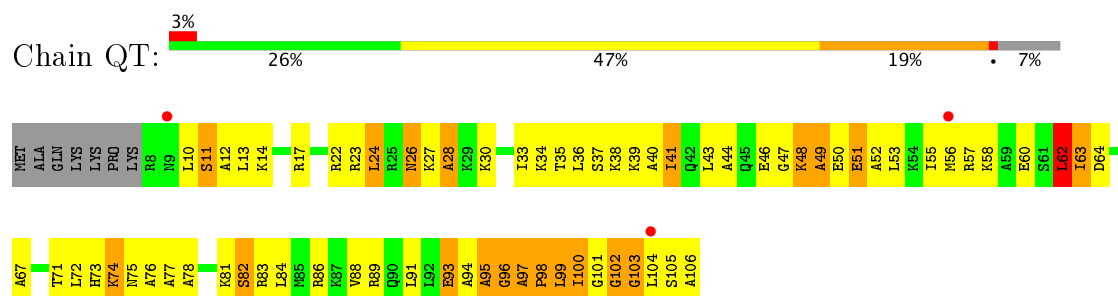
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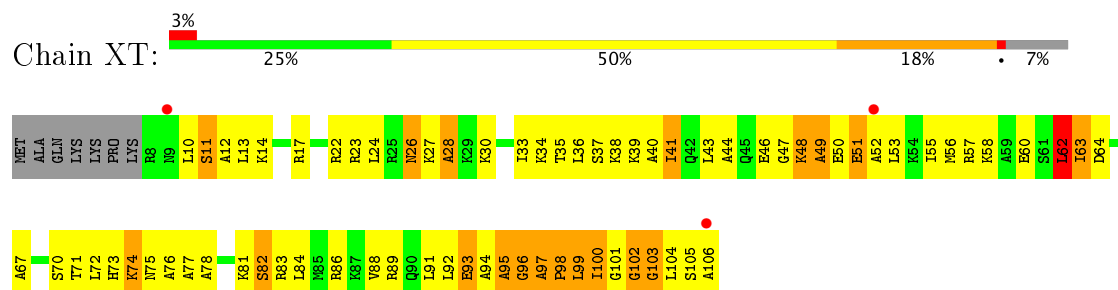
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20



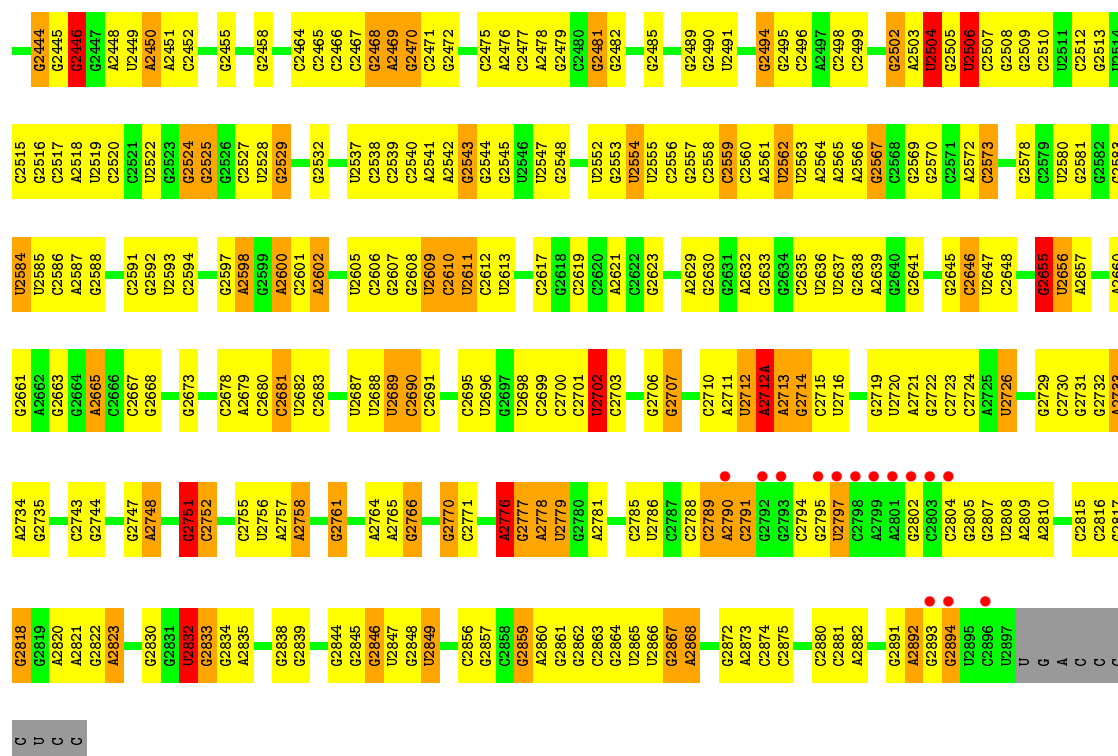


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| G1834 | A1759 | A1641 | C1564 | U1489 | U1445  | U1335 | G1259 | A1177 | A1096 | U1026 | U958  | G883 | A804 | C736 |
| G1835 | A1760 | C1644 | C1565 | C1493 | G1416  | U1336 | G1260 | C1178 | U1097 | A1027 | A959  | C884 | G805 | C737 |
| G1839 | C1761 | C1644 | A1566 | C1493 | C1417  | G1337 | C1261 | C1179 | A1098 | A1028 | A960  | C885 | C806 | G738 |
| G1845 | C1762 | C1644 | A1567 | A1494 | G1418  | G1338 | U1262 | C1180 | A1099 | A1029 | C961  | C886 | U807 | G739 |
| G1846 | C1763 | C1648 | A1568 | A1495 | A1419  | G1339 | U1263 | G1183 | G1100 | G1030 | G962  | C887 | G808 | G744 |
| A1847 | C1764 | C1648 | A1569 | A1496 | U1420  | G1340 | A1264 | G1184 | G1101 | U1033 | U963  | C888 | U810 | G745 |
| A1848 | G1769 | G1653 | A1570 | U1497 | G1421  | U1341 | A1265 | C1184 | C1102 | U1033 | C964  | C889 | A890 | G746 |
| G1849 | C1770 | A1654 | A1571 | C1498 | G1422  | U1341 | U1267 | G1187 | C1103 | C1041 | G966  | G892 | C812 | U747 |
| G1850 | C1771 | A1655 | C1577 | C1499 | G1425  | G1348 | U1268 | U1188 | C1104 | G1042 | U969  | C893 | G748 | G749 |
| G1858 | C1772 | A1658 | U1578 | C1501 | G1426  | A1349 | A1269 | U1189 | G1110 | C1043 | C970  | C896 | G818 | A750 |
| G1864 | C1773 | C1658 | A1579 | C1502 | A1427  | G1350 | C1270 | G1190 | A1111 | C1044 | C971  | C897 | A819 | A751 |
| U1864 | C1774 | U1659 | A1580 | G1503 | G1428  | C1351 | G1271 | G1191 | G1112 | A1045 | G972  | C898 | A752 | A752 |
| G1869 | U1775 | C1660 | G1581 | C1504 | G1429  | U1352 | A1272 | G1192 | U1113 | A1046 | G973  | C899 | C753 | C753 |
| A1871 | C1776 | G1661 | C1582 | C1505 | U1431  | A1353 | U1273 | G1193 | G1114 | A1048 | G974  | A900 | C754 | C755 |
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| G1883 | A1786 | U1671 | C1588 | C1509 | G1434  | U1357 | G1279 | C1202 | G1125 | G1055 | A983  | C905 | U828 | A761 |
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| G1903 | G1799 | C1695 | U1608 | G1527 | G1455  | U1379 | G1224 | G1224 | U1142 | G1068 | C995  | U922 | G776 | G776 |
| G1904 | A1801 | C1698 | A1609 | G1530 | C1458  | G1380 | G1296 | A1227 | A1143 | A1070 | G997  | C924 | A849 | A777 |
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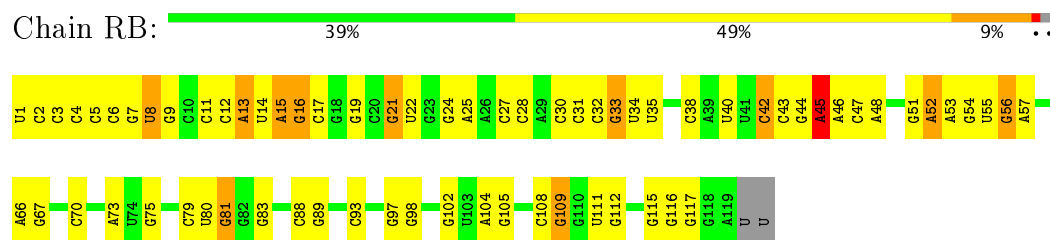




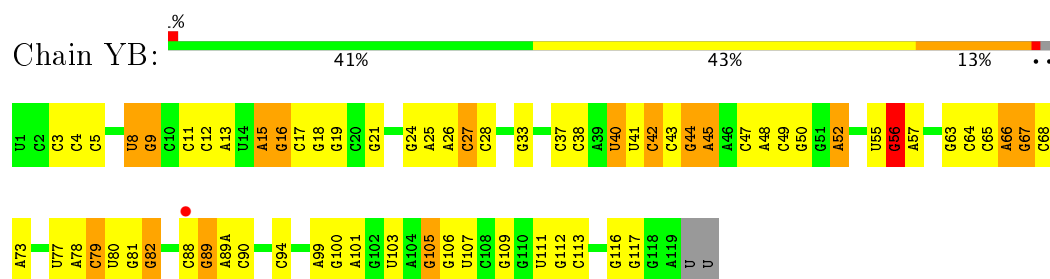




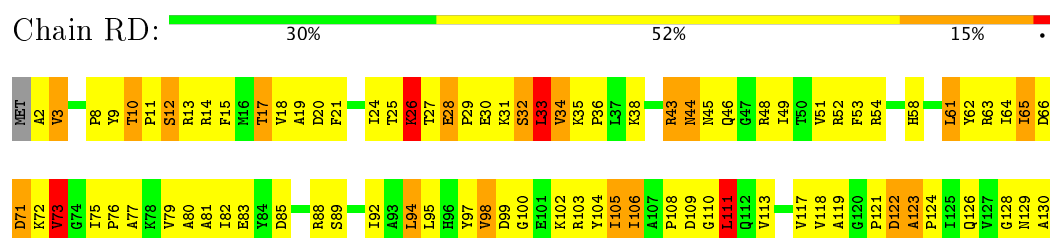
### • Molecule 23: 5S Ribosomal RNA



### • Molecule 23: 5S Ribosomal RNA



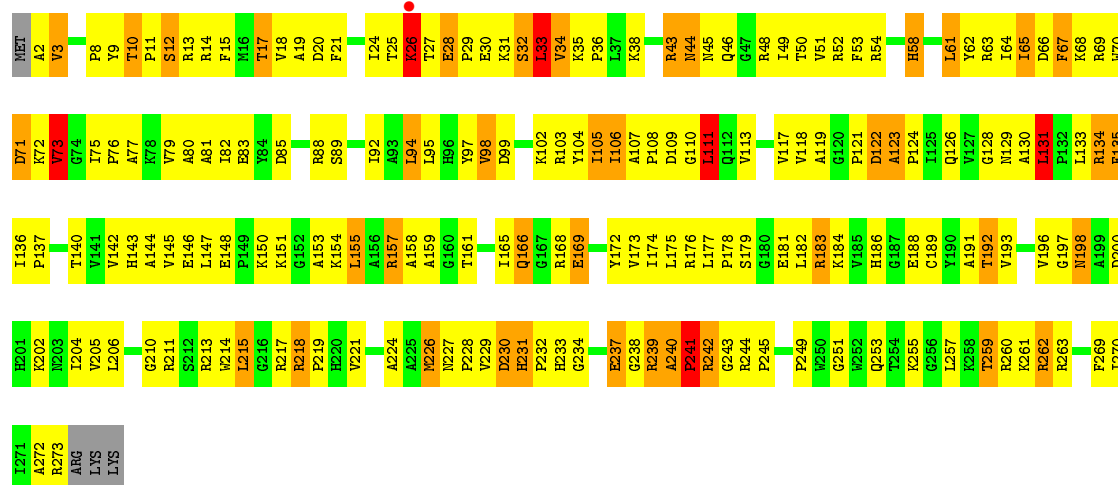
### • Molecule 24: 50S ribosomal protein L2





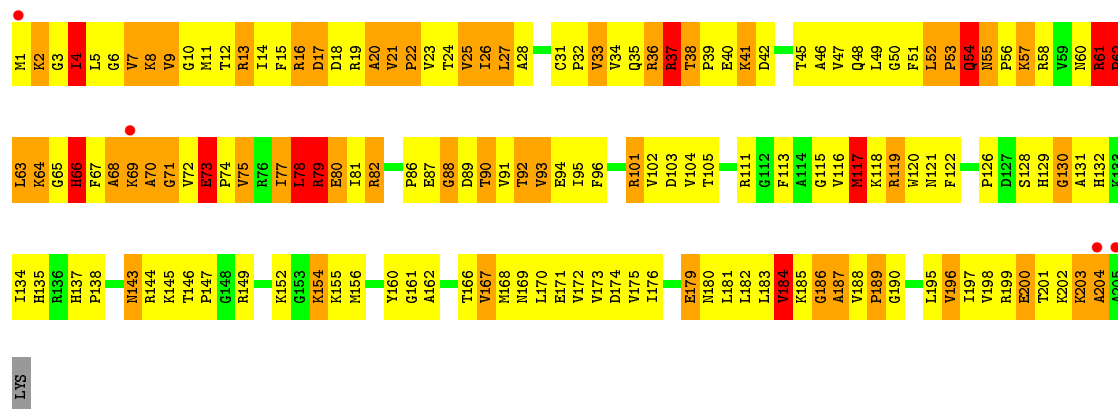
• Molecule 24: 50S ribosomal protein L2

Chain YD: 30% 51% 14% ..



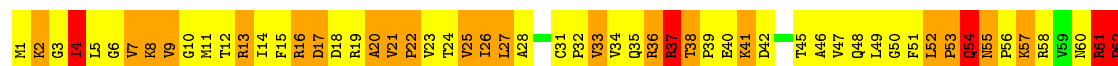
• Molecule 25: 50S ribosomal protein L3

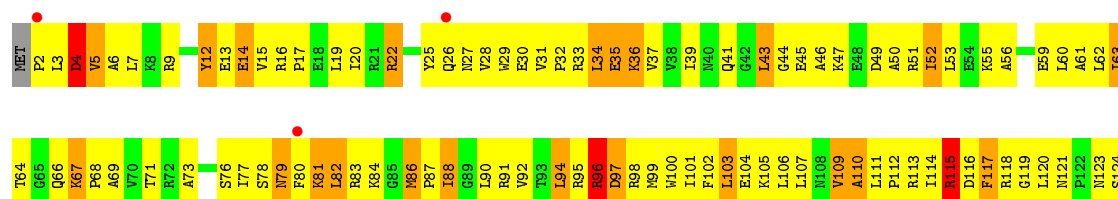
Chain RE: 2% 23% 48% 24% 5%

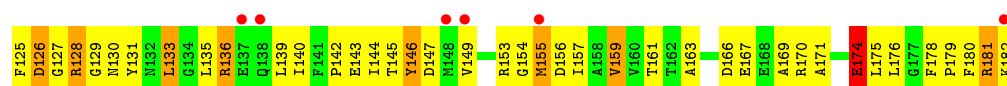


• Molecule 25: 50S ribosomal protein L3

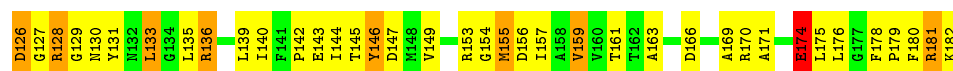
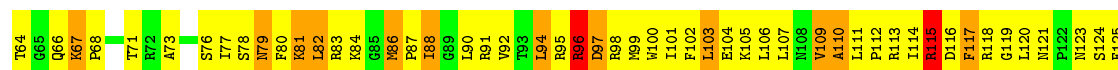
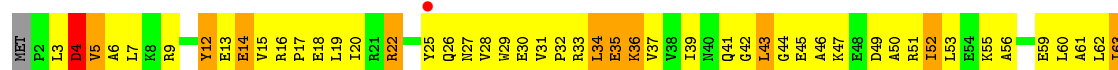
Chain YE: 23% 48% 24% 5%



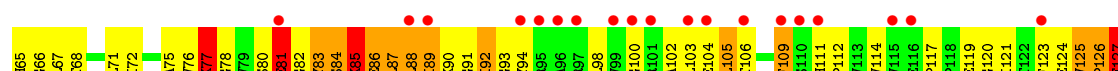
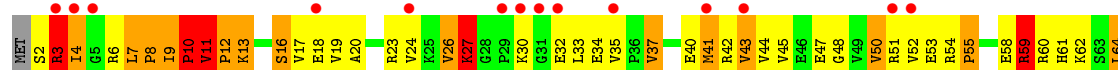




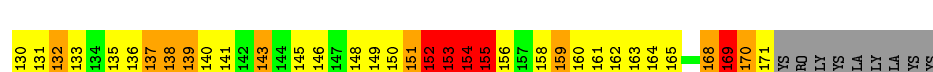
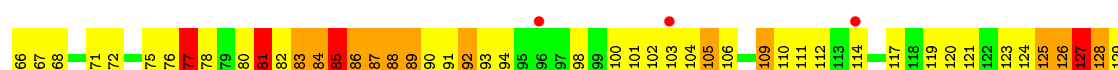
• Molecule 27: 50S ribosomal protein L5



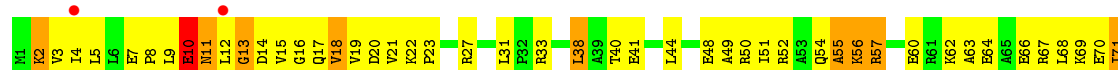
• Molecule 28: 50S ribosomal protein L6

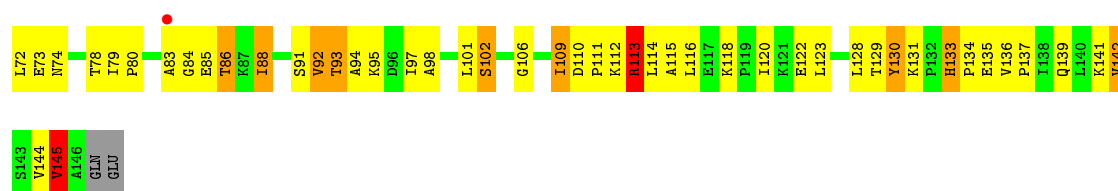


• Molecule 28: 50S ribosomal protein L6

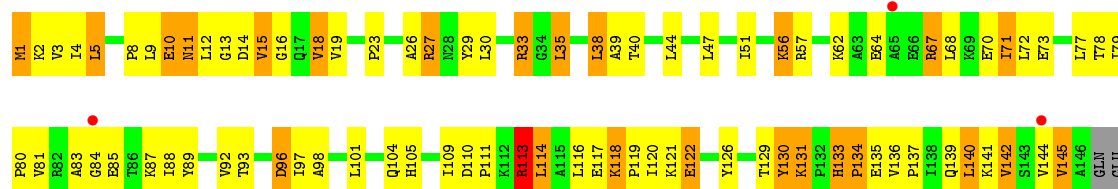


• Molecule 29: 50S ribosomal protein L9





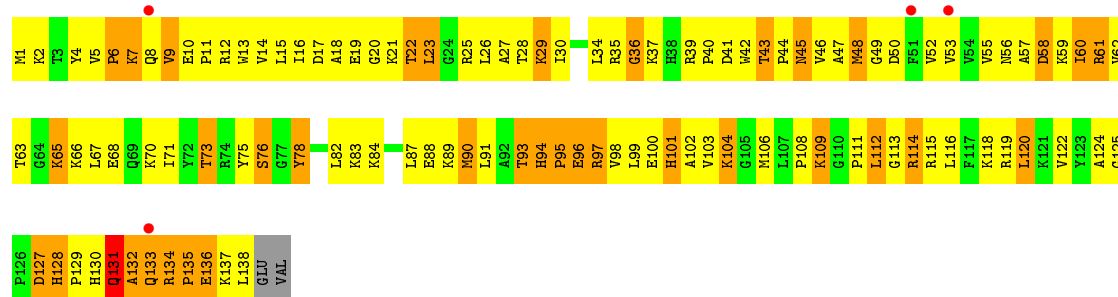
- Molecule 29: 50S ribosomal protein L9



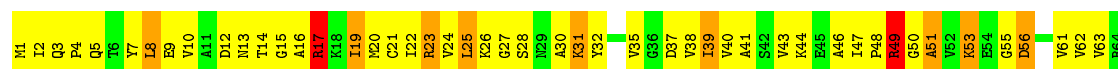
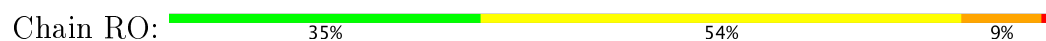
- Molecule 30: 50S ribosomal protein L13

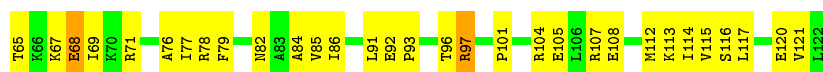


- Molecule 30: 50S ribosomal protein L13



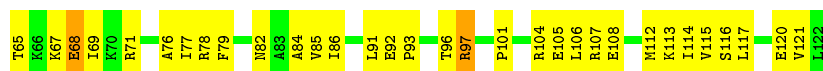
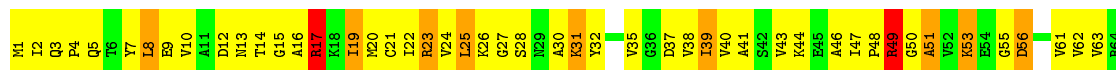
- Molecule 31: 50S ribosomal protein L14





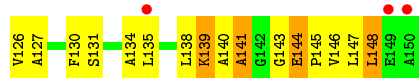
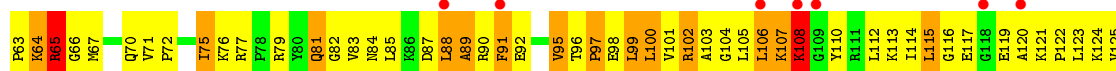
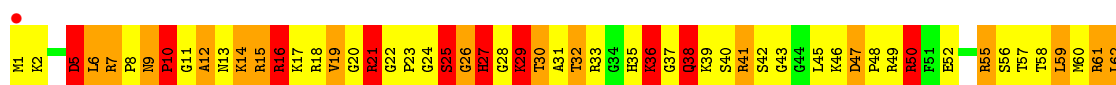
• Molecule 31: 50S ribosomal protein L14

Chain YO: 34% 55% 9% 2%



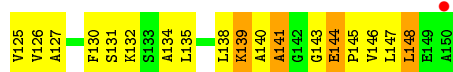
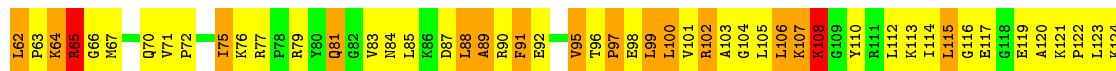
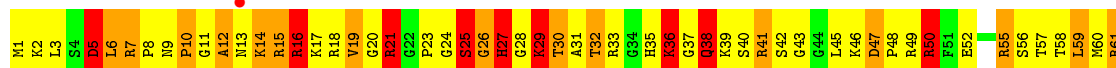
• Molecule 32: 50S ribosomal protein L15

Chain RP: 7% 19% 51% 23% 8%



• Molecule 32: 50S ribosomal protein L15

Chain YP: 19% 51% 23% 7%

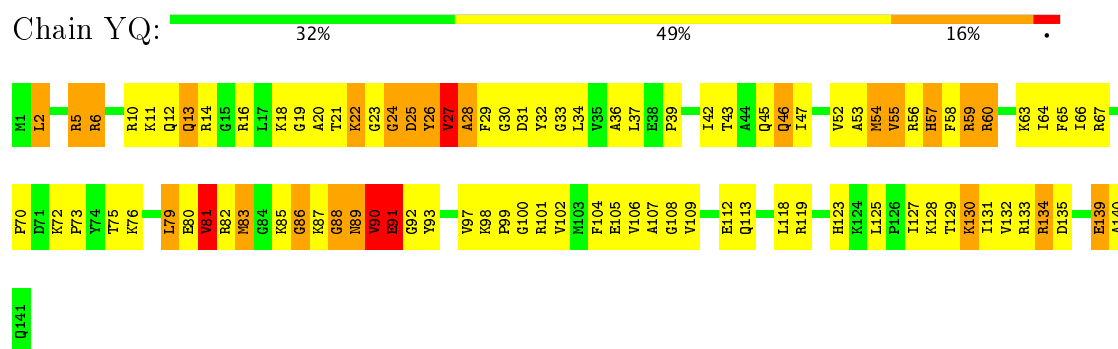


• Molecule 33: 50S ribosomal protein L16

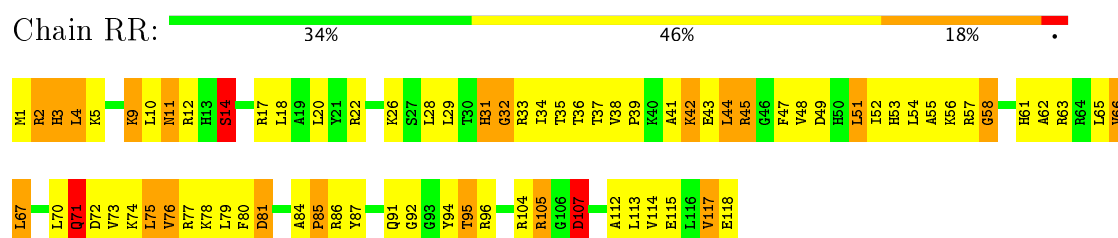
Chain RQ: 2% 33% 49% 16% 2%



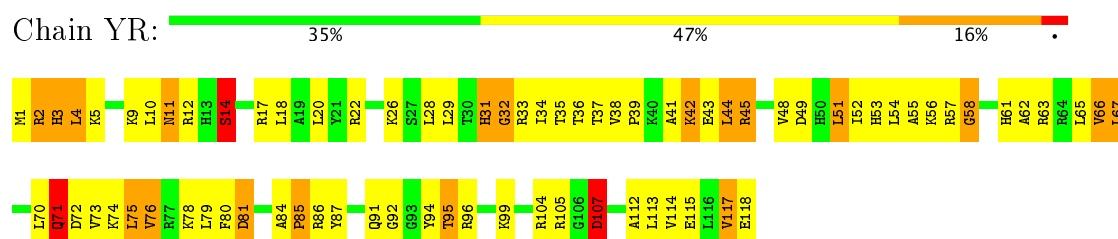
- Molecule 33: 50S ribosomal protein L16



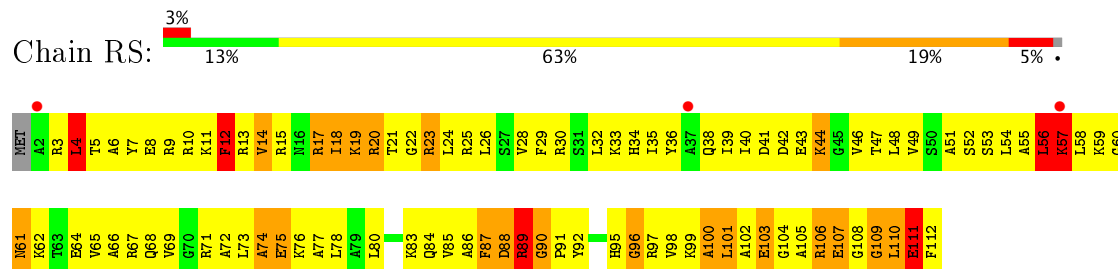
- Molecule 34: 50S ribosomal protein L17



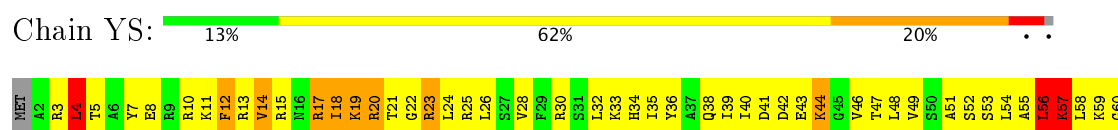
- Molecule 34: 50S ribosomal protein L17

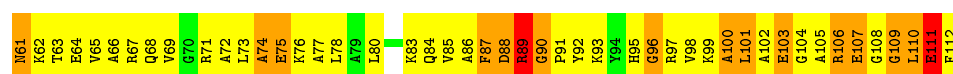


- Molecule 35: 50S ribosomal protein L18



- Molecule 35: 50S ribosomal protein L18

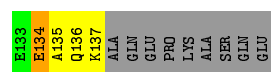
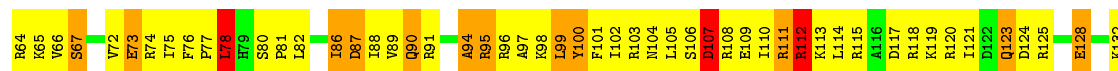




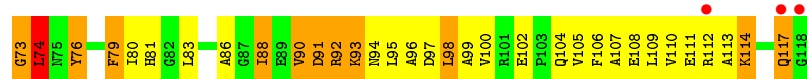
• Molecule 36: 50S ribosomal protein L19



• Molecule 36: 50S ribosomal protein L19



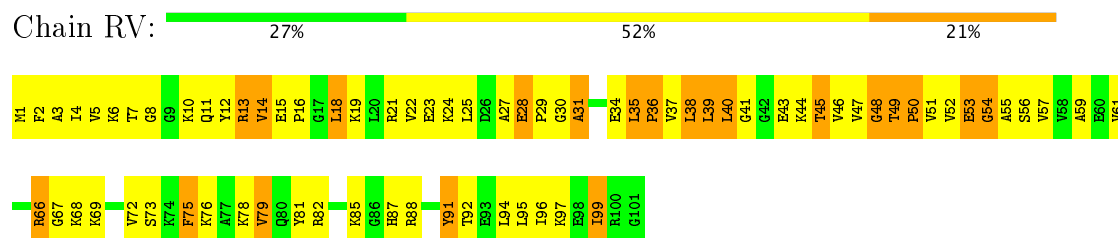
• Molecule 37: 50S ribosomal protein L20



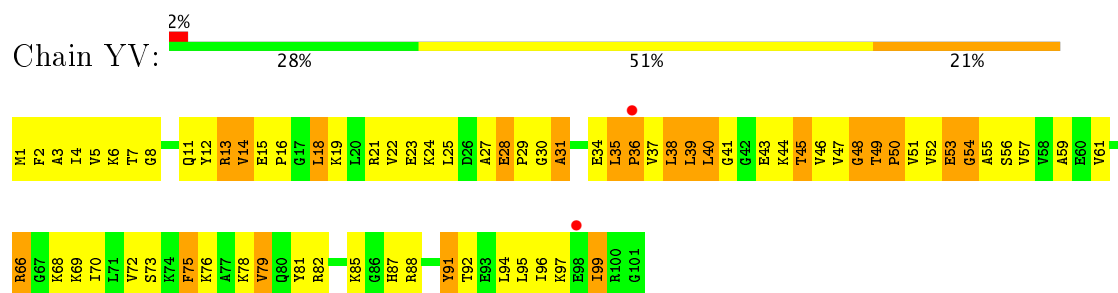
• Molecule 37: 50S ribosomal protein L20



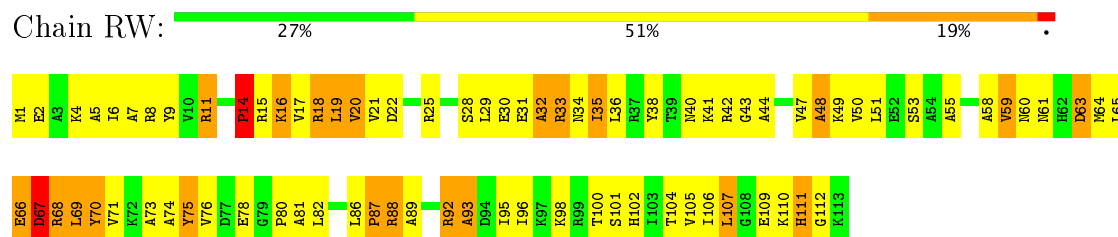
• Molecule 38: 50S ribosomal protein L21



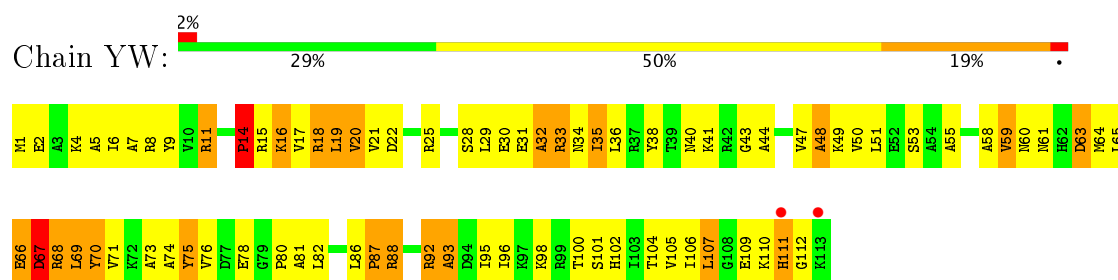
• Molecule 38: 50S ribosomal protein L21



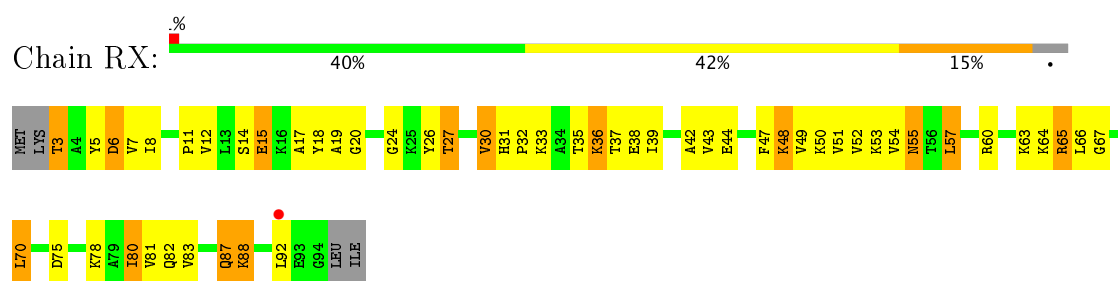
• Molecule 39: 50S ribosomal protein L22



• Molecule 39: 50S ribosomal protein L22

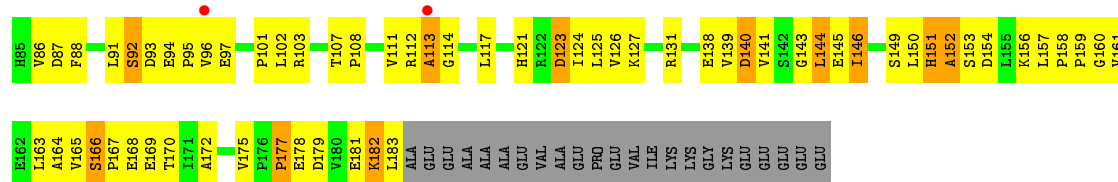


• Molecule 40: 50S ribosomal protein L23

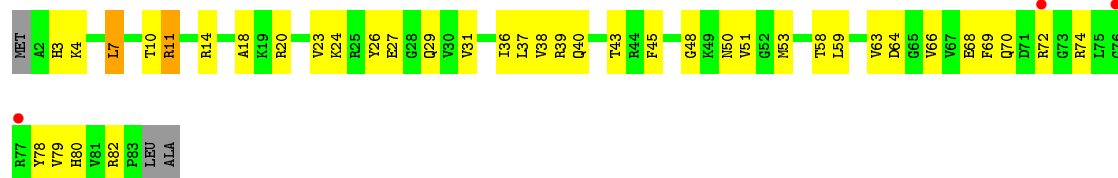


• Molecule 40: 50S ribosomal protein L23

| Category | Count |
|----------|-------|
| M1       | 10    |
| E2       | 10    |
| Y3       | 10    |
| R4       | 10    |
| L5       | 10    |
| K6       | 10    |
| A7       | 10    |
| Y8       | 10    |
| Y9       | 10    |
| R10      | 10    |
| E13      | 10    |
| S16      | 10    |
| R19      | 10    |
| R20      | 10    |
| L24      | 10    |
| M28      | 10    |
| N34      | 10    |
| R35      | 10    |
| K36      | 10    |
| V37      | 10    |
| Y38      | 10    |
| V39      | 10    |
| D40      | 10    |
| L41      | 10    |
| D45      | 10    |
| K46      | 10    |
| V47      | 10    |
| F48      | 10    |
| R49      | 10    |
| Q50      | 10    |
| A51      | 10    |
| S52      | 10    |
| I53      | 10    |
| V58      | 10    |
| L59      | 10    |
| B60      | 10    |
| L61      | 10    |
| P62      | 10    |
| D63      | 10    |
| S66      | 10    |
| T69      | 10    |
| L70      | 10    |
| V71      | 10    |
| R72      | 10    |
| L76      | 10    |
| R81      | 10    |
| F84      | 10    |



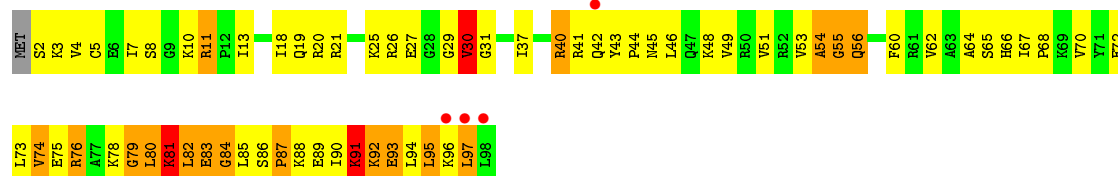
- Molecule 43: 50S ribosomal protein L27



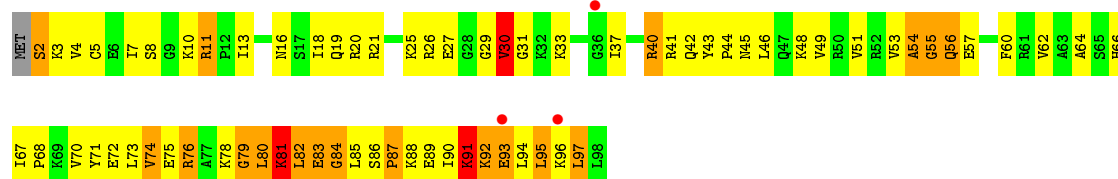
- Molecule 43: 50S ribosomal protein L27



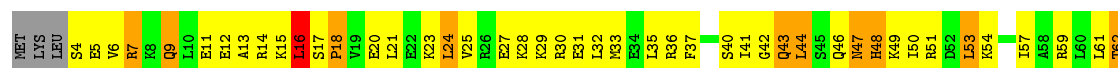
- Molecule 44: 50S ribosomal protein L28

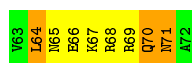


- Molecule 44: 50S ribosomal protein L28

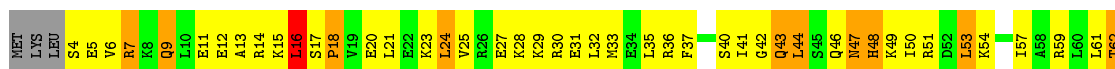


- Molecule 45: 50S ribosomal protein L29

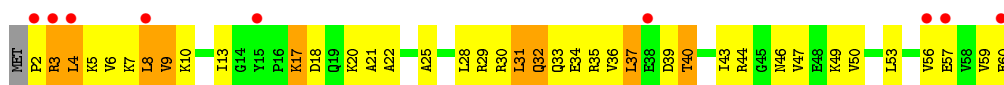




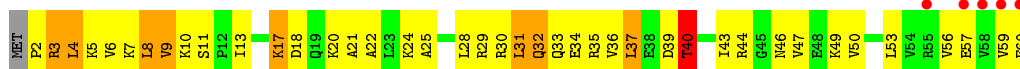
- Molecule 45: 50S ribosomal protein L29



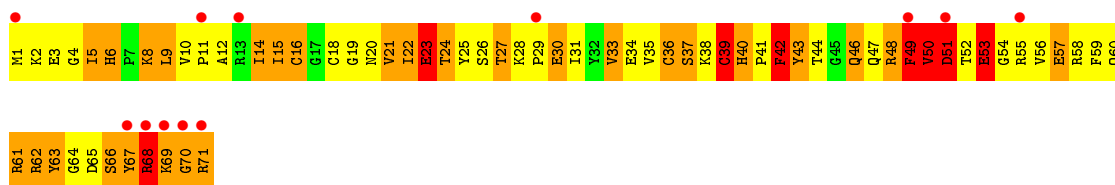
- Molecule 46: 50S ribosomal protein L30



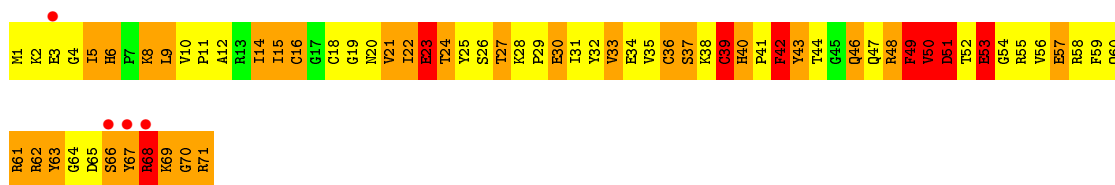
- Molecule 46: 50S ribosomal protein L30



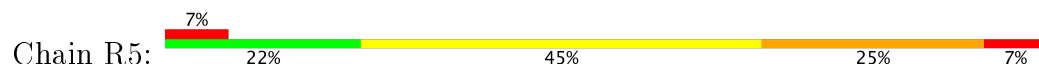
- Molecule 47: 50S ribosomal protein L31



- Molecule 47: 50S ribosomal protein L31



- Molecule 48: 50S ribosomal protein L32

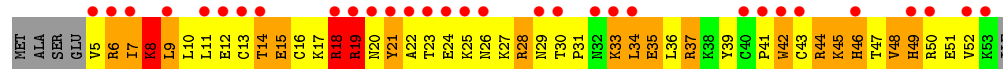




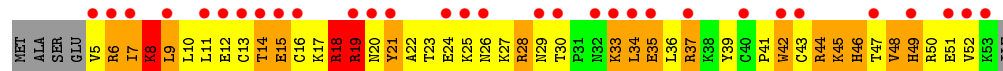
- Molecule 48: 50S ribosomal protein L32



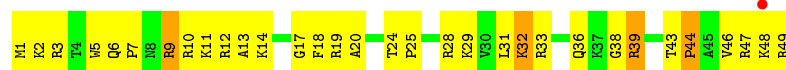
- Molecule 49: 50S ribosomal protein L33



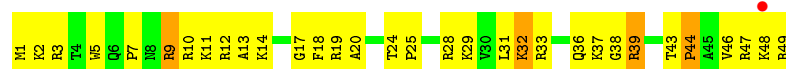
- Molecule 49: 50S ribosomal protein L33



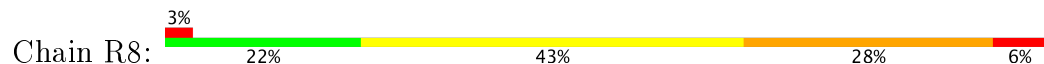
- Molecule 50: 50S ribosomal protein L34



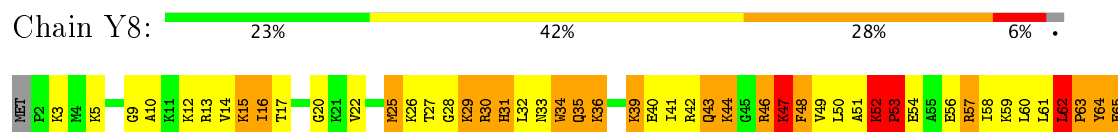
- Molecule 50: 50S ribosomal protein L34



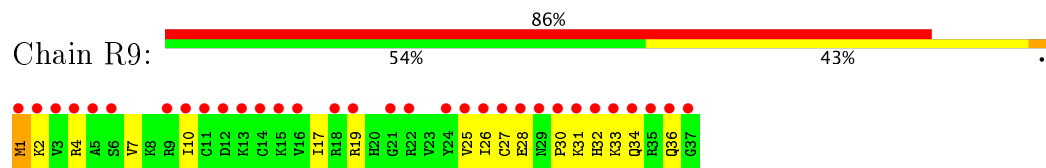
- Molecule 51: 50S ribosomal protein L35



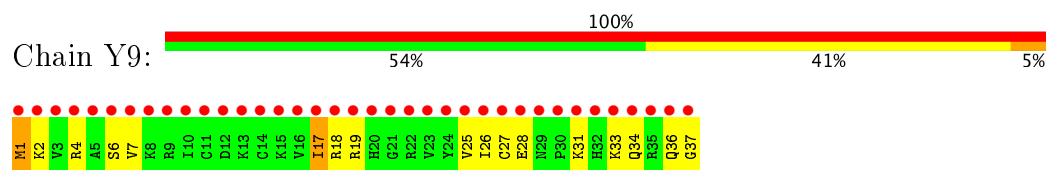
- Molecule 51: 50S ribosomal protein L35



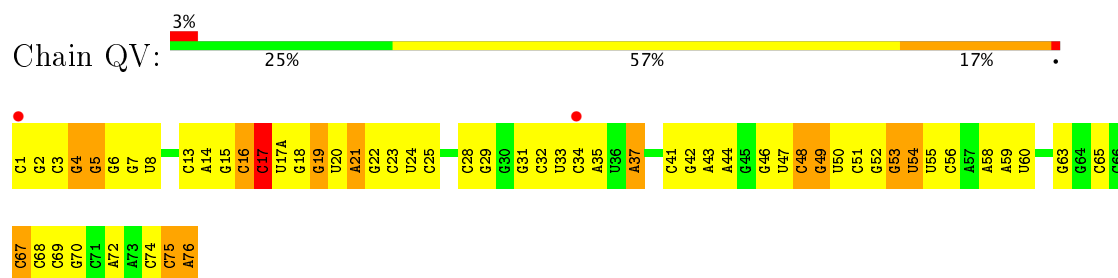
- Molecule 52: 50S ribosomal protein L36



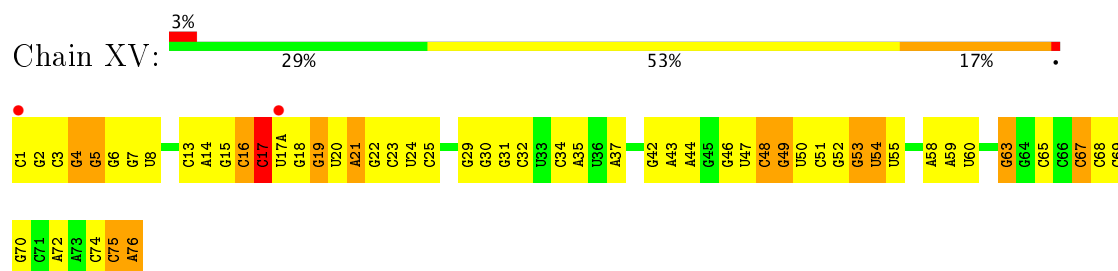
- Molecule 52: 50S ribosomal protein L36



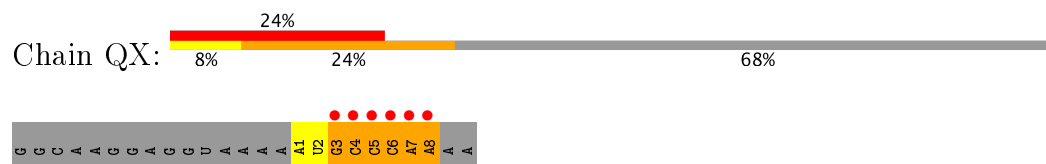
- Molecule 53: P-site tRNA fMet



- Molecule 53: P-site tRNA fMet



- Molecule 54: A-site ASL SufA6

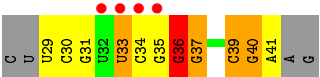


- Molecule 54: A-site ASL SufA6

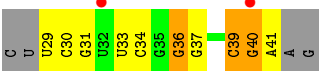
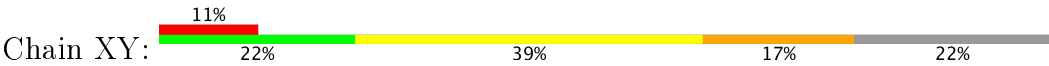




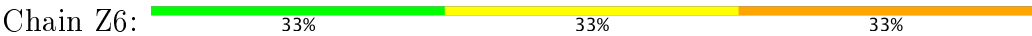
• Molecule 55: messenger RNA



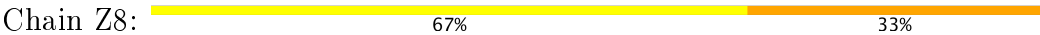
• Molecule 55: messenger RNA



• Molecule 56: tRNA acceptor end mimic



• Molecule 56: tRNA acceptor end mimic



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.24Å 446.10Å 623.32Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.68 – 3.90<br>49.68 – 3.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (49.68-3.90)<br>99.1 (49.68-3.70)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.31  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.66 (at 3.67Å)   | Xtriage          |
| Refinement program  | PHENIX  | Depositor        |
| R, $R_{free}$   | 0.235 , 0.278<br>0.235 , 0.278                              | Depositor<br>DCC |
| $R_{free}$ test set   | 23244 reflections (4.44%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 88.0  | Xtriage          |
| Anisotropy  | 0.281   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 47.0   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 291950  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 64.0  | wwPDB-VP         |

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

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 1MG, PPU

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

| Mol | Chain | Bond lengths |              | Bond angles |                 |
|-----|-------|--------------|--------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$  | RMSZ        | # $ Z  > 5$     |
| 1   | QA    | 0.43         | 0/36098      | 0.95        | 64/56341 (0.1%) |
| 1   | XA    | 0.48         | 0/36101      | 1.01        | 70/56346 (0.1%) |
| 2   | QB    | 0.35         | 0/1959       | 0.65        | 0/2642          |
| 2   | XB    | 0.35         | 0/1959       | 0.65        | 0/2642          |
| 3   | QC    | 0.36         | 0/1629       | 0.60        | 0/2195          |
| 3   | XC    | 0.37         | 0/1629       | 0.60        | 0/2195          |
| 4   | QD    | 0.41         | 0/1733       | 0.68        | 1/2318 (0.0%)   |
| 4   | XD    | 0.44         | 0/1733       | 0.68        | 1/2318 (0.0%)   |
| 5   | QE    | 0.38         | 0/1171       | 0.66        | 0/1576          |
| 5   | XE    | 0.38         | 0/1171       | 0.66        | 0/1576          |
| 6   | QF    | 0.43         | 0/856        | 0.68        | 0/1154          |
| 6   | XF    | 0.43         | 0/856        | 0.68        | 0/1154          |
| 7   | QG    | 0.37         | 0/1276       | 0.60        | 0/1709          |
| 7   | XG    | 0.36         | 0/1276       | 0.60        | 0/1709          |
| 8   | QH    | 0.40         | 0/1136       | 0.69        | 0/1527          |
| 8   | XH    | 0.40         | 0/1136       | 0.69        | 0/1527          |
| 9   | QI    | 0.36         | 0/1029       | 0.67        | 0/1379          |
| 9   | XI    | 0.36         | 0/1029       | 0.67        | 0/1379          |
| 10  | QJ    | 0.35         | 0/814        | 0.61        | 0/1095          |
| 10  | XJ    | 0.36         | 0/814        | 0.61        | 0/1095          |
| 11  | QK    | 0.40         | 0/900        | 0.67        | 0/1213          |
| 11  | XK    | 0.40         | 0/900        | 0.67        | 0/1213          |
| 12  | QL    | 0.48         | 1/991 (0.1%) | 0.79        | 2/1327 (0.2%)   |
| 12  | XL    | 0.48         | 1/991 (0.1%) | 0.79        | 2/1327 (0.2%)   |
| 13  | QM    | 0.34         | 0/974        | 0.66        | 0/1303          |
| 13  | XM    | 0.34         | 0/974        | 0.66        | 0/1303          |
| 14  | QN    | 0.42         | 0/501        | 0.68        | 0/664           |
| 14  | XN    | 0.52         | 0/501        | 0.67        | 0/664           |
| 15  | QO    | 0.39         | 0/745        | 0.67        | 0/992           |
| 15  | XO    | 0.39         | 0/745        | 0.66        | 0/992           |
| 16  | QP    | 0.36         | 0/721        | 0.67        | 0/970           |
| 16  | XP    | 0.37         | 0/721        | 0.67        | 0/970           |

| Mol | Chain | Bond lengths |                | Bond angles |                   |
|-----|-------|--------------|----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5           |
| 17  | QQ    | 0.37         | 0/847          | 0.68        | 0/1131            |
| 17  | XQ    | 0.38         | 0/847          | 0.68        | 0/1131            |
| 18  | QR    | 0.39         | 0/579          | 0.72        | 0/768             |
| 18  | XR    | 0.39         | 0/579          | 0.72        | 0/768             |
| 19  | QS    | 0.36         | 0/689          | 0.84        | 2/926 (0.2%)      |
| 19  | XS    | 0.36         | 0/689          | 0.84        | 2/926 (0.2%)      |
| 20  | QT    | 0.33         | 0/765          | 0.69        | 0/1007            |
| 20  | XT    | 0.34         | 0/765          | 0.69        | 0/1007            |
| 21  | QU    | 0.37         | 0/221          | 0.63        | 0/288             |
| 21  | XU    | 0.37         | 0/221          | 0.63        | 0/288             |
| 22  | RA    | 0.53         | 2/69521 (0.0%) | 1.06        | 133/108529 (0.1%) |
| 22  | YA    | 0.59         | 2/69543 (0.0%) | 1.12        | 219/108563 (0.2%) |
| 23  | RB    | 0.41         | 0/2878         | 0.95        | 4/4490 (0.1%)     |
| 23  | YB    | 0.49         | 0/2878         | 1.04        | 4/4490 (0.1%)     |
| 24  | RD    | 0.59         | 2/2165 (0.1%)  | 0.90        | 4/2919 (0.1%)     |
| 24  | YD    | 0.56         | 1/2165 (0.0%)  | 0.90        | 4/2919 (0.1%)     |
| 25  | RE    | 0.52         | 0/1601         | 0.91        | 2/2160 (0.1%)     |
| 25  | YE    | 0.52         | 0/1601         | 0.91        | 2/2160 (0.1%)     |
| 26  | RF    | 0.50         | 0/1620         | 0.76        | 0/2194            |
| 26  | YF    | 0.50         | 0/1620         | 0.76        | 0/2194            |
| 27  | RG    | 0.40         | 0/1499         | 0.66        | 0/2016            |
| 27  | YG    | 0.40         | 0/1499         | 0.66        | 0/2016            |
| 28  | RH    | 0.45         | 0/1332         | 0.85        | 3/1802 (0.2%)     |
| 28  | YH    | 0.45         | 0/1332         | 0.85        | 4/1802 (0.2%)     |
| 29  | RI    | 0.54         | 2/1151 (0.2%)  | 0.68        | 1/1558 (0.1%)     |
| 29  | YI    | 0.34         | 0/1151         | 0.61        | 0/1558            |
| 30  | RN    | 0.46         | 0/1131         | 0.78        | 1/1525 (0.1%)     |
| 30  | YN    | 0.46         | 0/1131         | 0.78        | 1/1525 (0.1%)     |
| 31  | RO    | 0.54         | 0/943          | 0.71        | 0/1269            |
| 31  | YO    | 0.53         | 0/943          | 0.71        | 0/1269            |
| 32  | RP    | 0.50         | 0/1162         | 0.94        | 3/1544 (0.2%)     |
| 32  | YP    | 0.50         | 0/1162         | 0.95        | 3/1544 (0.2%)     |
| 33  | RQ    | 0.54         | 0/1143         | 0.91        | 3/1527 (0.2%)     |
| 33  | YQ    | 0.54         | 0/1143         | 0.89        | 3/1527 (0.2%)     |
| 34  | RR    | 0.45         | 0/982          | 0.80        | 1/1312 (0.1%)     |
| 34  | YR    | 0.45         | 0/982          | 0.80        | 1/1312 (0.1%)     |
| 35  | RS    | 0.46         | 0/892          | 0.82        | 1/1187 (0.1%)     |
| 35  | YS    | 0.45         | 0/892          | 0.83        | 1/1187 (0.1%)     |
| 36  | RT    | 0.47         | 0/1155         | 0.73        | 2/1542 (0.1%)     |
| 36  | YT    | 0.46         | 0/1155         | 0.73        | 2/1542 (0.1%)     |
| 37  | RU    | 0.48         | 0/982          | 0.78        | 0/1306            |
| 37  | YU    | 0.48         | 0/982          | 0.78        | 0/1306            |
| 38  | RV    | 0.47         | 0/790          | 0.82        | 0/1057            |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | YV    | 0.47         | 0/790            | 0.82        | 0/1057            |
| 39  | RW    | 0.45         | 0/911            | 0.75        | 0/1220            |
| 39  | YW    | 0.45         | 0/911            | 0.75        | 0/1220            |
| 40  | RX    | 0.56         | 0/739            | 0.77        | 0/993             |
| 40  | YX    | 0.56         | 0/739            | 0.77        | 0/993             |
| 41  | RY    | 0.52         | 0/798            | 0.80        | 0/1064            |
| 41  | YY    | 0.52         | 0/798            | 0.80        | 0/1064            |
| 42  | RZ    | 0.36         | 0/1493           | 0.58        | 0/2026            |
| 42  | YZ    | 0.36         | 0/1493           | 0.62        | 0/2026            |
| 43  | R0    | 0.42         | 0/657            | 0.63        | 0/874             |
| 43  | Y0    | 0.42         | 0/657            | 0.65        | 0/874             |
| 44  | R1    | 0.49         | 0/770            | 0.85        | 1/1022 (0.1%)     |
| 44  | Y1    | 0.49         | 0/770            | 0.85        | 1/1022 (0.1%)     |
| 45  | R2    | 0.50         | 0/583            | 0.84        | 1/771 (0.1%)      |
| 45  | Y2    | 0.51         | 0/583            | 0.84        | 1/771 (0.1%)      |
| 46  | R3    | 0.47         | 0/474            | 0.72        | 0/635             |
| 46  | Y3    | 0.43         | 0/474            | 0.71        | 0/635             |
| 47  | R4    | 0.38         | 0/594            | 0.78        | 1/795 (0.1%)      |
| 47  | Y4    | 0.38         | 0/594            | 0.78        | 1/795 (0.1%)      |
| 48  | R5    | 0.51         | 0/473            | 0.74        | 0/639             |
| 48  | Y5    | 0.50         | 0/465            | 0.74        | 0/629             |
| 49  | R6    | 0.42         | 0/431            | 0.76        | 0/575             |
| 49  | Y6    | 0.43         | 0/431            | 0.76        | 0/575             |
| 50  | R7    | 0.56         | 0/438            | 0.76        | 0/575             |
| 50  | Y7    | 0.56         | 0/438            | 0.76        | 0/575             |
| 51  | R8    | 0.62         | 0/525            | 0.93        | 1/691 (0.1%)      |
| 51  | Y8    | 0.62         | 0/525            | 0.93        | 1/691 (0.1%)      |
| 52  | R9    | 0.35         | 0/310            | 0.60        | 0/407             |
| 52  | Y9    | 0.37         | 0/310            | 0.61        | 0/407             |
| 53  | QV    | 0.51         | 0/1836           | 0.99        | 6/2859 (0.2%)     |
| 53  | XV    | 0.51         | 0/1836           | 0.99        | 6/2859 (0.2%)     |
| 54  | QX    | 0.74         | 0/188            | 0.84        | 0/290             |
| 54  | XX    | 0.48         | 0/188            | 0.74        | 0/290             |
| 55  | QY    | 0.78         | 1/311 (0.3%)     | 0.88        | 0/483             |
| 55  | XY    | 0.51         | 0/311            | 0.88        | 0/483             |
| 56  | Z6    | 0.79         | 0/40             | 1.79        | 1/60 (1.7%)       |
| 56  | Z8    | 0.79         | 0/40             | 1.83        | 1/60 (1.7%)       |
| All | All   | 0.50         | 12/316321 (0.0%) | 0.98        | 568/472911 (0.1%) |

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

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| Mol | Chain | Res     | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 24  | RD    | 236     | GLY  | C-N   | 8.53  | 1.53        | 1.34     |
| 29  | RI    | 54      | GLN  | C-O   | -7.01 | 1.10        | 1.23     |
| 55  | QY    | 36      | G    | C2-N2 | -6.93 | 1.27        | 1.34     |
| 22  | YA    | 1142(A) | A    | N9-C4 | -6.45 | 1.33        | 1.37     |
| 29  | RI    | 55      | ALA  | C-O   | 6.04  | 1.34        | 1.23     |

The worst 5 of 568 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 53  | XV    | 17  | C    | C2-N1-C1' | 11.79  | 131.77      | 118.80   |
| 53  | QV    | 17  | C    | C2-N1-C1' | 11.74  | 131.72      | 118.80   |
| 22  | YA    | 761 | A    | N1-C6-N6  | 11.29  | 125.37      | 118.60   |
| 1   | XA    | 328 | C    | C6-N1-C2  | -10.26 | 116.19      | 120.30   |
| 25  | YE    | 21  | VAL  | C-N-CD    | -10.09 | 98.39       | 120.60   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | QA    | 32247 | 0        | 16278    | 672     | 0            |
| 1   | XA    | 32249 | 0        | 16278    | 742     | 1            |
| 2   | QB    | 1924  | 0        | 1975     | 283     | 0            |
| 2   | XB    | 1924  | 0        | 1975     | 290     | 0            |
| 3   | QC    | 1605  | 0        | 1668     | 210     | 0            |
| 3   | XC    | 1605  | 0        | 1668     | 210     | 0            |
| 4   | QD    | 1703  | 0        | 1764     | 247     | 0            |
| 4   | XD    | 1703  | 0        | 1765     | 215     | 1            |
| 5   | QE    | 1155  | 0        | 1213     | 159     | 0            |
| 5   | XE    | 1155  | 0        | 1213     | 133     | 0            |
| 6   | QF    | 843   | 0        | 857      | 92      | 1            |
| 6   | XF    | 843   | 0        | 857      | 96      | 0            |
| 7   | QG    | 1257  | 0        | 1296     | 146     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | XG    | 1257  | 0        | 1294     | 147     | 0            |
| 8   | QH    | 1116  | 0        | 1175     | 151     | 0            |
| 8   | XH    | 1116  | 0        | 1177     | 149     | 0            |
| 9   | QI    | 1010  | 0        | 1037     | 140     | 0            |
| 9   | XI    | 1010  | 0        | 1037     | 153     | 0            |
| 10  | QJ    | 801   | 0        | 849      | 149     | 0            |
| 10  | XJ    | 801   | 0        | 849      | 135     | 0            |
| 11  | QK    | 885   | 0        | 904      | 103     | 0            |
| 11  | XK    | 885   | 0        | 904      | 110     | 0            |
| 12  | QL    | 975   | 0        | 1062     | 111     | 0            |
| 12  | XL    | 975   | 0        | 1062     | 116     | 0            |
| 13  | QM    | 964   | 0        | 1034     | 152     | 0            |
| 13  | XM    | 964   | 0        | 1034     | 216     | 0            |
| 14  | QN    | 492   | 0        | 529      | 103     | 0            |
| 14  | XN    | 492   | 0        | 529      | 95      | 0            |
| 15  | QO    | 734   | 0        | 771      | 78      | 0            |
| 15  | XO    | 734   | 0        | 771      | 72      | 0            |
| 16  | QP    | 705   | 0        | 725      | 115     | 0            |
| 16  | XP    | 705   | 0        | 725      | 105     | 0            |
| 17  | QQ    | 834   | 0        | 904      | 77      | 0            |
| 17  | XQ    | 834   | 0        | 904      | 71      | 0            |
| 18  | QR    | 574   | 0        | 644      | 69      | 0            |
| 18  | XR    | 574   | 0        | 644      | 68      | 0            |
| 19  | QS    | 674   | 0        | 699      | 117     | 0            |
| 19  | XS    | 674   | 0        | 699      | 150     | 0            |
| 20  | QT    | 763   | 0        | 860      | 109     | 0            |
| 20  | XT    | 763   | 0        | 861      | 102     | 0            |
| 21  | QU    | 217   | 0        | 234      | 25      | 0            |
| 21  | XU    | 217   | 0        | 234      | 26      | 0            |
| 22  | RA    | 62071 | 0        | 31286    | 1243    | 0            |
| 22  | YA    | 62091 | 0        | 31295    | 1282    | 0            |
| 23  | RB    | 2573  | 0        | 1306     | 68      | 0            |
| 23  | YB    | 2573  | 0        | 1306     | 57      | 0            |
| 24  | RD    | 2115  | 0        | 2195     | 320     | 0            |
| 24  | YD    | 2115  | 0        | 2195     | 323     | 0            |
| 25  | RE    | 1568  | 0        | 1634     | 268     | 0            |
| 25  | YE    | 1568  | 0        | 1634     | 272     | 0            |
| 26  | RF    | 1585  | 0        | 1632     | 178     | 0            |
| 26  | YF    | 1585  | 0        | 1632     | 179     | 0            |
| 27  | RG    | 1474  | 0        | 1535     | 202     | 0            |
| 27  | YG    | 1474  | 0        | 1535     | 204     | 0            |
| 28  | RH    | 1307  | 0        | 1382     | 220     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | YH    | 1307  | 0        | 1382     | 227     | 3            |
| 29  | RI    | 1136  | 0        | 1223     | 61      | 1            |
| 29  | YI    | 1136  | 0        | 1223     | 57      | 0            |
| 30  | RN    | 1104  | 0        | 1180     | 190     | 0            |
| 30  | YN    | 1104  | 0        | 1180     | 186     | 0            |
| 31  | RO    | 933   | 0        | 996      | 124     | 0            |
| 31  | YO    | 933   | 0        | 996      | 131     | 0            |
| 32  | RP    | 1145  | 0        | 1227     | 247     | 0            |
| 32  | YP    | 1145  | 0        | 1228     | 239     | 0            |
| 33  | RQ    | 1122  | 0        | 1179     | 150     | 0            |
| 33  | YQ    | 1122  | 0        | 1178     | 149     | 0            |
| 34  | RR    | 968   | 0        | 1033     | 110     | 0            |
| 34  | YR    | 968   | 0        | 1033     | 114     | 0            |
| 35  | RS    | 882   | 0        | 943      | 156     | 0            |
| 35  | YS    | 882   | 0        | 943      | 159     | 0            |
| 36  | RT    | 1141  | 0        | 1202     | 156     | 0            |
| 36  | YT    | 1141  | 0        | 1202     | 152     | 0            |
| 37  | RU    | 964   | 0        | 1022     | 128     | 0            |
| 37  | YU    | 964   | 0        | 1022     | 134     | 0            |
| 38  | RV    | 779   | 0        | 852      | 130     | 0            |
| 38  | YV    | 779   | 0        | 852      | 128     | 0            |
| 39  | RW    | 900   | 0        | 964      | 101     | 0            |
| 39  | YW    | 900   | 0        | 964      | 102     | 0            |
| 40  | RX    | 725   | 0        | 778      | 67      | 0            |
| 40  | YX    | 725   | 0        | 778      | 67      | 0            |
| 41  | RY    | 785   | 0        | 878      | 166     | 0            |
| 41  | YY    | 785   | 0        | 878      | 154     | 3            |
| 42  | RZ    | 1461  | 0        | 1493     | 63      | 0            |
| 42  | YZ    | 1461  | 0        | 1493     | 70      | 0            |
| 43  | R0    | 648   | 0        | 672      | 28      | 0            |
| 43  | Y0    | 648   | 0        | 672      | 44      | 0            |
| 44  | R1    | 763   | 0        | 848      | 143     | 0            |
| 44  | Y1    | 763   | 0        | 848      | 140     | 0            |
| 45  | R2    | 581   | 0        | 629      | 80      | 0            |
| 45  | Y2    | 581   | 0        | 629      | 79      | 0            |
| 46  | R3    | 469   | 0        | 518      | 41      | 0            |
| 46  | Y3    | 469   | 0        | 518      | 44      | 0            |
| 47  | R4    | 581   | 0        | 574      | 156     | 0            |
| 47  | Y4    | 581   | 0        | 574      | 225     | 0            |
| 48  | R5    | 459   | 0        | 480      | 74      | 0            |
| 48  | Y5    | 451   | 0        | 471      | 68      | 0            |
| 49  | R6    | 424   | 0        | 450      | 93      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 49  | Y6    | 424   | 0        | 450      | 90      | 0            |
| 50  | R7    | 430   | 0        | 480      | 42      | 0            |
| 50  | Y7    | 430   | 0        | 480      | 44      | 0            |
| 51  | R8    | 517   | 0        | 582      | 102     | 0            |
| 51  | Y8    | 517   | 0        | 582      | 102     | 0            |
| 52  | R9    | 307   | 0        | 335      | 16      | 0            |
| 52  | Y9    | 307   | 0        | 336      | 20      | 0            |
| 53  | QV    | 1644  | 0        | 836      | 63      | 0            |
| 53  | XV    | 1644  | 0        | 836      | 56      | 0            |
| 54  | QX    | 169   | 0        | 88       | 55      | 0            |
| 54  | XX    | 169   | 0        | 88       | 17      | 0            |
| 55  | QY    | 303   | 0        | 152      | 22      | 0            |
| 55  | XY    | 303   | 0        | 154      | 30      | 0            |
| 56  | Z6    | 74    | 0        | 51       | 24      | 0            |
| 56  | Z8    | 74    | 0        | 51       | 14      | 0            |
| 57  | QA    | 65    | 0        | 0        | 0       | 0            |
| 57  | QF    | 1     | 0        | 0        | 0       | 0            |
| 57  | QH    | 1     | 0        | 0        | 0       | 0            |
| 57  | QM    | 1     | 0        | 0        | 0       | 0            |
| 57  | QX    | 1     | 0        | 0        | 0       | 0            |
| 57  | R5    | 1     | 0        | 0        | 0       | 0            |
| 57  | R8    | 1     | 0        | 0        | 0       | 0            |
| 57  | RA    | 244   | 0        | 0        | 0       | 0            |
| 57  | RB    | 2     | 0        | 0        | 0       | 0            |
| 57  | RD    | 1     | 0        | 0        | 0       | 0            |
| 57  | RE    | 2     | 0        | 0        | 0       | 0            |
| 57  | RF    | 1     | 0        | 0        | 0       | 0            |
| 57  | RP    | 2     | 0        | 0        | 0       | 0            |
| 57  | RR    | 1     | 0        | 0        | 0       | 0            |
| 57  | RU    | 1     | 0        | 0        | 0       | 0            |
| 57  | XA    | 72    | 0        | 0        | 0       | 0            |
| 57  | XM    | 1     | 0        | 0        | 0       | 0            |
| 57  | XV    | 2     | 0        | 0        | 0       | 0            |
| 57  | XX    | 1     | 0        | 0        | 0       | 0            |
| 57  | Y5    | 1     | 0        | 0        | 0       | 0            |
| 57  | Y7    | 1     | 0        | 0        | 0       | 0            |
| 57  | YA    | 265   | 0        | 0        | 0       | 0            |
| 57  | YB    | 3     | 0        | 0        | 0       | 0            |
| 57  | YE    | 1     | 0        | 0        | 0       | 0            |
| 57  | YP    | 2     | 0        | 0        | 0       | 0            |
| 57  | YQ    | 1     | 0        | 0        | 0       | 0            |
| 57  | YX    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58  | QA    | 42     | 0        | 45       | 4       | 0            |
| 58  | XA    | 42     | 0        | 45       | 2       | 0            |
| 59  | QD    | 1      | 0        | 0        | 0       | 0            |
| 59  | QN    | 1      | 0        | 0        | 0       | 0            |
| 59  | R9    | 1      | 0        | 0        | 0       | 0            |
| 59  | XD    | 1      | 0        | 0        | 0       | 0            |
| 59  | XN    | 1      | 0        | 0        | 0       | 0            |
| 59  | Y9    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 291950 | 0        | 198321   | 15633   | 5            |

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 32.

The worst 5 of 15633 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:XA:1400:C:N4   | 53:XV:34:C:C6     | 1.71                     | 1.55              |
| 14:XN:32:SER:CB  | 14:XN:41:ARG:HB3  | 1.23                     | 1.55              |
| 14:XN:32:SER:HB3 | 14:XN:41:ARG:CB   | 1.27                     | 1.54              |
| 28:RH:127:GLU:CG | 28:RH:128:PRO:HD3 | 1.35                     | 1.53              |
| 28:YH:127:GLU:CG | 28:YH:128:PRO:HD3 | 1.35                     | 1.52              |

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------------|--------------------------|-------------------|
| 28:YH:45:VAL:O   | 41:YY:24:VAL:N[4_445]  | 1.97                     | 0.23              |
| 29:RI:91:SER:OG  | 1:XA:368:U:OP1[4_555]  | 2.05                     | 0.15              |
| 28:YH:44:VAL:CG2 | 41:YY:23:ARG:CD[4_445] | 2.08                     | 0.12              |
| 6:QF:15:ASP:OD2  | 4:XD:27:TYR:OH[4_555]  | 2.14                     | 0.06              |
| 28:YH:47:GLU:OE2 | 41:YY:79:CYS:CB[4_445] | 2.18                     | 0.02              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | QB    | 235/256 (92%) | 153 (65%) | 52 (22%) | 30 (13%) | 0           | 7  |
| 2   | XB    | 235/256 (92%) | 153 (65%) | 52 (22%) | 30 (13%) | 0           | 7  |
| 3   | QC    | 203/239 (85%) | 128 (63%) | 56 (28%) | 19 (9%)  | 1           | 14 |
| 3   | XC    | 203/239 (85%) | 129 (64%) | 55 (27%) | 19 (9%)  | 1           | 14 |
| 4   | QD    | 206/209 (99%) | 136 (66%) | 50 (24%) | 20 (10%) | 1           | 13 |
| 4   | XD    | 206/209 (99%) | 135 (66%) | 48 (23%) | 23 (11%) | 0           | 9  |
| 5   | QE    | 149/162 (92%) | 103 (69%) | 31 (21%) | 15 (10%) | 1           | 12 |
| 5   | XE    | 149/162 (92%) | 103 (69%) | 30 (20%) | 16 (11%) | 0           | 10 |
| 6   | QF    | 99/101 (98%)  | 66 (67%)  | 24 (24%) | 9 (9%)   | 1           | 15 |
| 6   | XF    | 99/101 (98%)  | 66 (67%)  | 24 (24%) | 9 (9%)   | 1           | 15 |
| 7   | QG    | 153/156 (98%) | 101 (66%) | 37 (24%) | 15 (10%) | 1           | 13 |
| 7   | XG    | 153/156 (98%) | 103 (67%) | 36 (24%) | 14 (9%)  | 1           | 15 |
| 8   | QH    | 136/138 (99%) | 92 (68%)  | 29 (21%) | 15 (11%) | 0           | 10 |
| 8   | XH    | 136/138 (99%) | 92 (68%)  | 29 (21%) | 15 (11%) | 0           | 10 |
| 9   | QI    | 125/128 (98%) | 77 (62%)  | 32 (26%) | 16 (13%) | 0           | 7  |
| 9   | XI    | 125/128 (98%) | 77 (62%)  | 32 (26%) | 16 (13%) | 0           | 7  |
| 10  | QJ    | 97/105 (92%)  | 68 (70%)  | 20 (21%) | 9 (9%)   | 1           | 14 |
| 10  | XJ    | 97/105 (92%)  | 68 (70%)  | 19 (20%) | 10 (10%) | 0           | 11 |
| 11  | QK    | 117/129 (91%) | 87 (74%)  | 22 (19%) | 8 (7%)   | 1           | 22 |
| 11  | XK    | 117/129 (91%) | 87 (74%)  | 22 (19%) | 8 (7%)   | 1           | 22 |
| 12  | QL    | 123/132 (93%) | 84 (68%)  | 23 (19%) | 16 (13%) | 0           | 6  |
| 12  | XL    | 123/132 (93%) | 84 (68%)  | 24 (20%) | 15 (12%) | 0           | 7  |
| 13  | QM    | 119/126 (94%) | 71 (60%)  | 29 (24%) | 19 (16%) | 0           | 4  |
| 13  | XM    | 119/126 (94%) | 71 (60%)  | 27 (23%) | 21 (18%) | 0           | 3  |
| 14  | QN    | 58/61 (95%)   | 31 (53%)  | 15 (26%) | 12 (21%) | 0           | 2  |
| 14  | XN    | 58/61 (95%)   | 33 (57%)  | 13 (22%) | 12 (21%) | 0           | 2  |
| 15  | QO    | 86/89 (97%)   | 61 (71%)  | 19 (22%) | 6 (7%)   | 1           | 21 |
| 15  | XO    | 86/89 (97%)   | 61 (71%)  | 19 (22%) | 6 (7%)   | 1           | 21 |
| 16  | QP    | 82/88 (93%)   | 48 (58%)  | 23 (28%) | 11 (13%) | 0           | 6  |
| 16  | XP    | 82/88 (93%)   | 48 (58%)  | 23 (28%) | 11 (13%) | 0           | 6  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 17  | QQ    | 98/105 (93%)  | 75 (76%)  | 15 (15%) | 8 (8%)   | 1           | 17 |
| 17  | XQ    | 98/105 (93%)  | 75 (76%)  | 15 (15%) | 8 (8%)   | 1           | 17 |
| 18  | QR    | 68/88 (77%)   | 45 (66%)  | 15 (22%) | 8 (12%)  | 0           | 8  |
| 18  | XR    | 68/88 (77%)   | 46 (68%)  | 14 (21%) | 8 (12%)  | 0           | 8  |
| 19  | QS    | 82/93 (88%)   | 47 (57%)  | 17 (21%) | 18 (22%) | 0           | 1  |
| 19  | XS    | 82/93 (88%)   | 46 (56%)  | 18 (22%) | 18 (22%) | 0           | 1  |
| 20  | QT    | 97/106 (92%)  | 63 (65%)  | 16 (16%) | 18 (19%) | 0           | 3  |
| 20  | XT    | 97/106 (92%)  | 63 (65%)  | 15 (16%) | 19 (20%) | 0           | 2  |
| 21  | QU    | 23/27 (85%)   | 15 (65%)  | 4 (17%)  | 4 (17%)  | 0           | 3  |
| 21  | XU    | 23/27 (85%)   | 15 (65%)  | 4 (17%)  | 4 (17%)  | 0           | 3  |
| 24  | RD    | 270/276 (98%) | 203 (75%) | 48 (18%) | 19 (7%)  | 1           | 21 |
| 24  | YD    | 270/276 (98%) | 204 (76%) | 47 (17%) | 19 (7%)  | 1           | 21 |
| 25  | RE    | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0           | 2  |
| 25  | YE    | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0           | 2  |
| 26  | RF    | 200/210 (95%) | 143 (72%) | 37 (18%) | 20 (10%) | 1           | 12 |
| 26  | YF    | 200/210 (95%) | 143 (72%) | 37 (18%) | 20 (10%) | 1           | 12 |
| 27  | RG    | 179/182 (98%) | 119 (66%) | 39 (22%) | 21 (12%) | 0           | 8  |
| 27  | YG    | 179/182 (98%) | 119 (66%) | 39 (22%) | 21 (12%) | 0           | 8  |
| 28  | RH    | 168/180 (93%) | 94 (56%)  | 36 (21%) | 38 (23%) | 0           | 1  |
| 28  | YH    | 168/180 (93%) | 94 (56%)  | 36 (21%) | 38 (23%) | 0           | 1  |
| 29  | RI    | 144/148 (97%) | 106 (74%) | 21 (15%) | 17 (12%) | 0           | 8  |
| 29  | YI    | 144/148 (97%) | 100 (69%) | 27 (19%) | 17 (12%) | 0           | 8  |
| 30  | RN    | 136/140 (97%) | 84 (62%)  | 30 (22%) | 22 (16%) | 0           | 4  |
| 30  | YN    | 136/140 (97%) | 84 (62%)  | 30 (22%) | 22 (16%) | 0           | 4  |
| 31  | RO    | 120/122 (98%) | 90 (75%)  | 21 (18%) | 9 (8%)   | 1           | 19 |
| 31  | YO    | 120/122 (98%) | 90 (75%)  | 21 (18%) | 9 (8%)   | 1           | 19 |
| 32  | RP    | 148/150 (99%) | 97 (66%)  | 19 (13%) | 32 (22%) | 0           | 2  |
| 32  | YP    | 148/150 (99%) | 97 (66%)  | 19 (13%) | 32 (22%) | 0           | 2  |
| 33  | RQ    | 139/141 (99%) | 95 (68%)  | 30 (22%) | 14 (10%) | 1           | 12 |
| 33  | YQ    | 139/141 (99%) | 97 (70%)  | 28 (20%) | 14 (10%) | 1           | 12 |
| 34  | RR    | 116/118 (98%) | 82 (71%)  | 20 (17%) | 14 (12%) | 0           | 8  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 34  | YR    | 116/118 (98%) | 82 (71%)  | 20 (17%) | 14 (12%) | 0           | 8  |
| 35  | RS    | 109/112 (97%) | 62 (57%)  | 28 (26%) | 19 (17%) | 0           | 3  |
| 35  | YS    | 109/112 (97%) | 62 (57%)  | 28 (26%) | 19 (17%) | 0           | 3  |
| 36  | RT    | 135/146 (92%) | 83 (62%)  | 32 (24%) | 20 (15%) | 0           | 5  |
| 36  | YT    | 135/146 (92%) | 83 (62%)  | 32 (24%) | 20 (15%) | 0           | 5  |
| 37  | RU    | 115/118 (98%) | 86 (75%)  | 20 (17%) | 9 (8%)   | 1           | 18 |
| 37  | YU    | 115/118 (98%) | 86 (75%)  | 20 (17%) | 9 (8%)   | 1           | 18 |
| 38  | RV    | 99/101 (98%)  | 73 (74%)  | 16 (16%) | 10 (10%) | 1           | 12 |
| 38  | YV    | 99/101 (98%)  | 73 (74%)  | 16 (16%) | 10 (10%) | 1           | 12 |
| 39  | RW    | 111/113 (98%) | 75 (68%)  | 22 (20%) | 14 (13%) | 0           | 7  |
| 39  | YW    | 111/113 (98%) | 75 (68%)  | 22 (20%) | 14 (13%) | 0           | 7  |
| 40  | RX    | 90/96 (94%)   | 77 (86%)  | 8 (9%)   | 5 (6%)   | 2           | 27 |
| 40  | YX    | 90/96 (94%)   | 77 (86%)  | 8 (9%)   | 5 (6%)   | 2           | 27 |
| 41  | RY    | 100/110 (91%) | 58 (58%)  | 16 (16%) | 26 (26%) | 0           | 1  |
| 41  | YY    | 100/110 (91%) | 57 (57%)  | 17 (17%) | 26 (26%) | 0           | 1  |
| 42  | RZ    | 181/206 (88%) | 131 (72%) | 28 (16%) | 22 (12%) | 0           | 7  |
| 42  | YZ    | 181/206 (88%) | 128 (71%) | 35 (19%) | 18 (10%) | 1           | 12 |
| 43  | R0    | 80/85 (94%)   | 67 (84%)  | 12 (15%) | 1 (1%)   | 14          | 57 |
| 43  | Y0    | 80/85 (94%)   | 67 (84%)  | 11 (14%) | 2 (2%)   | 6           | 44 |
| 44  | R1    | 95/98 (97%)   | 64 (67%)  | 20 (21%) | 11 (12%) | 0           | 8  |
| 44  | Y1    | 95/98 (97%)   | 64 (67%)  | 20 (21%) | 11 (12%) | 0           | 8  |
| 45  | R2    | 67/72 (93%)   | 47 (70%)  | 11 (16%) | 9 (13%)  | 0           | 6  |
| 45  | Y2    | 67/72 (93%)   | 46 (69%)  | 12 (18%) | 9 (13%)  | 0           | 6  |
| 46  | R3    | 57/60 (95%)   | 45 (79%)  | 9 (16%)  | 3 (5%)   | 2           | 28 |
| 46  | Y3    | 57/60 (95%)   | 45 (79%)  | 9 (16%)  | 3 (5%)   | 2           | 28 |
| 47  | R4    | 69/71 (97%)   | 23 (33%)  | 20 (29%) | 26 (38%) | 0           | 0  |
| 47  | Y4    | 69/71 (97%)   | 23 (33%)  | 20 (29%) | 26 (38%) | 0           | 0  |
| 48  | R5    | 57/60 (95%)   | 33 (58%)  | 9 (16%)  | 15 (26%) | 0           | 1  |
| 48  | Y5    | 56/60 (93%)   | 32 (57%)  | 9 (16%)  | 15 (27%) | 0           | 1  |
| 49  | R6    | 47/54 (87%)   | 15 (32%)  | 18 (38%) | 14 (30%) | 0           | 0  |
| 49  | Y6    | 47/54 (87%)   | 15 (32%)  | 18 (38%) | 14 (30%) | 0           | 0  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-------------------|------------|------------|------------|-------------|-----|
| 50  | R7    | 47/49 (96%)       | 37 (79%)   | 7 (15%)    | 3 (6%)     | 1           | 24  |
| 50  | Y7    | 47/49 (96%)       | 37 (79%)   | 7 (15%)    | 3 (6%)     | 1           | 24  |
| 51  | R8    | 62/65 (95%)       | 36 (58%)   | 15 (24%)   | 11 (18%)   | 0           | 3   |
| 51  | Y8    | 62/65 (95%)       | 36 (58%)   | 15 (24%)   | 11 (18%)   | 0           | 3   |
| 52  | R9    | 35/37 (95%)       | 31 (89%)   | 4 (11%)    | 0          | 100         | 100 |
| 52  | Y9    | 35/37 (95%)       | 31 (89%)   | 4 (11%)    | 0          | 100         | 100 |
| All | All   | 11469/12128 (95%) | 7649 (67%) | 2333 (20%) | 1487 (13%) | 0           | 6   |

5 of 1487 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | QB    | 205/220 (93%) | 181 (88%) | 24 (12%) | 6           | 33 |
| 2   | XB    | 205/220 (93%) | 181 (88%) | 24 (12%) | 6           | 33 |
| 3   | QC    | 159/188 (85%) | 143 (90%) | 16 (10%) | 9           | 38 |
| 3   | XC    | 159/188 (85%) | 143 (90%) | 16 (10%) | 9           | 38 |
| 4   | QD    | 180/181 (99%) | 160 (89%) | 20 (11%) | 7           | 35 |
| 4   | XD    | 180/181 (99%) | 165 (92%) | 15 (8%)  | 13          | 48 |
| 5   | QE    | 116/123 (94%) | 107 (92%) | 9 (8%)   | 15          | 50 |
| 5   | XE    | 116/123 (94%) | 107 (92%) | 9 (8%)   | 15          | 50 |
| 6   | QF    | 90/90 (100%)  | 76 (84%)  | 14 (16%) | 3           | 22 |
| 6   | XF    | 90/90 (100%)  | 76 (84%)  | 14 (16%) | 3           | 22 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 7   | QG    | 126/127 (99%)  | 114 (90%) | 12 (10%) | 10          | 41 |
| 7   | XG    | 126/127 (99%)  | 115 (91%) | 11 (9%)  | 12          | 45 |
| 8   | QH    | 119/119 (100%) | 106 (89%) | 13 (11%) | 7           | 36 |
| 8   | XH    | 119/119 (100%) | 106 (89%) | 13 (11%) | 7           | 36 |
| 9   | QI    | 98/99 (99%)    | 87 (89%)  | 11 (11%) | 7           | 35 |
| 9   | XI    | 98/99 (99%)    | 87 (89%)  | 11 (11%) | 7           | 35 |
| 10  | QJ    | 89/92 (97%)    | 81 (91%)  | 8 (9%)   | 11          | 44 |
| 10  | XJ    | 89/92 (97%)    | 81 (91%)  | 8 (9%)   | 11          | 44 |
| 11  | QK    | 90/99 (91%)    | 81 (90%)  | 9 (10%)  | 9           | 39 |
| 11  | XK    | 90/99 (91%)    | 81 (90%)  | 9 (10%)  | 9           | 39 |
| 12  | QL    | 104/109 (95%)  | 88 (85%)  | 16 (15%) | 3           | 22 |
| 12  | XL    | 104/109 (95%)  | 89 (86%)  | 15 (14%) | 4           | 26 |
| 13  | QM    | 97/101 (96%)   | 81 (84%)  | 16 (16%) | 2           | 19 |
| 13  | XM    | 97/101 (96%)   | 81 (84%)  | 16 (16%) | 2           | 19 |
| 14  | QN    | 49/50 (98%)    | 40 (82%)  | 9 (18%)  | 2           | 14 |
| 14  | XN    | 49/50 (98%)    | 44 (90%)  | 5 (10%)  | 8           | 38 |
| 15  | QO    | 79/80 (99%)    | 73 (92%)  | 6 (8%)   | 15          | 52 |
| 15  | XO    | 79/80 (99%)    | 73 (92%)  | 6 (8%)   | 15          | 52 |
| 16  | QP    | 72/74 (97%)    | 63 (88%)  | 9 (12%)  | 5           | 30 |
| 16  | XP    | 72/74 (97%)    | 63 (88%)  | 9 (12%)  | 5           | 30 |
| 17  | QQ    | 95/97 (98%)    | 89 (94%)  | 6 (6%)   | 21          | 57 |
| 17  | XQ    | 95/97 (98%)    | 89 (94%)  | 6 (6%)   | 21          | 57 |
| 18  | QR    | 61/77 (79%)    | 54 (88%)  | 7 (12%)  | 6           | 34 |
| 18  | XR    | 61/77 (79%)    | 54 (88%)  | 7 (12%)  | 6           | 34 |
| 19  | QS    | 73/80 (91%)    | 62 (85%)  | 11 (15%) | 3           | 23 |
| 19  | XS    | 73/80 (91%)    | 62 (85%)  | 11 (15%) | 3           | 23 |
| 20  | QT    | 76/82 (93%)    | 68 (90%)  | 8 (10%)  | 8           | 37 |
| 20  | XT    | 76/82 (93%)    | 69 (91%)  | 7 (9%)   | 11          | 43 |
| 21  | QU    | 20/22 (91%)    | 19 (95%)  | 1 (5%)   | 28          | 64 |
| 21  | XU    | 20/22 (91%)    | 19 (95%)  | 1 (5%)   | 28          | 64 |
| 24  | RD    | 214/218 (98%)  | 177 (83%) | 37 (17%) | 2           | 17 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 24  | YD    | 214/218 (98%)  | 178 (83%) | 36 (17%) | 2           | 19 |
| 25  | RE    | 165/166 (99%)  | 127 (77%) | 38 (23%) | 1           | 7  |
| 25  | YE    | 165/166 (99%)  | 127 (77%) | 38 (23%) | 1           | 7  |
| 26  | RF    | 161/166 (97%)  | 140 (87%) | 21 (13%) | 5           | 29 |
| 26  | YF    | 161/166 (97%)  | 140 (87%) | 21 (13%) | 5           | 29 |
| 27  | RG    | 155/156 (99%)  | 130 (84%) | 25 (16%) | 3           | 21 |
| 27  | YG    | 155/156 (99%)  | 131 (84%) | 24 (16%) | 3           | 22 |
| 28  | RH    | 142/148 (96%)  | 114 (80%) | 28 (20%) | 1           | 12 |
| 28  | YH    | 142/148 (96%)  | 114 (80%) | 28 (20%) | 1           | 12 |
| 29  | RI    | 122/124 (98%)  | 100 (82%) | 22 (18%) | 2           | 15 |
| 29  | YI    | 122/124 (98%)  | 101 (83%) | 21 (17%) | 2           | 17 |
| 30  | RN    | 117/119 (98%)  | 98 (84%)  | 19 (16%) | 3           | 20 |
| 30  | YN    | 117/119 (98%)  | 98 (84%)  | 19 (16%) | 3           | 20 |
| 31  | RO    | 100/100 (100%) | 90 (90%)  | 10 (10%) | 9           | 39 |
| 31  | YO    | 100/100 (100%) | 90 (90%)  | 10 (10%) | 9           | 39 |
| 32  | RP    | 116/116 (100%) | 89 (77%)  | 27 (23%) | 1           | 7  |
| 32  | YP    | 116/116 (100%) | 89 (77%)  | 27 (23%) | 1           | 7  |
| 33  | RQ    | 111/111 (100%) | 93 (84%)  | 18 (16%) | 3           | 20 |
| 33  | YQ    | 111/111 (100%) | 93 (84%)  | 18 (16%) | 3           | 20 |
| 34  | RR    | 101/101 (100%) | 84 (83%)  | 17 (17%) | 2           | 19 |
| 34  | YR    | 101/101 (100%) | 84 (83%)  | 17 (17%) | 2           | 19 |
| 35  | RS    | 87/88 (99%)    | 74 (85%)  | 13 (15%) | 3           | 24 |
| 35  | YS    | 87/88 (99%)    | 74 (85%)  | 13 (15%) | 3           | 24 |
| 36  | RT    | 120/127 (94%)  | 97 (81%)  | 23 (19%) | 1           | 13 |
| 36  | YT    | 120/127 (94%)  | 97 (81%)  | 23 (19%) | 1           | 13 |
| 37  | RU    | 93/94 (99%)    | 80 (86%)  | 13 (14%) | 4           | 27 |
| 37  | YU    | 93/94 (99%)    | 80 (86%)  | 13 (14%) | 4           | 27 |
| 38  | RV    | 82/82 (100%)   | 71 (87%)  | 11 (13%) | 4           | 28 |
| 38  | YV    | 82/82 (100%)   | 71 (87%)  | 11 (13%) | 4           | 28 |
| 39  | RW    | 92/92 (100%)   | 77 (84%)  | 15 (16%) | 3           | 20 |
| 39  | YW    | 92/92 (100%)   | 77 (84%)  | 15 (16%) | 3           | 20 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 40  | RX    | 74/78 (95%)      | 63 (85%)   | 11 (15%)   | 3           | 24 |
| 40  | YX    | 74/78 (95%)      | 63 (85%)   | 11 (15%)   | 3           | 24 |
| 41  | RY    | 85/91 (93%)      | 70 (82%)   | 15 (18%)   | 2           | 17 |
| 41  | YY    | 85/91 (93%)      | 70 (82%)   | 15 (18%)   | 2           | 17 |
| 42  | RZ    | 162/179 (90%)    | 141 (87%)  | 21 (13%)   | 5           | 29 |
| 42  | YZ    | 162/179 (90%)    | 139 (86%)  | 23 (14%)   | 4           | 27 |
| 43  | R0    | 65/67 (97%)      | 57 (88%)   | 8 (12%)    | 5           | 30 |
| 43  | Y0    | 65/67 (97%)      | 60 (92%)   | 5 (8%)     | 15          | 51 |
| 44  | R1    | 82/83 (99%)      | 67 (82%)   | 15 (18%)   | 2           | 14 |
| 44  | Y1    | 82/83 (99%)      | 67 (82%)   | 15 (18%)   | 2           | 14 |
| 45  | R2    | 64/67 (96%)      | 57 (89%)   | 7 (11%)    | 7           | 36 |
| 45  | Y2    | 64/67 (96%)      | 57 (89%)   | 7 (11%)    | 7           | 36 |
| 46  | R3    | 51/52 (98%)      | 40 (78%)   | 11 (22%)   | 1           | 9  |
| 46  | Y3    | 51/52 (98%)      | 40 (78%)   | 11 (22%)   | 1           | 9  |
| 47  | R4    | 63/63 (100%)     | 44 (70%)   | 19 (30%)   | 0           | 3  |
| 47  | Y4    | 63/63 (100%)     | 44 (70%)   | 19 (30%)   | 0           | 3  |
| 48  | R5    | 51/52 (98%)      | 39 (76%)   | 12 (24%)   | 1           | 7  |
| 48  | Y5    | 50/52 (96%)      | 38 (76%)   | 12 (24%)   | 1           | 6  |
| 49  | R6    | 48/52 (92%)      | 38 (79%)   | 10 (21%)   | 1           | 10 |
| 49  | Y6    | 48/52 (92%)      | 38 (79%)   | 10 (21%)   | 1           | 10 |
| 50  | R7    | 42/42 (100%)     | 39 (93%)   | 3 (7%)     | 17          | 54 |
| 50  | Y7    | 42/42 (100%)     | 39 (93%)   | 3 (7%)     | 17          | 54 |
| 51  | R8    | 54/55 (98%)      | 39 (72%)   | 15 (28%)   | 0           | 4  |
| 51  | Y8    | 54/55 (98%)      | 39 (72%)   | 15 (28%)   | 0           | 4  |
| 52  | R9    | 34/34 (100%)     | 32 (94%)   | 2 (6%)     | 23          | 60 |
| 52  | Y9    | 34/34 (100%)     | 32 (94%)   | 2 (6%)     | 23          | 60 |
| All | All   | 9701/10066 (96%) | 8295 (86%) | 1406 (14%) | 4           | 25 |

5 of 1406 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | R2    | 53  | LEU  |
| 6   | XF    | 97  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | YZ    | 139 | VAL  |
| 47  | R4    | 23  | GLU  |
| 2   | XB    | 23  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | R2    | 47  | ASN  |
| 6   | XF    | 64  | GLN  |
| 42  | YZ    | 32  | HIS  |
| 46  | R3    | 32  | GLN  |
| 2   | XB    | 204 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | QA    | 1499/1522 (98%) | 281 (18%)         | 47 (3%)         |
| 1   | XA    | 1498/1522 (98%) | 299 (19%)         | 52 (3%)         |
| 22  | RA    | 2879/2916 (98%) | 658 (22%)         | 65 (2%)         |
| 22  | YA    | 2880/2916 (98%) | 639 (22%)         | 65 (2%)         |
| 23  | RB    | 119/122 (97%)   | 20 (16%)          | 2 (1%)          |
| 23  | YB    | 119/122 (97%)   | 25 (21%)          | 1 (0%)          |
| 53  | QV    | 76/77 (98%)     | 30 (39%)          | 1 (1%)          |
| 53  | XV    | 76/77 (98%)     | 30 (39%)          | 1 (1%)          |
| 54  | QX    | 7/25 (28%)      | 5 (71%)           | 2 (28%)         |
| 54  | XX    | 7/25 (28%)      | 4 (57%)           | 1 (14%)         |
| 55  | QY    | 13/18 (72%)     | 6 (46%)           | 2 (15%)         |
| 55  | XY    | 13/18 (72%)     | 5 (38%)           | 1 (7%)          |
| 56  | Z6    | 1/3 (33%)       | 0                 | 0               |
| 56  | Z8    | 1/3 (33%)       | 0                 | 0               |
| All | All   | 9188/9366 (98%) | 2002 (21%)        | 240 (2%)        |

5 of 2002 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 6   | G    |
| 1   | QA    | 9   | G    |
| 1   | QA    | 22  | G    |
| 1   | QA    | 32  | A    |
| 1   | QA    | 39  | G    |

5 of 240 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | RA    | 2776 | A    |
| 1   | XA    | 530  | G    |
| 22  | YA    | 2566 | A    |
| 22  | RA    | 2867 | G    |
| 1   | XA    | 243  | A    |

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

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

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 55  | 1MG  | QY    | 37  | 55    | 18,26,27     | 1.76 | 2 (11%)  | 18,39,42    | 1.67 | 4 (22%)  |
| 55  | 1MG  | XY    | 37  | 55    | 18,26,27     | 2.73 | 3 (16%)  | 18,39,42    | 1.55 | 4 (22%)  |
| 56  | PPU  | Z6    | 76  | 56,22 | 31,40,41     | 2.57 | 6 (19%)  | 34,57,60    | 2.56 | 6 (17%)  |
| 56  | PPU  | Z8    | 76  | 56,22 | 31,40,41     | 2.57 | 6 (19%)  | 34,57,60    | 2.56 | 6 (17%)  |

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   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 55  | 1MG  | QY    | 37  | 55    | -       | 0/3/25/26  | 0/3/3/3 |
| 55  | 1MG  | XY    | 37  | 55    | -       | 0/3/25/26  | 0/3/3/3 |
| 56  | PPU  | Z6    | 76  | 56,22 | -       | 0/21/43/44 | 0/4/4/4 |
| 56  | PPU  | Z8    | 76  | 56,22 | -       | 0/21/43/44 | 0/4/4/4 |

The worst 5 of 17 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 56  | Z6    | 76  | PPU  | C9-N6 | -5.81 | 1.31        | 1.45     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 56  | Z8    | 76  | PPU  | C9-N6  | -5.75 | 1.32        | 1.45     |
| 56  | Z8    | 76  | PPU  | C10-N6 | -5.44 | 1.32        | 1.45     |
| 56  | Z6    | 76  | PPU  | C10-N6 | -5.41 | 1.32        | 1.45     |
| 56  | Z8    | 76  | PPU  | C5-N7  | -2.02 | 1.32        | 1.39     |

The worst 5 of 20 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 56  | Z8    | 76  | PPU  | N3-C2-N1  | -8.63 | 121.34      | 128.86   |
| 56  | Z6    | 76  | PPU  | C3'-N3'-C | -8.63 | 110.20      | 123.21   |
| 56  | Z8    | 76  | PPU  | C3'-N3'-C | -8.59 | 110.25      | 123.21   |
| 56  | Z6    | 76  | PPU  | N3-C2-N1  | -8.54 | 121.42      | 128.86   |
| 55  | QY    | 37  | 1MG  | C5-C6-N1  | -4.69 | 112.91      | 118.28   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 34 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 55  | QY    | 37  | 1MG  | 2       | 0            |
| 55  | XY    | 37  | 1MG  | 7       | 0            |
| 56  | Z6    | 76  | PPU  | 14      | 0            |
| 56  | Z8    | 76  | PPU  | 11      | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 684 ligands modelled in this entry, 682 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | PAR  | QA    | 1666 | -    | 45,45,45     | 1.33 | 7 (15%)  | 60,67,67    | 1.42 | 8 (13%)  |
| 58  | PAR  | XA    | 1673 | -    | 45,45,45     | 1.38 | 7 (15%)  | 60,67,67    | 1.36 | 5 (8%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 58  | PAR  | QA    | 1666 | -    | -       | 0/18/94/94 | 0/4/4/4 |
| 58  | PAR  | XA    | 1673 | -    | -       | 0/18/94/94 | 0/4/4/4 |

The worst 5 of 14 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 58  | XA    | 1673 | PAR  | C31-C21 | 2.06 | 1.56        | 1.53     |
| 58  | QA    | 1666 | PAR  | C14-C24 | 2.11 | 1.56        | 1.52     |
| 58  | QA    | 1666 | PAR  | C31-C21 | 2.18 | 1.56        | 1.53     |
| 58  | QA    | 1666 | PAR  | C11-C21 | 2.24 | 1.56        | 1.52     |
| 58  | XA    | 1673 | PAR  | C14-C24 | 2.26 | 1.56        | 1.52     |

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

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 58  | QA    | 1666 | PAR  | O11-C42-C32 | -3.15 | 101.67      | 108.96   |
| 58  | QA    | 1666 | PAR  | O54-C54-C44 | -2.09 | 105.81      | 109.66   |
| 58  | QA    | 1666 | PAR  | C22-C32-C42 | 2.01  | 114.67      | 109.54   |
| 58  | XA    | 1673 | PAR  | C11-O51-C51 | 2.70  | 118.80      | 113.72   |
| 58  | XA    | 1673 | PAR  | O54-C54-C64 | 2.83  | 111.36      | 106.01   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58  | QA    | 1666 | PAR  | 4       | 0            |
| 58  | XA    | 1673 | PAR  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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   | QA    | 1500/1522 (98%) | -0.09  | 26 (1%) 70 61 | 22, 75, 152, 231      | 0     |
| 1   | XA    | 1500/1522 (98%) | -0.25  | 9 (0%) 89 84  | 7, 55, 142, 232       | 0     |
| 2   | QB    | 237/256 (92%)   | 0.39   | 16 (6%) 18 14 | 47, 109, 145, 182     | 0     |
| 2   | XB    | 237/256 (92%)   | 0.18   | 9 (3%) 41 32  | 38, 88, 133, 159      | 0     |
| 3   | QC    | 205/239 (85%)   | 0.14   | 4 (1%) 65 56  | 39, 98, 133, 150      | 0     |
| 3   | XC    | 205/239 (85%)   | -0.18  | 2 (0%) 82 74  | 20, 67, 110, 138      | 0     |
| 4   | QD    | 208/209 (99%)   | 0.14   | 2 (0%) 82 74  | 29, 79, 128, 167      | 0     |
| 4   | XD    | 208/209 (99%)   | 0.05   | 2 (0%) 82 74  | 10, 72, 110, 139      | 0     |
| 5   | QE    | 151/162 (93%)   | 0.28   | 6 (3%) 39 30  | 25, 85, 122, 159      | 0     |
| 5   | XE    | 151/162 (93%)   | -0.03  | 2 (1%) 77 68  | 1, 62, 104, 134       | 0     |
| 6   | QF    | 101/101 (100%)  | 0.15   | 1 (0%) 82 74  | 16, 74, 116, 131      | 0     |
| 6   | XF    | 101/101 (100%)  | -0.03  | 1 (0%) 82 74  | 16, 65, 110, 133      | 0     |
| 7   | QG    | 155/156 (99%)   | 0.47   | 17 (10%) 6 6  | 30, 84, 125, 149      | 0     |
| 7   | XG    | 155/156 (99%)   | 0.18   | 6 (3%) 40 32  | 20, 71, 109, 131      | 0     |
| 8   | QH    | 138/138 (100%)  | 0.31   | 3 (2%) 62 53  | 45, 88, 124, 156      | 0     |
| 8   | XH    | 138/138 (100%)  | 0.10   | 1 (0%) 87 81  | 19, 70, 102, 125      | 0     |
| 9   | QI    | 127/128 (99%)   | 0.72   | 12 (9%) 9 8   | 46, 97, 137, 144      | 0     |
| 9   | XI    | 127/128 (99%)   | 0.20   | 3 (2%) 59 49  | 16, 79, 119, 129      | 0     |
| 10  | QJ    | 99/105 (94%)    | 1.05   | 19 (19%) 1 2  | 44, 108, 142, 161     | 0     |
| 10  | XJ    | 99/105 (94%)    | 0.56   | 11 (11%) 6 6  | 9, 83, 129, 147       | 0     |
| 11  | QK    | 119/129 (92%)   | 0.40   | 14 (11%) 5 6  | 18, 71, 123, 149      | 0     |
| 11  | XK    | 119/129 (92%)   | 0.26   | 5 (4%) 37 29  | 15, 63, 110, 147      | 0     |
| 12  | QL    | 125/132 (94%)   | 0.45   | 8 (6%) 20 14  | 20, 72, 108, 139      | 0     |
| 12  | XL    | 125/132 (94%)   | -0.02  | 2 (1%) 72 63  | 0, 48, 91, 134        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | QM    | 121/126 (96%)   | 0.52   | 13 (10%) 7 6  | 39, 96, 131, 170      | 0     |
| 13  | XM    | 121/126 (96%)   | -0.00  | 3 (2%) 58 47  | 4, 68, 125, 149       | 0     |
| 14  | QN    | 60/61 (98%)     | 0.64   | 6 (10%) 8 7   | 52, 98, 137, 146      | 0     |
| 14  | XN    | 60/61 (98%)     | -0.07  | 0 100 100     | 4, 60, 100, 120       | 0     |
| 15  | QO    | 88/89 (98%)     | 0.14   | 6 (6%) 18 14  | 30, 79, 120, 136      | 0     |
| 15  | XO    | 88/89 (98%)     | 0.01   | 1 (1%) 80 72  | 10, 64, 93, 107       | 0     |
| 16  | QP    | 84/88 (95%)     | 0.32   | 2 (2%) 59 49  | 12, 68, 103, 138      | 0     |
| 16  | XP    | 84/88 (95%)     | 0.46   | 2 (2%) 59 49  | 30, 70, 106, 135      | 0     |
| 17  | QQ    | 100/105 (95%)   | 0.56   | 7 (7%) 17 13  | 33, 82, 115, 141      | 0     |
| 17  | XQ    | 100/105 (95%)   | 0.21   | 0 100 100     | 14, 64, 102, 124      | 0     |
| 18  | QR    | 70/88 (79%)     | 0.53   | 9 (12%) 4 4   | 18, 78, 119, 147      | 0     |
| 18  | XR    | 70/88 (79%)     | 0.38   | 4 (5%) 24 19  | 22, 67, 109, 135      | 0     |
| 19  | QS    | 84/93 (90%)     | 0.68   | 7 (8%) 12 10  | 60, 102, 132, 147     | 0     |
| 19  | XS    | 84/93 (90%)     | 0.21   | 2 (2%) 59 49  | 15, 73, 112, 164      | 0     |
| 20  | QT    | 99/106 (93%)    | 0.19   | 3 (3%) 51 40  | 3, 77, 111, 131       | 0     |
| 20  | XT    | 99/106 (93%)    | 0.30   | 3 (3%) 51 40  | 19, 77, 117, 126      | 0     |
| 21  | QU    | 25/27 (92%)     | 1.78   | 9 (36%) 0 1   | 37, 85, 131, 145      | 0     |
| 21  | XU    | 25/27 (92%)     | 0.97   | 3 (12%) 5 6   | 30, 75, 103, 134      | 0     |
| 22  | RA    | 2882/2916 (98%) | -0.18  | 97 (3%) 46 36 | 2, 45, 174, 236       | 0     |
| 22  | YA    | 2883/2916 (98%) | -0.27  | 71 (2%) 58 47 | 1, 35, 165, 227       | 0     |
| 23  | RB    | 120/122 (98%)   | -0.17  | 0 100 100     | 46, 89, 131, 153      | 0     |
| 23  | YB    | 120/122 (98%)   | -0.48  | 1 (0%) 86 79  | 18, 58, 93, 139       | 0     |
| 24  | RD    | 272/276 (98%)   | -0.11  | 0 100 100     | 4, 41, 81, 123        | 0     |
| 24  | YD    | 272/276 (98%)   | -0.05  | 1 (0%) 92 88  | 1, 33, 74, 140        | 0     |
| 25  | RE    | 205/206 (99%)   | 0.12   | 4 (1%) 65 56  | 7, 62, 112, 141       | 0     |
| 25  | YE    | 205/206 (99%)   | 0.04   | 2 (0%) 82 74  | 6, 56, 103, 125       | 0     |
| 26  | RF    | 202/210 (96%)   | -0.04  | 2 (0%) 82 74  | 1, 64, 110, 129       | 0     |
| 26  | YF    | 202/210 (96%)   | -0.06  | 2 (0%) 82 74  | 1, 47, 95, 112        | 0     |
| 27  | RG    | 181/182 (99%)   | 0.37   | 9 (4%) 30 24  | 34, 99, 142, 166      | 0     |
| 27  | YG    | 181/182 (99%)   | -0.06  | 1 (0%) 89 84  | 9, 66, 115, 163       | 0     |
| 28  | RH    | 170/180 (94%)   | 1.11   | 37 (21%) 1 2  | 32, 108, 152, 170     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | YH    | 170/180 (94%)  | 0.20   | 5 (2%) 52 42  | 14, 68, 110, 133      | 0     |
| 29  | RI    | 146/148 (98%)  | 0.36   | 3 (2%) 64 54  | 16, 78, 122, 154      | 0     |
| 29  | YI    | 146/148 (98%)  | 0.17   | 3 (2%) 64 54  | 8, 72, 119, 159       | 0     |
| 30  | RN    | 138/140 (98%)  | 0.31   | 5 (3%) 43 34  | 14, 70, 110, 124      | 0     |
| 30  | YN    | 138/140 (98%)  | 0.03   | 4 (2%) 52 42  | 8, 55, 103, 128       | 0     |
| 31  | RO    | 122/122 (100%) | 0.15   | 0 100 100     | 5, 56, 97, 126        | 0     |
| 31  | YO    | 122/122 (100%) | -0.01  | 0 100 100     | 0, 42, 79, 94         | 0     |
| 32  | RP    | 150/150 (100%) | 0.49   | 11 (7%) 16 12 | 6, 65, 126, 159       | 0     |
| 32  | YP    | 150/150 (100%) | 0.04   | 2 (1%) 77 68  | 5, 53, 105, 154       | 0     |
| 33  | RQ    | 141/141 (100%) | 0.18   | 3 (2%) 64 54  | 2, 62, 106, 142       | 0     |
| 33  | YQ    | 141/141 (100%) | -0.12  | 0 100 100     | 3, 42, 94, 132        | 0     |
| 34  | RR    | 118/118 (100%) | -0.05  | 0 100 100     | 8, 50, 92, 118        | 0     |
| 34  | YR    | 118/118 (100%) | -0.07  | 0 100 100     | 7, 43, 89, 109        | 0     |
| 35  | RS    | 111/112 (99%)  | 0.36   | 3 (2%) 55 45  | 35, 78, 114, 141      | 0     |
| 35  | YS    | 111/112 (99%)  | 0.01   | 0 100 100     | 7, 61, 94, 111        | 0     |
| 36  | RT    | 137/146 (93%)  | 0.11   | 2 (1%) 74 64  | 13, 64, 125, 165      | 0     |
| 36  | YT    | 137/146 (93%)  | -0.10  | 1 (0%) 87 81  | 10, 58, 111, 158      | 0     |
| 37  | RU    | 117/118 (99%)  | -0.06  | 3 (2%) 56 46  | 10, 61, 104, 147      | 0     |
| 37  | YU    | 117/118 (99%)  | -0.16  | 2 (1%) 70 61  | 0, 44, 108, 129       | 0     |
| 38  | RV    | 101/101 (100%) | 0.07   | 0 100 100     | 20, 75, 116, 144      | 0     |
| 38  | YV    | 101/101 (100%) | 0.19   | 2 (1%) 65 56  | 11, 65, 104, 156      | 0     |
| 39  | RW    | 113/113 (100%) | 0.10   | 0 100 100     | 3, 43, 93, 149        | 0     |
| 39  | YW    | 113/113 (100%) | -0.09  | 2 (1%) 69 59  | 2, 42, 91, 144        | 0     |
| 40  | RX    | 92/96 (95%)    | -0.09  | 1 (1%) 80 72  | 15, 52, 96, 125       | 0     |
| 40  | YX    | 92/96 (95%)    | -0.11  | 0 100 100     | 3, 37, 76, 96         | 0     |
| 41  | RY    | 102/110 (92%)  | 1.27   | 28 (27%) 1 1  | 26, 88, 132, 159      | 0     |
| 41  | YY    | 102/110 (92%)  | 0.34   | 4 (3%) 40 32  | 9, 63, 120, 140       | 0     |
| 42  | RZ    | 183/206 (88%)  | 0.39   | 10 (5%) 26 20 | 21, 88, 133, 152      | 0     |
| 42  | YZ    | 183/206 (88%)  | 0.01   | 3 (1%) 72 63  | 20, 70, 123, 155      | 0     |
| 43  | R0    | 82/85 (96%)    | 0.36   | 3 (3%) 42 33  | 14, 48, 79, 112       | 0     |
| 43  | Y0    | 82/85 (96%)    | 0.18   | 1 (1%) 79 70  | 3, 36, 66, 97         | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | R1    | 97/98 (98%)       | 0.47   | 4 (4%) 38 30   | 5, 53, 126, 159       | 0     |
| 44  | Y1    | 97/98 (98%)       | 0.29   | 3 (3%) 49 39   | 5, 43, 104, 139       | 0     |
| 45  | R2    | 69/72 (95%)       | 0.05   | 0 100 100      | 13, 72, 111, 129      | 0     |
| 45  | Y2    | 69/72 (95%)       | -0.21  | 0 100 100      | 5, 50, 104, 121       | 0     |
| 46  | R3    | 59/60 (98%)       | 1.17   | 9 (15%) 2 3    | 12, 63, 111, 139      | 0     |
| 46  | Y3    | 59/60 (98%)       | 0.47   | 5 (8%) 11 10   | 2, 44, 101, 174       | 0     |
| 47  | R4    | 71/71 (100%)      | 0.89   | 12 (16%) 2 3   | 75, 131, 170, 189     | 0     |
| 47  | Y4    | 71/71 (100%)      | 0.27   | 4 (5%) 25 20   | 46, 102, 154, 161     | 0     |
| 48  | R5    | 59/60 (98%)       | 0.11   | 4 (6%) 18 14   | 6, 55, 133, 141       | 0     |
| 48  | Y5    | 58/60 (96%)       | 0.14   | 2 (3%) 46 36   | 10, 59, 143, 162      | 0     |
| 49  | R6    | 49/54 (90%)       | 3.21   | 31 (63%) 0 1   | 83, 118, 150, 157     | 0     |
| 49  | Y6    | 49/54 (90%)       | 2.66   | 31 (63%) 0 1   | 51, 109, 141, 149     | 0     |
| 50  | R7    | 49/49 (100%)      | 0.07   | 1 (2%) 65 56   | 8, 35, 87, 146        | 0     |
| 50  | Y7    | 49/49 (100%)      | 0.08   | 1 (2%) 65 56   | 1, 29, 71, 121        | 0     |
| 51  | R8    | 64/65 (98%)       | 0.23   | 2 (3%) 49 39   | 1, 52, 96, 158        | 0     |
| 51  | Y8    | 64/65 (98%)       | 0.02   | 0 100 100      | 5, 40, 81, 149        | 0     |
| 52  | R9    | 37/37 (100%)      | 3.92   | 32 (86%) 0 0   | 66, 110, 156, 168     | 0     |
| 52  | Y9    | 37/37 (100%)      | 4.49   | 37 (100%) 0 0  | 78, 107, 132, 166     | 0     |
| 53  | QV    | 77/77 (100%)      | 0.13   | 2 (2%) 56 46   | 46, 99, 145, 169      | 0     |
| 53  | XV    | 77/77 (100%)      | 0.03   | 2 (2%) 56 46   | 28, 72, 119, 180      | 0     |
| 54  | QX    | 8/25 (32%)        | 3.09   | 6 (75%) 0 0    | 103, 130, 144, 183    | 0     |
| 54  | XX    | 8/25 (32%)        | 1.62   | 2 (25%) 1 1    | 56, 75, 115, 190      | 0     |
| 55  | QY    | 13/18 (72%)       | 1.53   | 4 (30%) 0 1    | 112, 161, 199, 206    | 0     |
| 55  | XY    | 13/18 (72%)       | 1.15   | 2 (15%) 2 3    | 72, 116, 180, 193     | 0     |
| 56  | Z6    | 2/3 (66%)         | 0.34   | 0 100 100      | 52, 52, 52, 57        | 0     |
| 56  | Z8    | 2/3 (66%)         | 0.56   | 0 100 100      | 46, 46, 46, 46        | 0     |
| All | All   | 20870/21494 (97%) | 0.06   | 785 (3%) 41 32 | 0, 61, 135, 236       | 0     |

The worst 5 of 785 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 52  | R9    | 11  | CYS  | 11.8 |
| 52  | Y9    | 34  | GLN  | 9.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 49  | R6    | 22  | ALA  | 9.7  |
| 52  | R9    | 14  | CYS  | 9.5  |
| 52  | R9    | 34  | GLN  | 8.4  |

## 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 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 56  | PPU  | Z8    | 76  | 37/38 | 0.93 | 0.33 | -    | 48,48,48,48                | 0     |
| 56  | PPU  | Z6    | 76  | 37/38 | 0.93 | 0.31 | -    | 51,51,51,51                | 0     |
| 55  | 1MG  | QY    | 37  | 24/25 | 0.84 | 0.31 | -    | 125,125,125,125            | 0     |
| 55  | 1MG  | XY    | 37  | 24/25 | 0.89 | 0.20 | -    | 64,64,64,64                | 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 |
|-----|------|-------|------|-------|------|------|--------|----------------------------|-------|
| 57  | MG   | RA    | 3003 | 1/1   | 0.87 | 1.15 | 132.21 | 50,50,50,50                | 0     |
| 57  | MG   | YA    | 3053 | 1/1   | 0.78 | 1.02 | 74.03  | 50,50,50,50                | 0     |
| 57  | MG   | RA    | 3007 | 1/1   | 0.81 | 1.30 | 73.04  | 50,50,50,50                | 0     |
| 57  | MG   | RA    | 3064 | 1/1   | 0.75 | 1.71 | 66.93  | 50,50,50,50                | 0     |
| 57  | MG   | YA    | 3026 | 1/1   | 0.94 | 1.28 | 66.88  | 50,50,50,50                | 0     |
| 57  | MG   | XA    | 1656 | 1/1   | 0.88 | 0.89 | 63.25  | 12,12,12,12                | 0     |
| 57  | MG   | RA    | 3100 | 1/1   | 0.95 | 1.01 | 61.99  | 50,50,50,50                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57  | MG   | XA    | 1603 | 1/1   | 0.90 | 0.95 | 51.89 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3261 | 1/1   | 0.78 | 0.96 | 46.98 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3065 | 1/1   | 0.71 | 1.23 | 45.98 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3051 | 1/1   | 0.85 | 0.83 | 44.16 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3093 | 1/1   | 0.89 | 0.71 | 43.07 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3061 | 1/1   | 0.94 | 0.77 | 43.02 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3009 | 1/1   | 0.96 | 0.74 | 41.99 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3164 | 1/1   | 0.78 | 0.55 | 37.48 | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3186 | 1/1   | 0.68 | 0.72 | 36.31 | 51,51,51,51                 | 0     |
| 57  | MG   | RA    | 3036 | 1/1   | 0.98 | 0.40 | 35.57 | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3031 | 1/1   | 0.86 | 1.04 | 34.99 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3049 | 1/1   | 0.94 | 1.10 | 34.88 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3259 | 1/1   | 0.78 | 0.66 | 33.02 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3034 | 1/1   | 0.78 | 1.60 | 32.93 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3079 | 1/1   | 0.80 | 1.26 | 32.21 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3257 | 1/1   | 0.97 | 0.78 | 31.67 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3009 | 1/1   | 0.96 | 0.56 | 30.89 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3042 | 1/1   | 0.96 | 0.58 | 30.85 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3019 | 1/1   | 0.91 | 0.80 | 29.28 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3035 | 1/1   | 0.91 | 0.81 | 29.16 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3180 | 1/1   | 0.89 | 0.72 | 28.88 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3015 | 1/1   | 0.96 | 0.77 | 28.21 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3056 | 1/1   | 0.93 | 0.88 | 28.09 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3217 | 1/1   | 0.84 | 0.62 | 27.60 | 52,52,52,52                 | 0     |
| 57  | MG   | YA    | 3193 | 1/1   | 0.82 | 0.74 | 26.55 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3005 | 1/1   | 0.87 | 0.81 | 26.51 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3098 | 1/1   | 0.91 | 0.84 | 24.01 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3127 | 1/1   | 0.72 | 0.52 | 23.74 | 15,15,15,15                 | 0     |
| 57  | MG   | XA    | 1625 | 1/1   | 0.88 | 0.48 | 23.54 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3219 | 1/1   | 0.80 | 0.56 | 22.90 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3057 | 1/1   | 0.95 | 0.77 | 22.32 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3123 | 1/1   | 0.79 | 0.94 | 22.08 | 50,50,50,50                 | 0     |
| 57  | MG   | XA    | 1635 | 1/1   | 0.73 | 1.57 | 21.76 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3153 | 1/1   | 0.90 | 0.41 | 21.40 | 36,36,36,36                 | 0     |
| 57  | MG   | XA    | 1664 | 1/1   | 0.83 | 0.39 | 21.24 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3242 | 1/1   | 0.94 | 0.61 | 20.86 | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3045 | 1/1   | 0.88 | 0.55 | 20.57 | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3060 | 1/1   | 0.96 | 0.71 | 20.12 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3157 | 1/1   | 0.84 | 0.32 | 19.76 | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3085 | 1/1   | 0.89 | 0.81 | 17.43 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3201 | 1/1   | 0.79 | 0.36 | 16.52 | 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 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57  | MG   | RA    | 3038 | 1/1   | 0.90 | 0.74 | 16.18 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3020 | 1/1   | 0.88 | 0.71 | 15.66 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3097 | 1/1   | 0.95 | 0.70 | 15.61 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3033 | 1/1   | 0.96 | 0.60 | 15.50 | 16,16,16,16                 | 0     |
| 57  | MG   | XA    | 1668 | 1/1   | 0.95 | 0.28 | 15.41 | 6,6,6,6                     | 0     |
| 57  | MG   | YA    | 3033 | 1/1   | 0.95 | 0.73 | 14.85 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3202 | 1/1   | 0.85 | 0.43 | 14.71 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3002 | 1/1   | 0.95 | 0.73 | 14.50 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3118 | 1/1   | 0.98 | 0.46 | 14.34 | 12,12,12,12                 | 0     |
| 57  | MG   | YA    | 3254 | 1/1   | 0.88 | 0.37 | 14.20 | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3042 | 1/1   | 0.98 | 0.46 | 14.11 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3023 | 1/1   | 0.98 | 0.46 | 13.88 | 5,5,5,5                     | 0     |
| 57  | MG   | XA    | 1604 | 1/1   | 0.96 | 1.07 | 13.86 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3169 | 1/1   | 0.88 | 0.86 | 13.71 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3182 | 1/1   | 0.92 | 0.63 | 13.62 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3206 | 1/1   | 0.84 | 0.29 | 13.60 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3041 | 1/1   | 0.82 | 0.85 | 13.55 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3222 | 1/1   | 0.87 | 0.37 | 13.36 | 4,4,4,4                     | 0     |
| 57  | MG   | QA    | 1617 | 1/1   | 0.91 | 0.44 | 13.22 | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3134 | 1/1   | 0.86 | 0.66 | 13.19 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3032 | 1/1   | 0.92 | 0.52 | 12.88 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3052 | 1/1   | 0.94 | 0.48 | 12.78 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3135 | 1/1   | 0.95 | 0.39 | 12.71 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3132 | 1/1   | 0.95 | 0.38 | 12.59 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3077 | 1/1   | 0.95 | 0.39 | 12.56 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3173 | 1/1   | 0.90 | 0.20 | 12.25 | 14,14,14,14                 | 0     |
| 57  | MG   | XA    | 1645 | 1/1   | 0.95 | 0.45 | 12.00 | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3099 | 1/1   | 0.98 | 0.33 | 11.72 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3044 | 1/1   | 0.95 | 0.53 | 11.72 | 16,16,16,16                 | 0     |
| 57  | MG   | YA    | 3099 | 1/1   | 0.92 | 0.79 | 11.61 | 50,50,50,50                 | 0     |
| 57  | MG   | QA    | 1613 | 1/1   | 0.95 | 0.42 | 11.56 | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3203 | 1/1   | 0.95 | 0.40 | 11.55 | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3027 | 1/1   | 0.83 | 0.97 | 11.52 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3048 | 1/1   | 0.93 | 0.46 | 11.13 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3116 | 1/1   | 0.89 | 0.40 | 11.07 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3106 | 1/1   | 0.95 | 0.49 | 10.94 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3184 | 1/1   | 0.82 | 0.36 | 10.92 | 40,40,40,40                 | 0     |
| 57  | MG   | RA    | 3226 | 1/1   | 0.93 | 0.32 | 10.86 | 29,29,29,29                 | 0     |
| 57  | MG   | YA    | 3024 | 1/1   | 0.84 | 0.53 | 10.77 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3181 | 1/1   | 0.73 | 0.33 | 10.75 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3122 | 1/1   | 0.89 | 0.30 | 10.07 | 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 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | XA    | 1644 | 1/1   | 0.96 | 0.30 | 9.98 | 11,11,11,11                 | 0     |
| 57  | MG   | QA    | 1610 | 1/1   | 0.85 | 0.57 | 9.89 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3178 | 1/1   | 0.89 | 0.53 | 9.77 | 32,32,32,32                 | 0     |
| 57  | MG   | YA    | 3114 | 1/1   | 0.96 | 0.29 | 9.63 | 16,16,16,16                 | 0     |
| 57  | MG   | YA    | 3057 | 1/1   | 0.95 | 0.50 | 9.53 | 8,8,8,8                     | 0     |
| 57  | MG   | QA    | 1646 | 1/1   | 0.92 | 0.58 | 9.27 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3079 | 1/1   | 0.99 | 0.40 | 9.17 | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3096 | 1/1   | 0.98 | 0.48 | 9.12 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3006 | 1/1   | 0.86 | 0.86 | 8.89 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3067 | 1/1   | 0.99 | 0.45 | 8.85 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3107 | 1/1   | 0.98 | 0.45 | 8.65 | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3011 | 1/1   | 0.99 | 0.41 | 8.62 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3050 | 1/1   | 0.96 | 0.50 | 8.53 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3176 | 1/1   | 0.86 | 0.31 | 8.51 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3023 | 1/1   | 0.86 | 0.49 | 8.43 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3037 | 1/1   | 0.95 | 0.34 | 8.38 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3179 | 1/1   | 0.91 | 0.27 | 8.24 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3034 | 1/1   | 0.95 | 0.34 | 8.04 | 7,7,7,7                     | 0     |
| 57  | MG   | XA    | 1619 | 1/1   | 0.94 | 0.41 | 7.98 | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3152 | 1/1   | 0.96 | 0.39 | 7.76 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3196 | 1/1   | 0.97 | 0.27 | 7.75 | 76,76,76,76                 | 0     |
| 57  | MG   | YA    | 3092 | 1/1   | 0.95 | 0.40 | 7.53 | 2,2,2,2                     | 0     |
| 57  | MG   | XA    | 1615 | 1/1   | 0.80 | 0.48 | 7.37 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3223 | 1/1   | 0.75 | 0.33 | 7.26 | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3124 | 1/1   | 0.96 | 0.29 | 7.24 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3226 | 1/1   | 0.90 | 0.23 | 6.95 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3073 | 1/1   | 0.90 | 0.29 | 6.91 | 4,4,4,4                     | 0     |
| 57  | MG   | XA    | 1650 | 1/1   | 0.73 | 0.31 | 6.81 | 22,22,22,22                 | 0     |
| 57  | MG   | YA    | 3142 | 1/1   | 0.93 | 0.27 | 6.79 | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3215 | 1/1   | 0.89 | 0.25 | 6.71 | 2,2,2,2                     | 0     |
| 57  | MG   | XA    | 1672 | 1/1   | 0.96 | 0.26 | 6.71 | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3087 | 1/1   | 0.92 | 0.43 | 6.58 | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3241 | 1/1   | 0.94 | 0.28 | 6.56 | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3140 | 1/1   | 0.92 | 0.21 | 6.35 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3163 | 1/1   | 0.57 | 0.31 | 6.33 | 9,9,9,9                     | 0     |
| 57  | MG   | QA    | 1604 | 1/1   | 0.95 | 0.37 | 6.19 | 7,7,7,7                     | 0     |
| 57  | MG   | XA    | 1634 | 1/1   | 0.79 | 0.21 | 6.05 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3205 | 1/1   | 0.91 | 0.24 | 5.93 | 40,40,40,40                 | 0     |
| 57  | MG   | YA    | 3093 | 1/1   | 0.94 | 0.48 | 5.92 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3262 | 1/1   | 0.86 | 0.33 | 5.89 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3086 | 1/1   | 0.96 | 0.30 | 5.81 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3062 | 1/1   | 0.97 | 0.49 | 5.73 | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3081 | 1/1   | 0.96 | 0.34 | 5.71 | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3025 | 1/1   | 0.97 | 0.25 | 5.70 | 7,7,7,7                     | 0     |
| 57  | MG   | QA    | 1639 | 1/1   | 0.85 | 0.27 | 5.66 | 27,27,27,27                 | 0     |
| 57  | MG   | RA    | 3037 | 1/1   | 0.94 | 0.43 | 5.49 | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3071 | 1/1   | 0.92 | 0.32 | 5.36 | 6,6,6,6                     | 0     |
| 57  | MG   | QA    | 1612 | 1/1   | 0.89 | 0.37 | 5.36 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3113 | 1/1   | 0.88 | 0.48 | 5.18 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3038 | 1/1   | 0.99 | 0.25 | 4.91 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3072 | 1/1   | 0.93 | 0.49 | 4.90 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3260 | 1/1   | 0.94 | 0.56 | 4.89 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3149 | 1/1   | 0.90 | 0.62 | 4.88 | 17,17,17,17                 | 0     |
| 57  | MG   | YA    | 3213 | 1/1   | 0.90 | 0.31 | 4.84 | 15,15,15,15                 | 0     |
| 58  | PAR  | QA    | 1666 | 42/42 | 0.80 | 0.38 | 4.77 | 104,104,104,104             | 0     |
| 57  | MG   | QA    | 1631 | 1/1   | 0.50 | 0.24 | 4.69 | 63,63,63,63                 | 0     |
| 57  | MG   | RA    | 3018 | 1/1   | 0.97 | 0.28 | 4.56 | 3,3,3,3                     | 0     |
| 57  | MG   | XV    | 101  | 1/1   | 0.92 | 0.39 | 4.43 | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3078 | 1/1   | 0.97 | 0.26 | 4.39 | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3066 | 1/1   | 0.98 | 0.24 | 4.35 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3211 | 1/1   | 0.87 | 0.25 | 4.25 | 11,11,11,11                 | 0     |
| 58  | PAR  | XA    | 1673 | 42/42 | 0.87 | 0.32 | 4.18 | 132,132,132,132             | 0     |
| 57  | MG   | RA    | 3126 | 1/1   | 0.95 | 0.22 | 4.18 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3083 | 1/1   | 0.96 | 0.38 | 4.16 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3184 | 1/1   | 0.97 | 0.32 | 4.15 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3138 | 1/1   | 0.96 | 0.37 | 3.99 | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3088 | 1/1   | 0.97 | 0.25 | 3.93 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3216 | 1/1   | 0.97 | 0.25 | 3.79 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3056 | 1/1   | 0.92 | 0.20 | 3.79 | 0,0,0,0                     | 0     |
| 57  | MG   | XA    | 1623 | 1/1   | 0.99 | 0.22 | 3.63 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3013 | 1/1   | 0.92 | 0.35 | 3.60 | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3177 | 1/1   | 0.95 | 0.27 | 3.57 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3240 | 1/1   | 0.89 | 0.67 | 3.56 | 12,12,12,12                 | 0     |
| 57  | MG   | YA    | 3156 | 1/1   | 0.65 | 0.24 | 3.45 | 8,8,8,8                     | 0     |
| 57  | MG   | YX    | 101  | 1/1   | 0.95 | 0.42 | 3.34 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3185 | 1/1   | 0.92 | 0.19 | 3.30 | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3088 | 1/1   | 0.97 | 0.26 | 3.22 | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3054 | 1/1   | 0.89 | 0.31 | 3.20 | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3209 | 1/1   | 0.95 | 0.20 | 3.10 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3101 | 1/1   | 0.92 | 0.27 | 3.09 | 9,9,9,9                     | 0     |
| 57  | MG   | XA    | 1646 | 1/1   | 0.92 | 0.17 | 3.05 | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3172 | 1/1   | 0.93 | 0.27 | 3.00 | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3014 | 1/1   | 0.96 | 0.38 | 2.93 | 1,1,1,1                     | 0     |
| 57  | MG   | XA    | 1618 | 1/1   | 0.97 | 0.31 | 2.90 | 4,4,4,4                     | 0     |
| 57  | MG   | RP    | 201  | 1/1   | 0.95 | 0.43 | 2.89 | 85,85,85,85                 | 0     |
| 57  | MG   | XA    | 1610 | 1/1   | 0.96 | 0.26 | 2.87 | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3111 | 1/1   | 0.94 | 0.24 | 2.80 | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3107 | 1/1   | 0.95 | 0.26 | 2.79 | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3109 | 1/1   | 0.98 | 0.24 | 2.75 | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3173 | 1/1   | 0.94 | 0.35 | 2.67 | 3,3,3,3                     | 0     |
| 57  | MG   | XA    | 1611 | 1/1   | 0.96 | 0.33 | 2.60 | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3165 | 1/1   | 0.97 | 0.20 | 2.60 | 42,42,42,42                 | 0     |
| 57  | MG   | RA    | 3152 | 1/1   | 0.96 | 0.17 | 2.59 | 26,26,26,26                 | 0     |
| 57  | MG   | XA    | 1607 | 1/1   | 0.83 | 0.32 | 2.47 | 17,17,17,17                 | 0     |
| 57  | MG   | QA    | 1645 | 1/1   | 0.98 | 0.27 | 2.45 | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3017 | 1/1   | 0.96 | 0.28 | 2.42 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3151 | 1/1   | 0.73 | 0.55 | 2.40 | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3022 | 1/1   | 0.96 | 0.24 | 2.37 | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3191 | 1/1   | 0.84 | 0.39 | 2.36 | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3195 | 1/1   | 0.94 | 0.19 | 2.35 | 21,21,21,21                 | 0     |
| 57  | MG   | RA    | 3074 | 1/1   | 0.98 | 0.19 | 2.35 | 20,20,20,20                 | 0     |
| 57  | MG   | YA    | 3162 | 1/1   | 0.87 | 0.28 | 2.29 | 30,30,30,30                 | 0     |
| 57  | MG   | RA    | 3157 | 1/1   | 0.82 | 0.25 | 2.28 | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3025 | 1/1   | 0.98 | 0.27 | 2.25 | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3089 | 1/1   | 0.95 | 0.38 | 2.23 | 0,0,0,0                     | 0     |
| 57  | MG   | YB    | 203  | 1/1   | 0.96 | 0.18 | 2.21 | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3044 | 1/1   | 0.98 | 0.23 | 2.18 | 8,8,8,8                     | 0     |
| 57  | MG   | XA    | 1612 | 1/1   | 0.97 | 0.22 | 2.13 | 23,23,23,23                 | 0     |
| 57  | MG   | XA    | 1608 | 1/1   | 0.93 | 0.18 | 2.12 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3077 | 1/1   | 0.97 | 0.22 | 2.07 | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3118 | 1/1   | 0.90 | 0.20 | 2.02 | 1,1,1,1                     | 0     |
| 57  | MG   | XA    | 1626 | 1/1   | 0.98 | 0.21 | 1.99 | 1,1,1,1                     | 0     |
| 59  | ZN   | XD    | 301  | 1/1   | 0.94 | 0.39 | 1.91 | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3183 | 1/1   | 0.87 | 0.19 | 1.85 | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3214 | 1/1   | 0.93 | 0.21 | 1.83 | 43,43,43,43                 | 0     |
| 57  | MG   | RA    | 3243 | 1/1   | 0.94 | 0.38 | 1.82 | 18,18,18,18                 | 0     |
| 57  | MG   | YP    | 202  | 1/1   | 0.97 | 0.33 | 1.74 | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3194 | 1/1   | 0.85 | 0.15 | 1.73 | 82,82,82,82                 | 0     |
| 57  | MG   | XA    | 1636 | 1/1   | 0.97 | 0.23 | 1.72 | 9,9,9,9                     | 0     |
| 57  | MG   | Y7    | 101  | 1/1   | 0.89 | 0.27 | 1.70 | 14,14,14,14                 | 0     |
| 57  | MG   | QA    | 1615 | 1/1   | 0.96 | 0.18 | 1.64 | 54,54,54,54                 | 0     |
| 57  | MG   | RA    | 3015 | 1/1   | 0.97 | 0.29 | 1.56 | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3076 | 1/1   | 0.95 | 0.17 | 1.49 | 3,3,3,3                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57  | MG   | YA    | 3058 | 1/1   | 0.99 | 0.20 | 1.49  | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3008 | 1/1   | 0.95 | 0.21 | 1.36  | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3162 | 1/1   | 0.92 | 0.21 | 1.34  | 18,18,18,18                 | 0     |
| 57  | MG   | YA    | 3005 | 1/1   | 0.89 | 0.21 | 1.28  | 2,2,2,2                     | 0     |
| 57  | MG   | RP    | 202  | 1/1   | 0.86 | 0.31 | 1.26  | 75,75,75,75                 | 0     |
| 57  | MG   | YA    | 3109 | 1/1   | 0.94 | 0.20 | 1.24  | 9,9,9,9                     | 0     |
| 57  | MG   | XA    | 1638 | 1/1   | 0.86 | 0.17 | 1.24  | 27,27,27,27                 | 0     |
| 57  | MG   | XA    | 1633 | 1/1   | 0.93 | 0.18 | 1.23  | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3064 | 1/1   | 0.95 | 0.17 | 1.07  | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3207 | 1/1   | 0.89 | 0.25 | 1.04  | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3028 | 1/1   | 0.98 | 0.22 | 0.97  | 8,8,8,8                     | 0     |
| 57  | MG   | QA    | 1619 | 1/1   | 0.95 | 0.25 | 0.94  | 29,29,29,29                 | 0     |
| 57  | MG   | QF    | 201  | 1/1   | 0.69 | 0.32 | 0.84  | 40,40,40,40                 | 0     |
| 57  | MG   | XA    | 1671 | 1/1   | 0.87 | 0.18 | 0.80  | 28,28,28,28                 | 0     |
| 57  | MG   | RD    | 301  | 1/1   | 0.89 | 0.28 | 0.77  | 15,15,15,15                 | 0     |
| 57  | MG   | XA    | 1614 | 1/1   | 0.93 | 0.31 | 0.74  | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3224 | 1/1   | 0.92 | 0.17 | 0.73  | 16,16,16,16                 | 0     |
| 57  | MG   | RR    | 201  | 1/1   | 0.97 | 0.27 | 0.73  | 9,9,9,9                     | 0     |
| 57  | MG   | XA    | 1629 | 1/1   | 0.90 | 0.14 | 0.72  | 32,32,32,32                 | 0     |
| 57  | MG   | XA    | 1637 | 1/1   | 0.97 | 0.27 | 0.70  | 13,13,13,13                 | 0     |
| 57  | MG   | QA    | 1659 | 1/1   | 0.93 | 0.19 | 0.61  | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3163 | 1/1   | 0.96 | 0.18 | 0.61  | 38,38,38,38                 | 0     |
| 57  | MG   | YA    | 3236 | 1/1   | 0.88 | 0.19 | 0.60  | 12,12,12,12                 | 0     |
| 57  | MG   | QA    | 1616 | 1/1   | 0.97 | 0.28 | 0.58  | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3040 | 1/1   | 0.97 | 0.23 | 0.56  | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3036 | 1/1   | 0.93 | 0.19 | 0.47  | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3114 | 1/1   | 0.89 | 0.18 | 0.42  | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3161 | 1/1   | 0.95 | 0.14 | 0.41  | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3210 | 1/1   | 0.91 | 0.15 | 0.36  | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3168 | 1/1   | 0.85 | 0.16 | 0.24  | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3068 | 1/1   | 0.97 | 0.26 | 0.16  | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3016 | 1/1   | 0.91 | 0.20 | 0.05  | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3204 | 1/1   | 0.83 | 0.16 | -0.01 | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3112 | 1/1   | 0.90 | 0.21 | -0.02 | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3110 | 1/1   | 0.97 | 0.16 | -0.08 | 5,5,5,5                     | 0     |
| 57  | MG   | QA    | 1608 | 1/1   | 0.89 | 0.23 | -0.09 | 63,63,63,63                 | 0     |
| 57  | MG   | RA    | 3187 | 1/1   | 0.93 | 0.16 | -0.21 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3123 | 1/1   | 0.96 | 0.18 | -0.25 | 0,0,0,0                     | 0     |
| 57  | MG   | RE    | 302  | 1/1   | 0.94 | 0.20 | -0.27 | 15,15,15,15                 | 0     |
| 57  | MG   | RF    | 301  | 1/1   | 0.94 | 0.27 | -0.31 | 10,10,10,10                 | 0     |
| 57  | MG   | XA    | 1655 | 1/1   | 0.96 | 0.22 | -0.32 | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3228 | 1/1   | 0.99 | 0.17 | -0.37 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 57  | MG   | XA    | 1620 | 1/1   | 0.96 | 0.15 | -0.38 | 0,0,0,0                    | 0     |
| 57  | MG   | XA    | 1659 | 1/1   | 0.91 | 0.16 | -0.43 | 15,15,15,15                | 0     |
| 57  | MG   | RA    | 3082 | 1/1   | 0.98 | 0.14 | -0.47 | 5,5,5,5                    | 0     |
| 57  | MG   | QA    | 1630 | 1/1   | 0.94 | 0.13 | -0.58 | 14,14,14,14                | 0     |
| 57  | MG   | YA    | 3103 | 1/1   | 0.89 | 0.14 | -0.60 | 31,31,31,31                | 0     |
| 57  | MG   | RA    | 3199 | 1/1   | 0.99 | 0.16 | -0.60 | 1,1,1,1                    | 0     |
| 57  | MG   | RA    | 3026 | 1/1   | 0.91 | 0.17 | -0.62 | 13,13,13,13                | 0     |
| 57  | MG   | RA    | 3104 | 1/1   | 0.94 | 0.13 | -0.63 | 5,5,5,5                    | 0     |
| 59  | ZN   | R9    | 101  | 1/1   | 0.30 | 0.76 | -0.66 | 177,177,177,177            | 0     |
| 57  | MG   | RA    | 3156 | 1/1   | 0.89 | 0.16 | -0.74 | 7,7,7,7                    | 0     |
| 57  | MG   | YA    | 3175 | 1/1   | 0.96 | 0.12 | -0.75 | 2,2,2,2                    | 0     |
| 57  | MG   | RA    | 3159 | 1/1   | 0.99 | 0.14 | -0.78 | 18,18,18,18                | 0     |
| 57  | MG   | QA    | 1621 | 1/1   | 0.94 | 0.19 | -0.79 | 35,35,35,35                | 0     |
| 57  | MG   | RA    | 3193 | 1/1   | 0.94 | 0.15 | -0.80 | 17,17,17,17                | 0     |
| 57  | MG   | YA    | 3136 | 1/1   | 0.98 | 0.12 | -0.80 | 1,1,1,1                    | 0     |
| 57  | MG   | XA    | 1666 | 1/1   | 0.92 | 0.21 | -0.83 | 34,34,34,34                | 0     |
| 57  | MG   | RA    | 3190 | 1/1   | 0.91 | 0.14 | -0.88 | 4,4,4,4                    | 0     |
| 59  | ZN   | XN    | 101  | 1/1   | 0.95 | 0.18 | -0.90 | 59,59,59,59                | 0     |
| 57  | MG   | YA    | 3166 | 1/1   | 0.94 | 0.13 | -0.91 | 14,14,14,14                | 0     |
| 59  | ZN   | QD    | 301  | 1/1   | 0.99 | 0.19 | -0.98 | 12,12,12,12                | 0     |
| 57  | MG   | XA    | 1628 | 1/1   | 0.86 | 0.14 | -0.99 | 2,2,2,2                    | 0     |
| 57  | MG   | YA    | 3188 | 1/1   | 0.92 | 0.12 | -1.03 | 36,36,36,36                | 0     |
| 57  | MG   | RA    | 3067 | 1/1   | 0.97 | 0.17 | -1.05 | 6,6,6,6                    | 0     |
| 57  | MG   | RA    | 3188 | 1/1   | 0.91 | 0.13 | -1.10 | 16,16,16,16                | 0     |
| 57  | MG   | RA    | 3208 | 1/1   | 0.95 | 0.14 | -1.22 | 50,50,50,50                | 0     |
| 57  | MG   | YA    | 3055 | 1/1   | 0.90 | 0.19 | -1.26 | 24,24,24,24                | 0     |
| 59  | ZN   | QN    | 101  | 1/1   | 0.96 | 0.13 | -1.35 | 56,56,56,56                | 0     |
| 57  | MG   | YA    | 3130 | 1/1   | 0.89 | 0.10 | -1.38 | 3,3,3,3                    | 0     |
| 57  | MG   | RA    | 3148 | 1/1   | 0.91 | 0.13 | -1.45 | 0,0,0,0                    | 0     |
| 57  | MG   | YA    | 3222 | 1/1   | 0.94 | 0.12 | -1.53 | 2,2,2,2                    | 0     |
| 57  | MG   | RA    | 3133 | 1/1   | 0.95 | 0.14 | -1.58 | 4,4,4,4                    | 0     |
| 57  | MG   | QA    | 1635 | 1/1   | 0.98 | 0.14 | -1.62 | 11,11,11,11                | 0     |
| 57  | MG   | YP    | 201  | 1/1   | 0.98 | 0.05 | -1.82 | 83,83,83,83                | 0     |
| 57  | MG   | QM    | 201  | 1/1   | 0.97 | 0.10 | -1.83 | 34,34,34,34                | 0     |
| 57  | MG   | QA    | 1657 | 1/1   | 0.89 | 0.10 | -1.89 | 19,19,19,19                | 0     |
| 57  | MG   | QA    | 1661 | 1/1   | 0.94 | 0.10 | -2.13 | 44,44,44,44                | 0     |
| 57  | MG   | QA    | 1607 | 1/1   | 0.99 | 0.06 | -2.13 | 30,30,30,30                | 0     |
| 57  | MG   | RA    | 3167 | 1/1   | 0.90 | 0.09 | -2.20 | 26,26,26,26                | 0     |
| 57  | MG   | YA    | 3233 | 1/1   | 0.95 | 0.10 | -2.24 | 3,3,3,3                    | 0     |
| 57  | MG   | YA    | 3069 | 1/1   | 0.96 | 0.10 | -2.25 | 8,8,8,8                    | 0     |
| 57  | MG   | YA    | 3060 | 1/1   | 0.98 | 0.09 | -2.35 | 9,9,9,9                    | 0     |
| 57  | MG   | QA    | 1654 | 1/1   | 0.98 | 0.12 | -2.43 | 17,17,17,17                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57  | MG   | XA    | 1661 | 1/1   | 0.99 | 0.07 | -2.43 | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3102 | 1/1   | 0.95 | 0.13 | -2.43 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3133 | 1/1   | 0.94 | 0.08 | -2.60 | 12,12,12,12                 | 0     |
| 57  | MG   | YA    | 3238 | 1/1   | 0.99 | 0.10 | -2.62 | 33,33,33,33                 | 0     |
| 57  | MG   | QA    | 1629 | 1/1   | 0.99 | 0.08 | -2.76 | 38,38,38,38                 | 0     |
| 57  | MG   | QA    | 1609 | 1/1   | 0.98 | 0.12 | -2.79 | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3127 | 1/1   | 0.98 | 0.10 | -2.79 | 12,12,12,12                 | 0     |
| 57  | MG   | RA    | 3134 | 1/1   | 0.91 | 0.09 | -2.81 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3143 | 1/1   | 0.95 | 0.08 | -2.87 | 12,12,12,12                 | 0     |
| 57  | MG   | QA    | 1643 | 1/1   | 0.76 | 0.14 | -2.95 | 20,20,20,20                 | 0     |
| 57  | MG   | RA    | 3125 | 1/1   | 0.97 | 0.07 | -3.11 | 14,14,14,14                 | 0     |
| 59  | ZN   | Y9    | 101  | 1/1   | 0.71 | 0.53 | -3.21 | 158,158,158,158             | 0     |
| 57  | MG   | QA    | 1649 | 1/1   | 0.95 | 0.10 | -3.96 | 19,19,19,19                 | 0     |
| 57  | MG   | XA    | 1660 | 1/1   | 0.91 | 0.10 | -4.13 | 19,19,19,19                 | 0     |
| 57  | MG   | RB    | 201  | 1/1   | 0.98 | 0.08 | -4.17 | 38,38,38,38                 | 0     |
| 57  | MG   | QA    | 1606 | 1/1   | 0.98 | 0.06 | -4.64 | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3137 | 1/1   | 0.99 | 0.10 | -5.64 | 3,3,3,3                     | 0     |
| 57  | MG   | XA    | 1622 | 1/1   | 0.98 | 0.11 | -6.19 | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3058 | 1/1   | 0.99 | 0.29 | -     | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3187 | 1/1   | 0.82 | 0.21 | -     | 47,47,47,47                 | 0     |
| 57  | MG   | YA    | 3237 | 1/1   | 0.96 | 0.20 | -     | 38,38,38,38                 | 0     |
| 57  | MG   | QA    | 1638 | 1/1   | 0.73 | 0.20 | -     | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3160 | 1/1   | 0.87 | 0.34 | -     | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3228 | 1/1   | 0.88 | 0.15 | -     | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3235 | 1/1   | 0.96 | 0.14 | -     | 2,2,2,2                     | 0     |
| 57  | MG   | QA    | 1634 | 1/1   | 0.99 | 0.12 | -     | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3014 | 1/1   | 0.91 | 0.90 | -     | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3124 | 1/1   | 0.95 | 0.28 | -     | 13,13,13,13                 | 0     |
| 57  | MG   | RA    | 3115 | 1/1   | 0.97 | 0.16 | -     | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3174 | 1/1   | 0.99 | 0.37 | -     | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3227 | 1/1   | 0.96 | 0.14 | -     | 39,39,39,39                 | 0     |
| 57  | MG   | QA    | 1603 | 1/1   | 0.80 | 0.52 | -     | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3004 | 1/1   | 0.71 | 0.44 | -     | 9,9,9,9                     | 0     |
| 57  | MG   | RE    | 301  | 1/1   | 0.96 | 0.13 | -     | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3053 | 1/1   | 0.98 | 0.63 | -     | 50,50,50,50                 | 0     |
| 57  | MG   | QA    | 1664 | 1/1   | 0.79 | 0.34 | -     | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3117 | 1/1   | 0.72 | 0.80 | -     | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3059 | 1/1   | 0.95 | 0.30 | -     | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3263 | 1/1   | 0.97 | 0.29 | -     | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3137 | 1/1   | 0.79 | 0.28 | -     | 22,22,22,22                 | 0     |
| 57  | MG   | QA    | 1642 | 1/1   | 0.93 | 0.16 | -     | 9,9,9,9                     | 0     |
| 57  | MG   | RA    | 3075 | 1/1   | 0.94 | 0.36 | -     | 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 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3078 | 1/1   | 0.85 | 0.83 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3094 | 1/1   | 0.96 | 0.38 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | QA    | 1624 | 1/1   | 0.94 | 0.29 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | YA    | 3201 | 1/1   | 0.96 | 0.16 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3232 | 1/1   | 0.94 | 0.30 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3021 | 1/1   | 0.87 | 1.12 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | XA    | 1647 | 1/1   | 0.96 | 0.34 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3186 | 1/1   | 0.94 | 0.18 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | XA    | 1649 | 1/1   | 0.77 | 0.39 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | QA    | 1626 | 1/1   | 0.92 | 0.17 | -    | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3017 | 1/1   | 0.97 | 0.30 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3047 | 1/1   | 0.84 | 1.00 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | QA    | 1640 | 1/1   | 0.69 | 0.23 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3103 | 1/1   | 0.94 | 0.21 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | XA    | 1657 | 1/1   | 0.92 | 0.27 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3091 | 1/1   | 0.89 | 0.49 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | QA    | 1633 | 1/1   | 0.90 | 0.43 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3177 | 1/1   | 0.97 | 0.07 | -    | 92,92,92,92                 | 0     |
| 57  | MG   | YA    | 3208 | 1/1   | 0.97 | 0.16 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3007 | 1/1   | 0.94 | 0.23 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3236 | 1/1   | 0.97 | 0.49 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3039 | 1/1   | 0.95 | 0.23 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3070 | 1/1   | 0.98 | 0.15 | -    | 21,21,21,21                 | 0     |
| 57  | MG   | RA    | 3016 | 1/1   | 0.93 | 0.65 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3062 | 1/1   | 0.89 | 0.23 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3213 | 1/1   | 0.94 | 0.31 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3220 | 1/1   | 0.88 | 0.15 | -    | 26,26,26,26                 | 0     |
| 57  | MG   | RU    | 201  | 1/1   | 0.94 | 0.16 | -    | 86,86,86,86                 | 0     |
| 57  | MG   | RA    | 3128 | 1/1   | 0.83 | 0.23 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | YA    | 3227 | 1/1   | 0.92 | 0.17 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | YA    | 3096 | 1/1   | 0.99 | 0.24 | -    | 17,17,17,17                 | 0     |
| 57  | MG   | YA    | 3132 | 1/1   | 0.93 | 0.37 | -    | 26,26,26,26                 | 0     |
| 57  | MG   | XA    | 1639 | 1/1   | 0.97 | 0.06 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | XA    | 1627 | 1/1   | 0.97 | 0.35 | -    | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3146 | 1/1   | 0.96 | 0.20 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3212 | 1/1   | 0.75 | 0.26 | -    | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3256 | 1/1   | 0.96 | 0.14 | -    | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3022 | 1/1   | 0.96 | 0.75 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | XA    | 1624 | 1/1   | 0.95 | 0.60 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | XA    | 1663 | 1/1   | 0.96 | 0.17 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3174 | 1/1   | 0.87 | 0.15 | -    | 40,40,40,40                 | 0     |
| 57  | MG   | R5    | 101  | 1/1   | 0.95 | 0.15 | -    | 14,14,14,14                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 57  | MG   | YA    | 3121 | 1/1   | 0.96 | 0.16 | -    | 8,8,8,8                    | 0     |
| 57  | MG   | QA    | 1658 | 1/1   | 0.86 | 0.42 | -    | 46,46,46,46                | 0     |
| 57  | MG   | RA    | 3197 | 1/1   | 0.90 | 0.16 | -    | 9,9,9,9                    | 0     |
| 57  | MG   | RA    | 3131 | 1/1   | 0.86 | 0.18 | -    | 25,25,25,25                | 0     |
| 57  | MG   | RA    | 3136 | 1/1   | 0.85 | 0.24 | -    | 14,14,14,14                | 0     |
| 57  | MG   | YA    | 3210 | 1/1   | 0.96 | 0.30 | -    | 30,30,30,30                | 0     |
| 57  | MG   | YA    | 3027 | 1/1   | 0.89 | 0.17 | -    | 1,1,1,1                    | 0     |
| 57  | MG   | RA    | 3168 | 1/1   | 0.94 | 0.23 | -    | 10,10,10,10                | 0     |
| 57  | MG   | RA    | 3006 | 1/1   | 0.90 | 1.07 | -    | 50,50,50,50                | 0     |
| 57  | MG   | QA    | 1653 | 1/1   | 0.95 | 0.11 | -    | 6,6,6,6                    | 0     |
| 57  | MG   | QA    | 1627 | 1/1   | 0.92 | 0.15 | -    | 1,1,1,1                    | 0     |
| 57  | MG   | RA    | 3179 | 1/1   | 0.95 | 0.24 | -    | 10,10,10,10                | 0     |
| 57  | MG   | YA    | 3154 | 1/1   | 0.84 | 0.26 | -    | 5,5,5,5                    | 0     |
| 57  | MG   | YA    | 3214 | 1/1   | 0.91 | 0.24 | -    | 23,23,23,23                | 0     |
| 57  | MG   | QA    | 1605 | 1/1   | 0.93 | 0.53 | -    | 4,4,4,4                    | 0     |
| 57  | MG   | QX    | 101  | 1/1   | 0.85 | 0.15 | -    | 6,6,6,6                    | 0     |
| 57  | MG   | RA    | 3031 | 1/1   | 0.93 | 0.77 | -    | 50,50,50,50                | 0     |
| 57  | MG   | XA    | 1652 | 1/1   | 0.86 | 0.26 | -    | 50,50,50,50                | 0     |
| 57  | MG   | YA    | 3029 | 1/1   | 0.97 | 0.32 | -    | 6,6,6,6                    | 0     |
| 57  | MG   | YA    | 3185 | 1/1   | 0.84 | 0.16 | -    | 74,74,74,74                | 0     |
| 57  | MG   | YA    | 3207 | 1/1   | 0.89 | 0.25 | -    | 0,0,0,0                    | 0     |
| 57  | MG   | XA    | 1654 | 1/1   | 0.93 | 0.43 | -    | 17,17,17,17                | 0     |
| 57  | MG   | XA    | 1632 | 1/1   | 0.95 | 0.41 | -    | 2,2,2,2                    | 0     |
| 57  | MG   | YA    | 3232 | 1/1   | 0.89 | 0.22 | -    | 15,15,15,15                | 0     |
| 57  | MG   | RA    | 3154 | 1/1   | 0.93 | 0.45 | -    | 6,6,6,6                    | 0     |
| 57  | MG   | YE    | 301  | 1/1   | 0.94 | 0.23 | -    | 1,1,1,1                    | 0     |
| 57  | MG   | XV    | 102  | 1/1   | 0.94 | 0.16 | -    | 16,16,16,16                | 0     |
| 57  | MG   | YA    | 3164 | 1/1   | 0.97 | 0.76 | -    | 97,97,97,97                | 0     |
| 57  | MG   | RA    | 3151 | 1/1   | 0.87 | 0.35 | -    | 37,37,37,37                | 0     |
| 57  | MG   | YA    | 3061 | 1/1   | 0.96 | 0.49 | -    | 9,9,9,9                    | 0     |
| 57  | MG   | QA    | 1625 | 1/1   | 0.95 | 0.08 | -    | 74,74,74,74                | 0     |
| 57  | MG   | RA    | 3140 | 1/1   | 0.75 | 0.25 | -    | 61,61,61,61                | 0     |
| 57  | MG   | YA    | 3265 | 1/1   | 0.93 | 0.65 | -    | 11,11,11,11                | 0     |
| 57  | MG   | YA    | 3251 | 1/1   | 0.94 | 1.32 | -    | 50,50,50,50                | 0     |
| 57  | MG   | YA    | 3170 | 1/1   | 0.88 | 0.28 | -    | 8,8,8,8                    | 0     |
| 57  | MG   | RA    | 3189 | 1/1   | 0.94 | 0.17 | -    | 16,16,16,16                | 0     |
| 57  | MG   | XA    | 1662 | 1/1   | 0.62 | 0.74 | -    | 50,50,50,50                | 0     |
| 57  | MG   | RA    | 3117 | 1/1   | 0.97 | 0.35 | -    | 4,4,4,4                    | 0     |
| 57  | MG   | RA    | 3230 | 1/1   | 0.47 | 0.47 | -    | 45,45,45,45                | 0     |
| 57  | MG   | YA    | 3181 | 1/1   | 0.94 | 0.57 | -    | 5,5,5,5                    | 0     |
| 57  | MG   | YA    | 3223 | 1/1   | 0.76 | 0.92 | -    | 11,11,11,11                | 0     |
| 57  | MG   | YA    | 3081 | 1/1   | 0.91 | 0.28 | -    | 7,7,7,7                    | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3024 | 1/1   | 0.98 | 0.36 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3116 | 1/1   | 0.70 | 0.32 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | XA    | 1605 | 1/1   | 0.78 | 0.61 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | QA    | 1622 | 1/1   | 0.81 | 0.45 | -    | 52,52,52,52                 | 0     |
| 57  | MG   | RA    | 3147 | 1/1   | 0.93 | 0.24 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3048 | 1/1   | 0.94 | 1.15 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3243 | 1/1   | 0.93 | 0.76 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3239 | 1/1   | 0.92 | 0.79 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | XA    | 1613 | 1/1   | 0.97 | 0.08 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | QA    | 1628 | 1/1   | 0.61 | 0.43 | -    | 21,21,21,21                 | 0     |
| 57  | MG   | QA    | 1651 | 1/1   | 0.83 | 0.43 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3105 | 1/1   | 0.96 | 0.21 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3147 | 1/1   | 0.94 | 0.17 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3197 | 1/1   | 0.88 | 1.38 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3218 | 1/1   | 0.91 | 0.35 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | XX    | 101  | 1/1   | 0.89 | 0.17 | -    | 88,88,88,88                 | 0     |
| 57  | MG   | YA    | 3258 | 1/1   | 0.92 | 0.52 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3045 | 1/1   | 0.92 | 0.29 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3190 | 1/1   | 0.90 | 0.51 | -    | 17,17,17,17                 | 0     |
| 57  | MG   | YA    | 3119 | 1/1   | 0.80 | 0.41 | -    | 66,66,66,66                 | 0     |
| 57  | MG   | YA    | 3129 | 1/1   | 0.97 | 0.11 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3206 | 1/1   | 0.87 | 0.25 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3095 | 1/1   | 0.97 | 0.32 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3238 | 1/1   | 0.92 | 0.71 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3191 | 1/1   | 0.98 | 0.25 | -    | 38,38,38,38                 | 0     |
| 57  | MG   | RA    | 3072 | 1/1   | 0.90 | 0.35 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3063 | 1/1   | 0.99 | 0.29 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | YA    | 3054 | 1/1   | 0.92 | 0.59 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3097 | 1/1   | 0.96 | 0.60 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3224 | 1/1   | 0.97 | 0.80 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3069 | 1/1   | 0.87 | 0.26 | -    | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3250 | 1/1   | 0.76 | 1.15 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | R8    | 101  | 1/1   | 0.82 | 0.38 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | YA    | 3247 | 1/1   | 0.74 | 0.58 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | QA    | 1614 | 1/1   | 0.92 | 0.24 | -    | 21,21,21,21                 | 0     |
| 57  | MG   | YA    | 3089 | 1/1   | 0.95 | 0.25 | -    | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3189 | 1/1   | 0.91 | 0.42 | -    | 7,7,7,7                     | 0     |
| 57  | MG   | Y5    | 101  | 1/1   | 0.95 | 0.14 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3010 | 1/1   | 0.97 | 0.60 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3241 | 1/1   | 0.87 | 0.38 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3183 | 1/1   | 0.97 | 0.49 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3182 | 1/1   | 0.90 | 0.50 | -    | 10,10,10,10                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3104 | 1/1   | 0.98 | 0.13 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3146 | 1/1   | 0.86 | 0.41 | -    | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3221 | 1/1   | 0.91 | 0.24 | -    | 7,7,7,7                     | 0     |
| 57  | MG   | YA    | 3161 | 1/1   | 0.98 | 0.35 | -    | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3212 | 1/1   | 0.96 | 0.24 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3198 | 1/1   | 0.86 | 0.28 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3249 | 1/1   | 0.87 | 0.70 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | XA    | 1602 | 1/1   | 0.92 | 0.92 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3084 | 1/1   | 0.94 | 0.28 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3046 | 1/1   | 0.93 | 0.45 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3178 | 1/1   | 0.89 | 0.37 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3145 | 1/1   | 0.90 | 0.21 | -    | 25,25,25,25                 | 0     |
| 57  | MG   | RA    | 3141 | 1/1   | 0.96 | 0.45 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3225 | 1/1   | 0.96 | 0.36 | -    | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3073 | 1/1   | 0.96 | 0.28 | -    | 36,36,36,36                 | 0     |
| 57  | MG   | RA    | 3203 | 1/1   | 0.90 | 0.20 | -    | 34,34,34,34                 | 0     |
| 57  | MG   | XA    | 1631 | 1/1   | 0.92 | 0.18 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3145 | 1/1   | 0.97 | 0.42 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3141 | 1/1   | 0.94 | 0.10 | -    | 18,18,18,18                 | 0     |
| 57  | MG   | XA    | 1670 | 1/1   | 0.93 | 0.19 | -    | 44,44,44,44                 | 0     |
| 57  | MG   | RA    | 3158 | 1/1   | 0.95 | 0.26 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | QA    | 1665 | 1/1   | 0.75 | 0.48 | -    | 37,37,37,37                 | 0     |
| 57  | MG   | YA    | 3246 | 1/1   | 0.89 | 0.51 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | QH    | 201  | 1/1   | 0.31 | 0.27 | -    | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3150 | 1/1   | 0.71 | 0.58 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3029 | 1/1   | 0.98 | 0.24 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | XA    | 1658 | 1/1   | 0.94 | 0.28 | -    | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3121 | 1/1   | 0.87 | 0.15 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | XA    | 1642 | 1/1   | 0.95 | 0.23 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3194 | 1/1   | 0.92 | 0.19 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3028 | 1/1   | 0.91 | 0.23 | -    | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3011 | 1/1   | 0.91 | 0.39 | -    | 7,7,7,7                     | 0     |
| 57  | MG   | XA    | 1609 | 1/1   | 0.87 | 0.55 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3234 | 1/1   | 0.87 | 0.09 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3091 | 1/1   | 0.95 | 0.58 | -    | 12,12,12,12                 | 0     |
| 57  | MG   | YB    | 201  | 1/1   | 0.85 | 0.29 | -    | 14,14,14,14                 | 0     |
| 57  | MG   | RA    | 3055 | 1/1   | 0.99 | 0.29 | -    | 12,12,12,12                 | 0     |
| 57  | MG   | XA    | 1641 | 1/1   | 0.86 | 0.33 | -    | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3192 | 1/1   | 0.96 | 0.15 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | XA    | 1651 | 1/1   | 0.92 | 0.17 | -    | 84,84,84,84                 | 0     |
| 57  | MG   | YA    | 3245 | 1/1   | 0.80 | 0.57 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3139 | 1/1   | 0.88 | 0.54 | -    | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | XA    | 1617 | 1/1   | 0.96 | 0.26 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3085 | 1/1   | 0.86 | 0.22 | -    | 27,27,27,27                 | 0     |
| 57  | MG   | QA    | 1663 | 1/1   | 0.98 | 0.09 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3076 | 1/1   | 0.96 | 0.39 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3111 | 1/1   | 0.96 | 0.44 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3153 | 1/1   | 0.73 | 0.28 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | QA    | 1632 | 1/1   | 0.97 | 0.10 | -    | 71,71,71,71                 | 0     |
| 57  | MG   | YA    | 3242 | 1/1   | 0.86 | 0.20 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3090 | 1/1   | 0.93 | 0.22 | -    | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3010 | 1/1   | 0.90 | 0.30 | -    | 56,56,56,56                 | 0     |
| 57  | MG   | RA    | 3225 | 1/1   | 0.81 | 0.29 | -    | 47,47,47,47                 | 0     |
| 57  | MG   | RA    | 3231 | 1/1   | 0.82 | 0.35 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3110 | 1/1   | 0.98 | 0.10 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3092 | 1/1   | 0.90 | 0.23 | -    | 59,59,59,59                 | 0     |
| 57  | MG   | XA    | 1601 | 1/1   | 0.74 | 1.10 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3108 | 1/1   | 0.93 | 0.24 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3150 | 1/1   | 0.99 | 0.26 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | QA    | 1611 | 1/1   | 0.91 | 0.27 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3255 | 1/1   | 0.93 | 1.37 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3240 | 1/1   | 0.99 | 0.14 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | QA    | 1641 | 1/1   | 0.96 | 0.08 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3205 | 1/1   | 0.74 | 0.46 | -    | 33,33,33,33                 | 0     |
| 57  | MG   | YA    | 3101 | 1/1   | 0.98 | 0.12 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | RA    | 3106 | 1/1   | 0.99 | 0.26 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3018 | 1/1   | 0.94 | 0.82 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3155 | 1/1   | 0.96 | 0.18 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3030 | 1/1   | 0.90 | 0.73 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3108 | 1/1   | 0.98 | 0.12 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | RA    | 3233 | 1/1   | 0.93 | 1.47 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | XA    | 1630 | 1/1   | 0.92 | 0.31 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3119 | 1/1   | 0.85 | 0.25 | -    | 88,88,88,88                 | 0     |
| 57  | MG   | YA    | 3230 | 1/1   | 0.99 | 0.20 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3086 | 1/1   | 0.92 | 0.42 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3080 | 1/1   | 0.91 | 0.83 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3040 | 1/1   | 0.89 | 0.69 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3180 | 1/1   | 0.87 | 0.36 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | XA    | 1643 | 1/1   | 0.92 | 0.74 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3171 | 1/1   | 0.81 | 0.22 | -    | 7,7,7,7                     | 0     |
| 57  | MG   | QA    | 1620 | 1/1   | 0.96 | 0.12 | -    | 21,21,21,21                 | 0     |
| 57  | MG   | RA    | 3039 | 1/1   | 0.87 | 0.66 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | QA    | 1637 | 1/1   | 0.85 | 0.26 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3148 | 1/1   | 0.50 | 0.23 | -    | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3144 | 1/1   | 0.94 | 0.18 | -    | 29,29,29,29                 | 0     |
| 57  | MG   | RA    | 3084 | 1/1   | 0.97 | 0.31 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | QA    | 1655 | 1/1   | 0.80 | 0.39 | -    | 66,66,66,66                 | 0     |
| 57  | MG   | RA    | 3195 | 1/1   | 0.92 | 0.14 | -    | 23,23,23,23                 | 0     |
| 57  | MG   | RA    | 3059 | 1/1   | 0.97 | 0.50 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3200 | 1/1   | 0.96 | 0.15 | -    | 35,35,35,35                 | 0     |
| 57  | MG   | YA    | 3199 | 1/1   | 0.93 | 0.18 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3004 | 1/1   | 0.97 | 0.43 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3047 | 1/1   | 0.95 | 0.16 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | RA    | 3217 | 1/1   | 0.67 | 0.91 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3002 | 1/1   | 0.94 | 0.19 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3172 | 1/1   | 0.91 | 0.14 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3066 | 1/1   | 0.99 | 0.19 | -    | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3125 | 1/1   | 0.85 | 0.45 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | YA    | 3012 | 1/1   | 0.56 | 1.42 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3229 | 1/1   | 0.95 | 0.13 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3218 | 1/1   | 0.98 | 0.27 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | RA    | 3176 | 1/1   | 0.94 | 0.28 | -    | 30,30,30,30                 | 0     |
| 57  | MG   | YA    | 3131 | 1/1   | 0.88 | 0.50 | -    | 17,17,17,17                 | 0     |
| 57  | MG   | RA    | 3229 | 1/1   | 0.52 | 0.33 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3051 | 1/1   | 0.99 | 0.21 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3235 | 1/1   | 0.64 | 0.47 | -    | 34,34,34,34                 | 0     |
| 57  | MG   | QA    | 1660 | 1/1   | 0.99 | 0.33 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | XA    | 1616 | 1/1   | 0.86 | 0.77 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3130 | 1/1   | 0.94 | 0.17 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | XA    | 1648 | 1/1   | 0.91 | 0.19 | -    | 10,10,10,10                 | 0     |
| 57  | MG   | QA    | 1602 | 1/1   | 0.78 | 1.00 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3144 | 1/1   | 0.94 | 0.54 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3050 | 1/1   | 0.81 | 0.14 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3035 | 1/1   | 0.91 | 0.80 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3071 | 1/1   | 0.57 | 0.89 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3128 | 1/1   | 0.88 | 0.23 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3098 | 1/1   | 0.96 | 0.40 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | YB    | 202  | 1/1   | 0.86 | 0.43 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3052 | 1/1   | 0.98 | 0.33 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3120 | 1/1   | 0.96 | 0.15 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3068 | 1/1   | 0.98 | 0.48 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3149 | 1/1   | 0.92 | 0.76 | -    | 7,7,7,7                     | 0     |
| 57  | MG   | RA    | 3166 | 1/1   | 0.86 | 0.94 | -    | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3115 | 1/1   | 0.87 | 0.29 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | XA    | 1621 | 1/1   | 0.92 | 0.57 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RB    | 202  | 1/1   | 0.98 | 0.20 | -    | 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 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | YA    | 3138 | 1/1   | 0.88 | 0.49 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3248 | 1/1   | 0.91 | 0.87 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3112 | 1/1   | 0.96 | 0.38 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | YA    | 3100 | 1/1   | 0.93 | 0.71 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | RA    | 3175 | 1/1   | 0.87 | 0.28 | -    | 12,12,12,12                 | 0     |
| 57  | MG   | RA    | 3008 | 1/1   | 0.93 | 0.28 | -    | 0,0,0,0                     | 0     |
| 57  | MG   | YA    | 3143 | 1/1   | 0.91 | 0.23 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3003 | 1/1   | 0.94 | 0.46 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3094 | 1/1   | 0.98 | 0.36 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3043 | 1/1   | 0.77 | 1.09 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3211 | 1/1   | 0.93 | 0.13 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | RA    | 3012 | 1/1   | 0.96 | 0.27 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3219 | 1/1   | 0.93 | 0.10 | -    | 22,22,22,22                 | 0     |
| 57  | MG   | XA    | 1640 | 1/1   | 0.94 | 0.14 | -    | 119,119,119,119             | 0     |
| 57  | MG   | YA    | 3020 | 1/1   | 0.91 | 0.58 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | YQ    | 201  | 1/1   | 0.96 | 0.21 | -    | 79,79,79,79                 | 0     |
| 57  | MG   | RA    | 3155 | 1/1   | 0.95 | 0.19 | -    | 9,9,9,9                     | 0     |
| 57  | MG   | YA    | 3160 | 1/1   | 0.92 | 0.38 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3204 | 1/1   | 0.98 | 0.53 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | RA    | 3063 | 1/1   | 0.81 | 0.11 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | RA    | 3200 | 1/1   | 0.94 | 0.20 | -    | 31,31,31,31                 | 0     |
| 57  | MG   | YA    | 3264 | 1/1   | 0.87 | 0.53 | -    | 14,14,14,14                 | 0     |
| 57  | MG   | YA    | 3252 | 1/1   | 0.96 | 0.15 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | QA    | 1652 | 1/1   | 0.95 | 0.21 | -    | 24,24,24,24                 | 0     |
| 57  | MG   | RA    | 3032 | 1/1   | 0.97 | 0.68 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3220 | 1/1   | 0.91 | 0.15 | -    | 25,25,25,25                 | 0     |
| 57  | MG   | YA    | 3083 | 1/1   | 0.86 | 0.21 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3221 | 1/1   | 0.90 | 0.70 | -    | 79,79,79,79                 | 0     |
| 57  | MG   | RA    | 3196 | 1/1   | 0.88 | 0.33 | -    | 22,22,22,22                 | 0     |
| 57  | MG   | RA    | 3080 | 1/1   | 0.95 | 0.16 | -    | 5,5,5,5                     | 0     |
| 57  | MG   | YA    | 3070 | 1/1   | 0.75 | 0.30 | -    | 33,33,33,33                 | 0     |
| 57  | MG   | RA    | 3216 | 1/1   | 0.90 | 0.30 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | QA    | 1636 | 1/1   | 0.98 | 0.18 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3013 | 1/1   | 0.96 | 0.37 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3209 | 1/1   | 0.98 | 0.12 | -    | 44,44,44,44                 | 0     |
| 57  | MG   | YA    | 3102 | 1/1   | 0.93 | 0.84 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3234 | 1/1   | 0.93 | 0.85 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | QA    | 1647 | 1/1   | 0.96 | 0.15 | -    | 55,55,55,55                 | 0     |
| 57  | MG   | QA    | 1648 | 1/1   | 0.96 | 0.19 | -    | 16,16,16,16                 | 0     |
| 57  | MG   | RA    | 3192 | 1/1   | 0.96 | 0.16 | -    | 27,27,27,27                 | 0     |
| 57  | MG   | YA    | 3021 | 1/1   | 0.95 | 0.56 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3090 | 1/1   | 0.91 | 0.45 | -    | 4,4,4,4                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3215 | 1/1   | 0.93 | 0.28 | -    | 14,14,14,14                 | 0     |
| 57  | MG   | XA    | 1606 | 1/1   | 0.86 | 0.64 | -    | 13,13,13,13                 | 0     |
| 57  | MG   | RA    | 3113 | 1/1   | 0.94 | 0.30 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | YA    | 3046 | 1/1   | 0.97 | 0.26 | -    | 12,12,12,12                 | 0     |
| 57  | MG   | QA    | 1650 | 1/1   | 0.93 | 0.24 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3202 | 1/1   | 0.88 | 0.31 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | XM    | 201  | 1/1   | 0.85 | 0.17 | -    | 78,78,78,78                 | 0     |
| 57  | MG   | YA    | 3167 | 1/1   | 0.98 | 0.19 | -    | 39,39,39,39                 | 0     |
| 57  | MG   | QA    | 1656 | 1/1   | 0.92 | 0.09 | -    | 63,63,63,63                 | 0     |
| 57  | MG   | YA    | 3244 | 1/1   | 0.91 | 0.48 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3129 | 1/1   | 0.98 | 0.10 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3122 | 1/1   | 0.97 | 0.58 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3030 | 1/1   | 0.87 | 0.89 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3105 | 1/1   | 0.83 | 0.74 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3170 | 1/1   | 0.96 | 0.41 | -    | 2,2,2,2                     | 0     |
| 57  | MG   | QA    | 1662 | 1/1   | 0.96 | 0.08 | -    | 39,39,39,39                 | 0     |
| 57  | MG   | YA    | 3087 | 1/1   | 0.99 | 0.37 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | YA    | 3126 | 1/1   | 0.75 | 0.33 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3239 | 1/1   | 0.98 | 0.12 | -    | 13,13,13,13                 | 0     |
| 57  | MG   | XA    | 1669 | 1/1   | 0.92 | 0.08 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | YA    | 3158 | 1/1   | 0.93 | 0.24 | -    | 6,6,6,6                     | 0     |
| 57  | MG   | RA    | 3244 | 1/1   | 0.92 | 0.20 | -    | 9,9,9,9                     | 0     |
| 57  | MG   | QA    | 1644 | 1/1   | 0.96 | 0.29 | -    | 24,24,24,24                 | 0     |
| 57  | MG   | QA    | 1623 | 1/1   | 0.86 | 0.52 | -    | 13,13,13,13                 | 0     |
| 57  | MG   | YA    | 3231 | 1/1   | 0.97 | 0.36 | -    | 11,11,11,11                 | 0     |
| 57  | MG   | YA    | 3139 | 1/1   | 0.96 | 0.27 | -    | 13,13,13,13                 | 0     |
| 57  | MG   | RA    | 3135 | 1/1   | 0.95 | 0.13 | -    | 28,28,28,28                 | 0     |
| 57  | MG   | RA    | 3120 | 1/1   | 0.94 | 0.20 | -    | 31,31,31,31                 | 0     |
| 57  | MG   | RA    | 3165 | 1/1   | 0.95 | 0.25 | -    | 3,3,3,3                     | 0     |
| 57  | MG   | YA    | 3001 | 1/1   | 0.89 | 1.16 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | XA    | 1667 | 1/1   | 0.91 | 0.14 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | YA    | 3074 | 1/1   | 0.87 | 0.61 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | XA    | 1665 | 1/1   | 0.84 | 0.19 | -    | 18,18,18,18                 | 0     |
| 57  | MG   | RA    | 3198 | 1/1   | 0.97 | 0.06 | -    | 35,35,35,35                 | 0     |
| 57  | MG   | RA    | 3169 | 1/1   | 0.95 | 0.12 | -    | 19,19,19,19                 | 0     |
| 57  | MG   | YA    | 3159 | 1/1   | 0.97 | 0.19 | -    | 22,22,22,22                 | 0     |
| 57  | MG   | XA    | 1653 | 1/1   | 0.84 | 0.15 | -    | 29,29,29,29                 | 0     |
| 57  | MG   | QA    | 1601 | 1/1   | 0.79 | 0.40 | -    | 21,21,21,21                 | 0     |
| 57  | MG   | QA    | 1618 | 1/1   | 0.88 | 0.42 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | YA    | 3082 | 1/1   | 0.95 | 0.58 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3001 | 1/1   | 0.83 | 0.78 | -    | 1,1,1,1                     | 0     |
| 57  | MG   | RA    | 3019 | 1/1   | 0.94 | 1.19 | -    | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | RA    | 3043 | 1/1   | 0.85 | 0.71 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3075 | 1/1   | 0.90 | 1.18 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3142 | 1/1   | 0.92 | 0.44 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3095 | 1/1   | 0.97 | 0.42 | -    | 24,24,24,24                 | 0     |
| 57  | MG   | RA    | 3041 | 1/1   | 0.80 | 0.64 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | YA    | 3253 | 1/1   | 0.82 | 1.86 | -    | 50,50,50,50                 | 0     |
| 57  | MG   | RA    | 3237 | 1/1   | 0.87 | 0.23 | -    | 4,4,4,4                     | 0     |
| 57  | MG   | RA    | 3171 | 1/1   | 0.93 | 0.44 | -    | 15,15,15,15                 | 0     |
| 57  | MG   | YA    | 3065 | 1/1   | 0.94 | 0.75 | -    | 8,8,8,8                     | 0     |
| 57  | MG   | RA    | 3049 | 1/1   | 0.99 | 0.34 | -    | 1,1,1,1                     | 0     |

## 6.5 Other polymers

There are no such residues in this entry.