



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:43 am GMT

PDB ID : 2A68  
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic rifabutin  
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-07-01  
Resolution : 2.50 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 : trunk28620  
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) : recalc28949

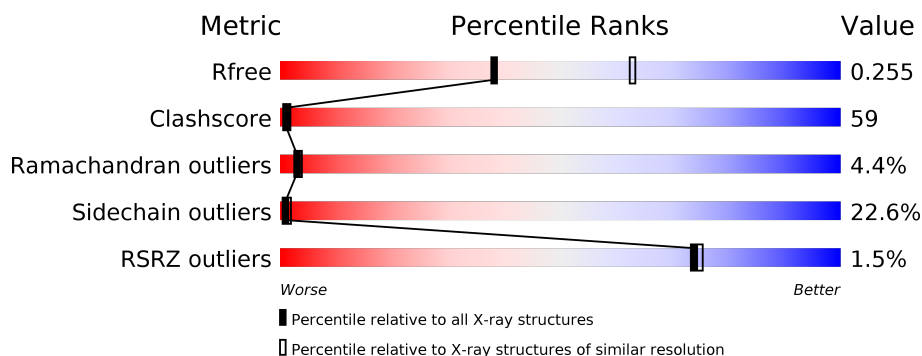
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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                      | 3846 (2.50-2.50)                                      |
| Clashscore            | 112137                      | 4554 (2.50-2.50)                                      |
| Ramachandran outliers | 110173                      | 4463 (2.50-2.50)                                      |
| Sidechain outliers    | 110143                      | 4465 (2.50-2.50)                                      |
| RSRZ outliers         | 101464                      | 3876 (2.50-2.50)                                      |

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   | A     | 315    |                  |
| 1   | B     | 315    |                  |
| 1   | K     | 315    |                  |
| 1   | L     | 315    |                  |
| 2   | C     | 1119   |                  |
| 2   | M     | 1119   |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | D     | 1524   |                  |
| 3   | N     | 1524   |                  |
| 4   | E     | 99     |                  |
| 4   | O     | 99     |                  |
| 5   | F     | 423    |                  |
| 5   | P     | 423    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 7   | RBT  | C     | 8001 | -         | -        | -       | X                |

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61089 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 1   | B     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 1   | K     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 1   | L     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |
| 2   | M     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1392     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10797 | 6819 | 1925 | 2020 | 33 |         |         |       |
| 3   | N     | 1392     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10797 | 6819 | 1925 | 2020 | 33 |         |         |       |

- Molecule 4 is a protein called RNA polymerase omega chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 488 | 133 | 144 | 4 |         |         |       |
| 4   | O     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 488 | 133 | 144 | 4 |         |         |       |

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2771  | 1744 | 504 | 519 | 4 |         |         |       |
| 5   | P     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2771  | 1744 | 504 | 519 | 4 |         |         |       |

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | P     | 20       | Total | Mg  | 0       | 0       |
|     |       |          | 20    | 20  |         |         |
| 6   | D     | 137      | Total | Mg  | 0       | 0       |
|     |       |          | 137   | 137 |         |         |
| 6   | K     | 21       | Total | Mg  | 0       | 0       |
|     |       |          | 21    | 21  |         |         |
| 6   | E     | 10       | Total | Mg  | 0       | 0       |
|     |       |          | 10    | 10  |         |         |
| 6   | B     | 23       | Total | Mg  | 0       | 0       |
|     |       |          | 23    | 23  |         |         |
| 6   | C     | 81       | Total | Mg  | 0       | 0       |
|     |       |          | 81    | 81  |         |         |
| 6   | A     | 31       | Total | Mg  | 0       | 0       |
|     |       |          | 31    | 31  |         |         |
| 6   | N     | 108      | Total | Mg  | 0       | 0       |
|     |       |          | 108   | 108 |         |         |
| 6   | O     | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 6   | L     | 25       | Total | Mg  | 0       | 0       |
|     |       |          | 25    | 25  |         |         |
| 6   | F     | 31       | Total | Mg  | 0       | 0       |
|     |       |          | 31    | 31  |         |         |
| 6   | M     | 69       | Total | Mg  | 0       | 0       |
|     |       |          | 69    | 69  |         |         |

- Molecule 7 is RIFABUTIN (three-letter code: RBT) (formula: C<sub>46</sub>H<sub>62</sub>N<sub>4</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 7   | C     | 1        | Total<br>61 | C<br>46 | N<br>4 | O<br>11 | 0       | 0       |
| 7   | M     | 1        | Total<br>61 | C<br>46 | N<br>4 | O<br>11 | 0       | 0       |

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | D     | 2        | Total Zn<br>2 2 | 0       | 0       |
| 8   | N     | 2        | Total Zn<br>2 2 | 0       | 0       |

- Molecule 9 is water.

| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 9   | A     | 253      | Total O<br>253 253   | 0       | 0       |
| 9   | B     | 307      | Total O<br>307 307   | 0       | 0       |
| 9   | C     | 1000     | Total O<br>1000 1000 | 0       | 0       |
| 9   | D     | 1418     | Total O<br>1418 1418 | 0       | 0       |
| 9   | E     | 112      | Total O<br>112 112   | 0       | 0       |

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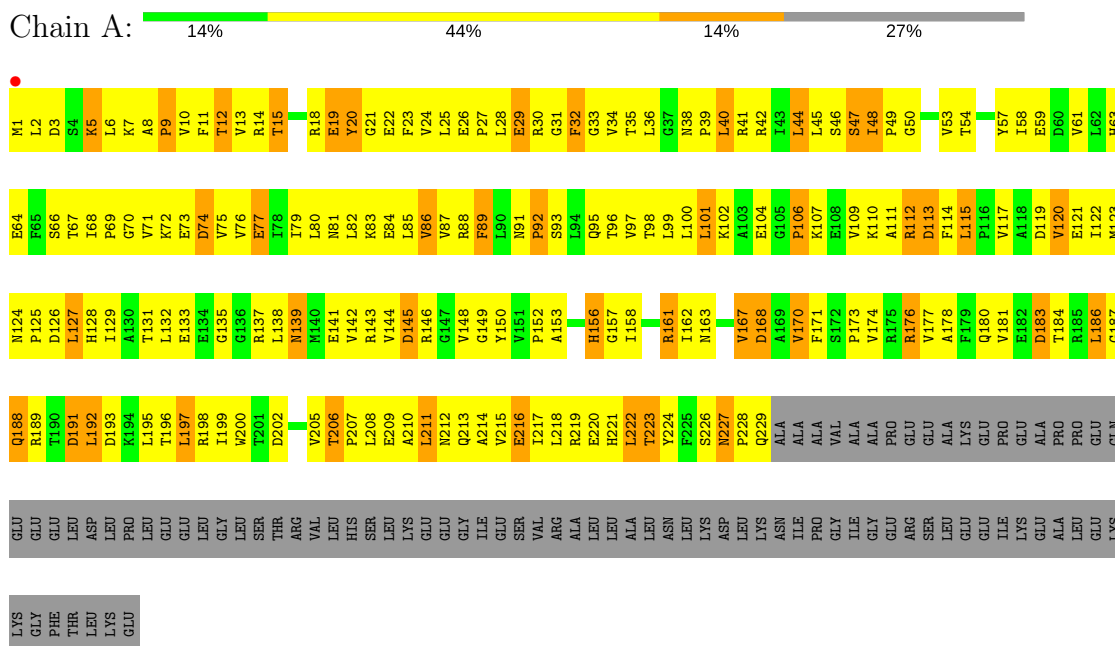
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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 9   | F     | 456      | Total<br>456  | O<br>456  | 0       | 0       |
| 9   | K     | 213      | Total<br>213  | O<br>213  | 0       | 0       |
| 9   | L     | 237      | Total<br>237  | O<br>237  | 0       | 0       |
| 9   | M     | 998      | Total<br>998  | O<br>998  | 0       | 0       |
| 9   | N     | 1357     | Total<br>1357 | O<br>1357 | 0       | 0       |
| 9   | O     | 117      | Total<br>117  | O<br>117  | 0       | 0       |
| 9   | P     | 377      | Total<br>377  | O<br>377  | 0       | 0       |

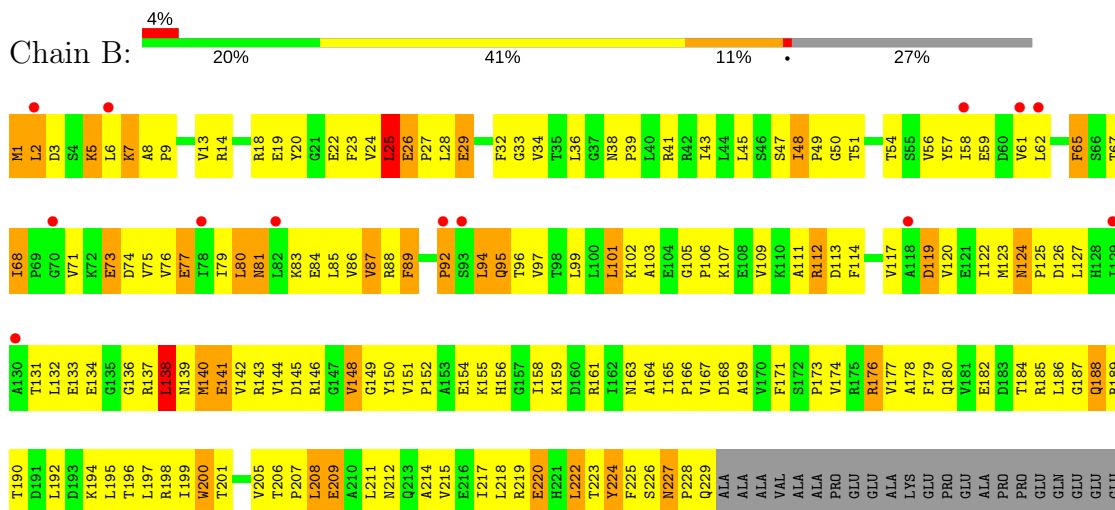
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

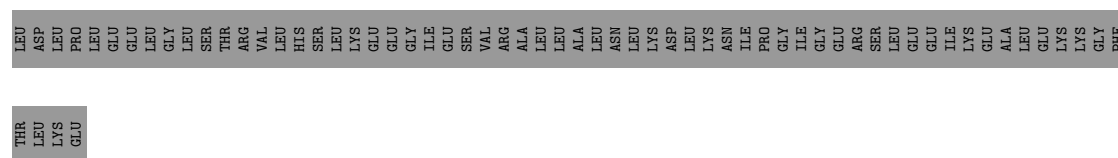
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



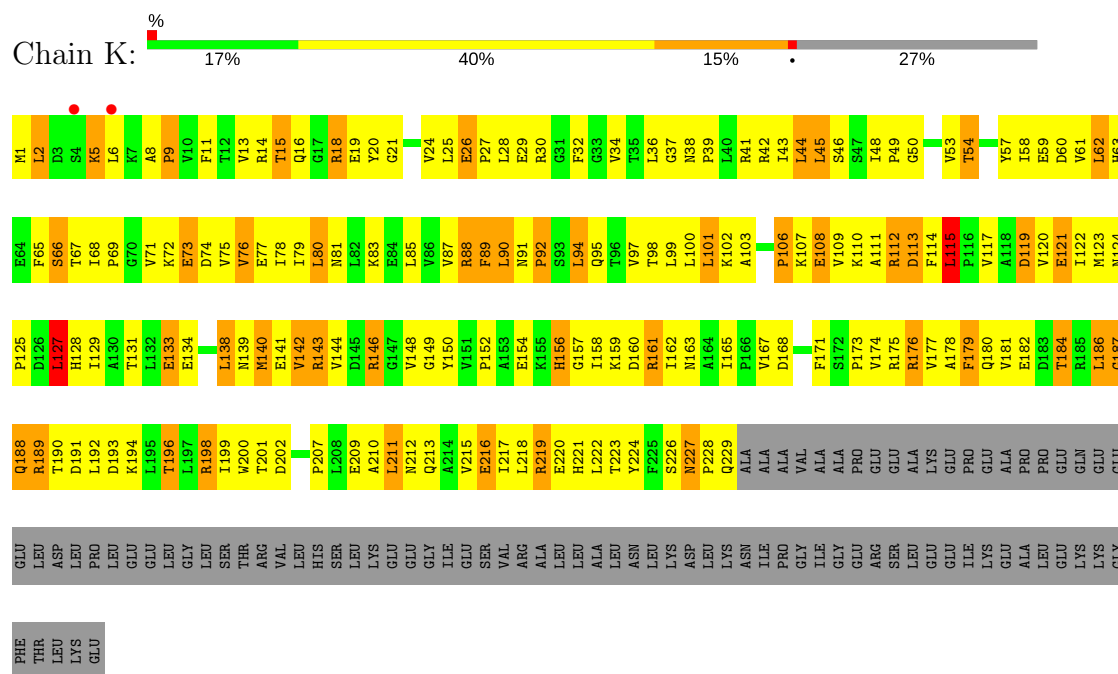
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



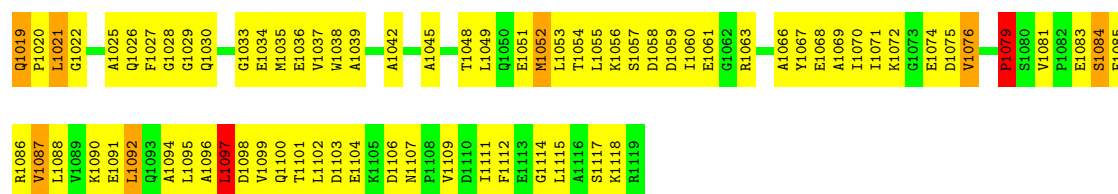




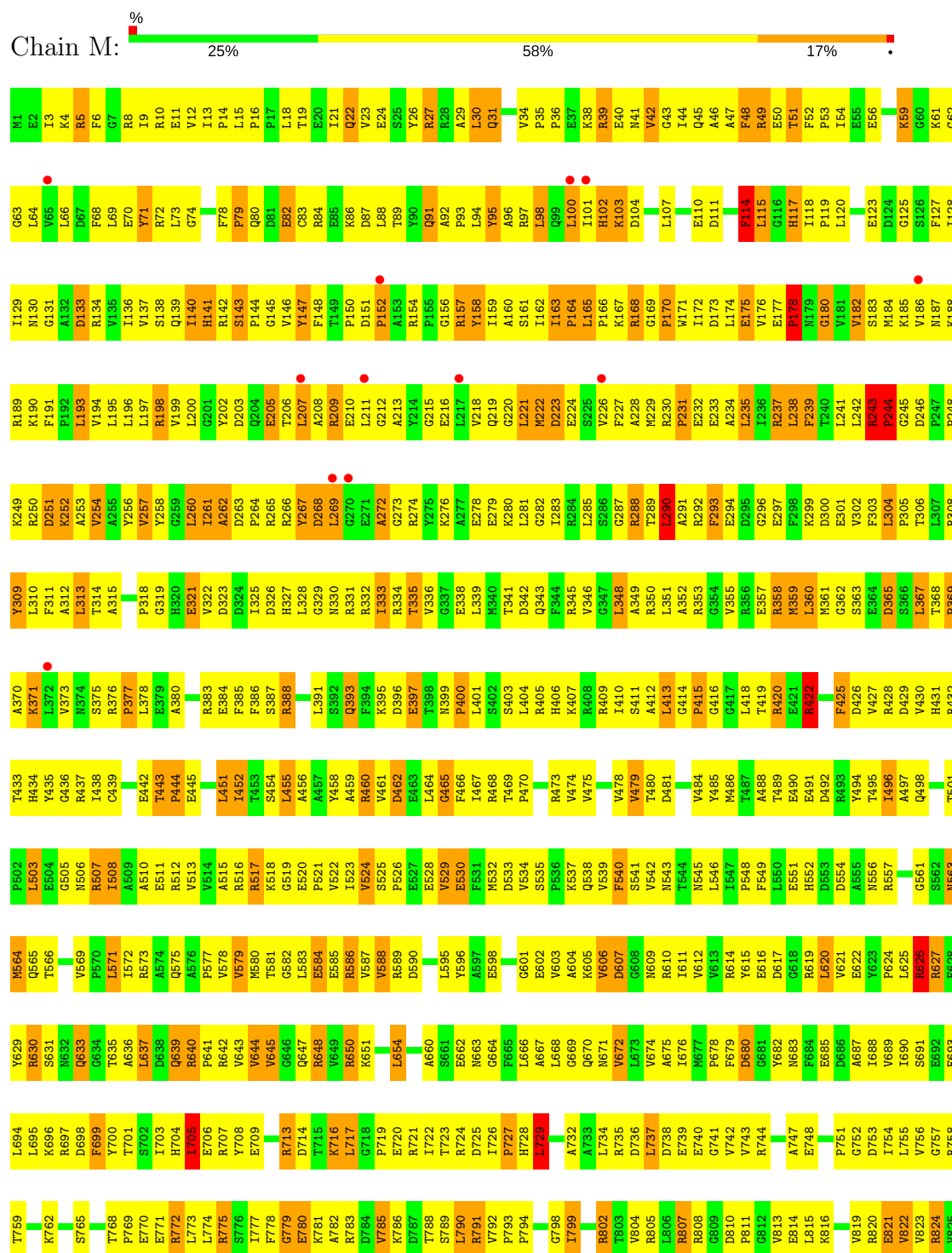
• Molecule 1: DNA-directed RNA polymerase alpha chain

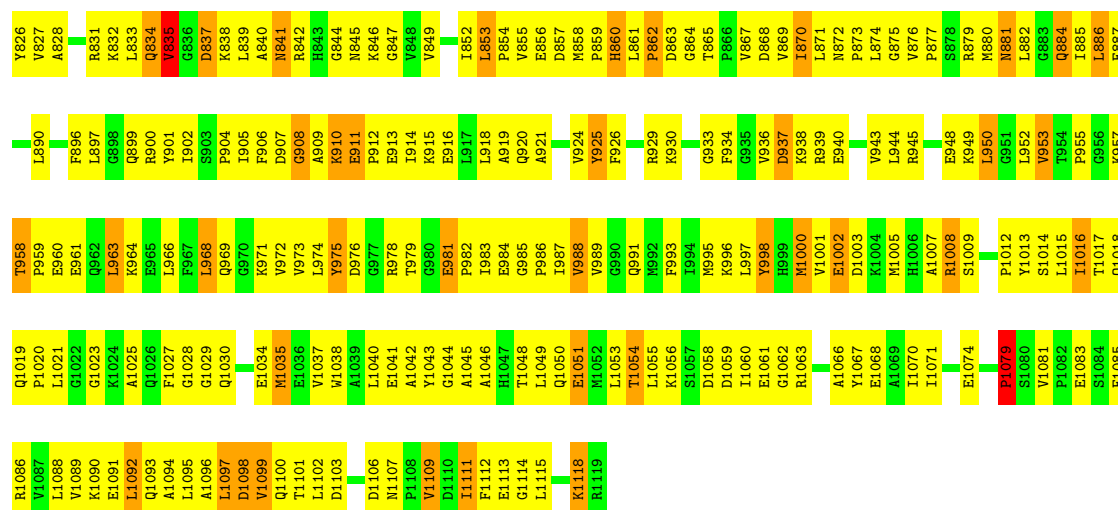




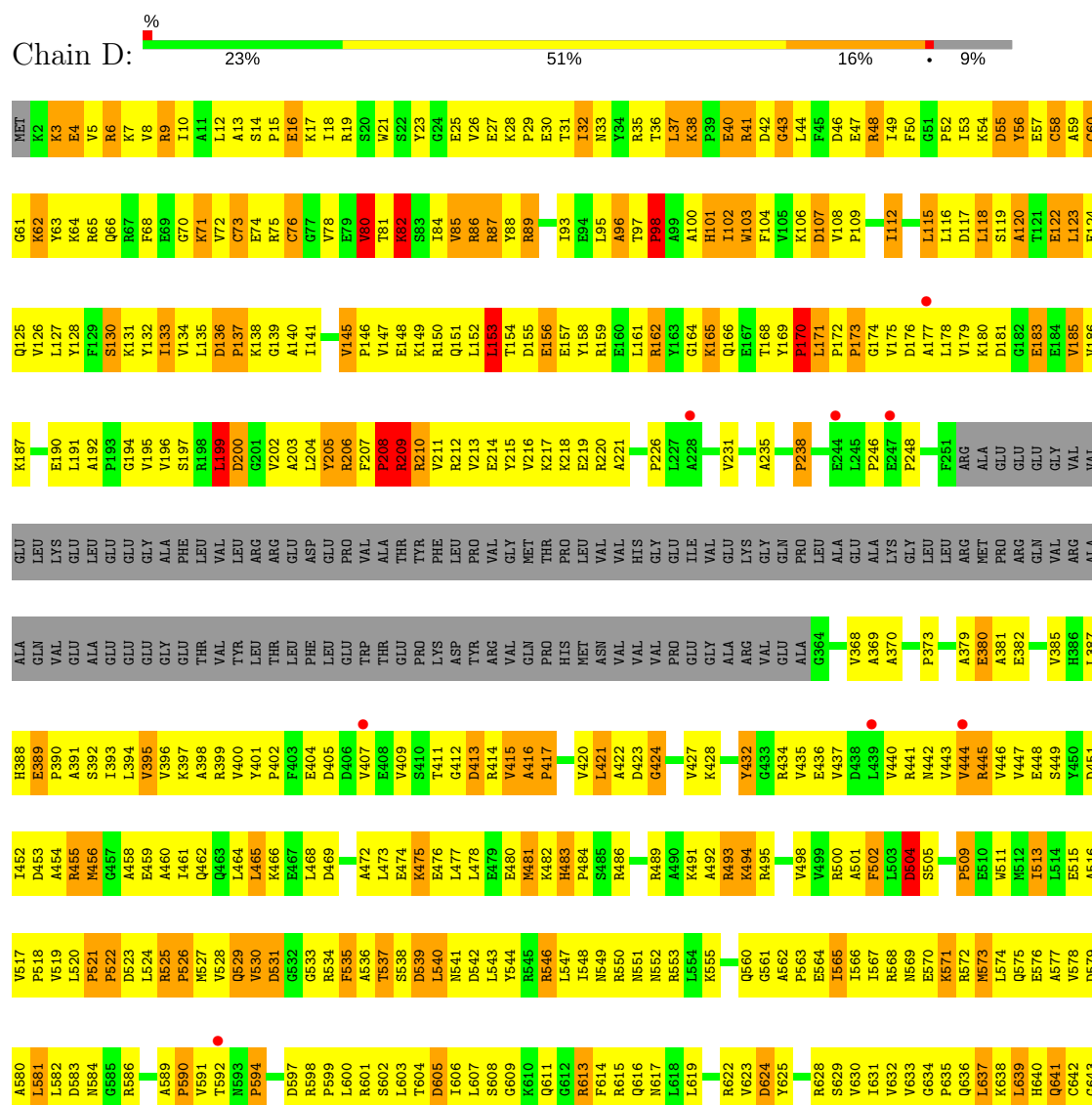


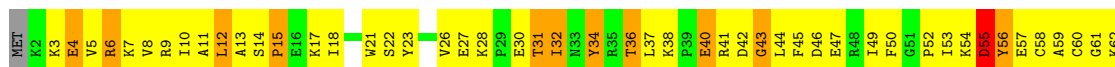
• Molecule 2: DNA-directed RNA polymerase beta chain



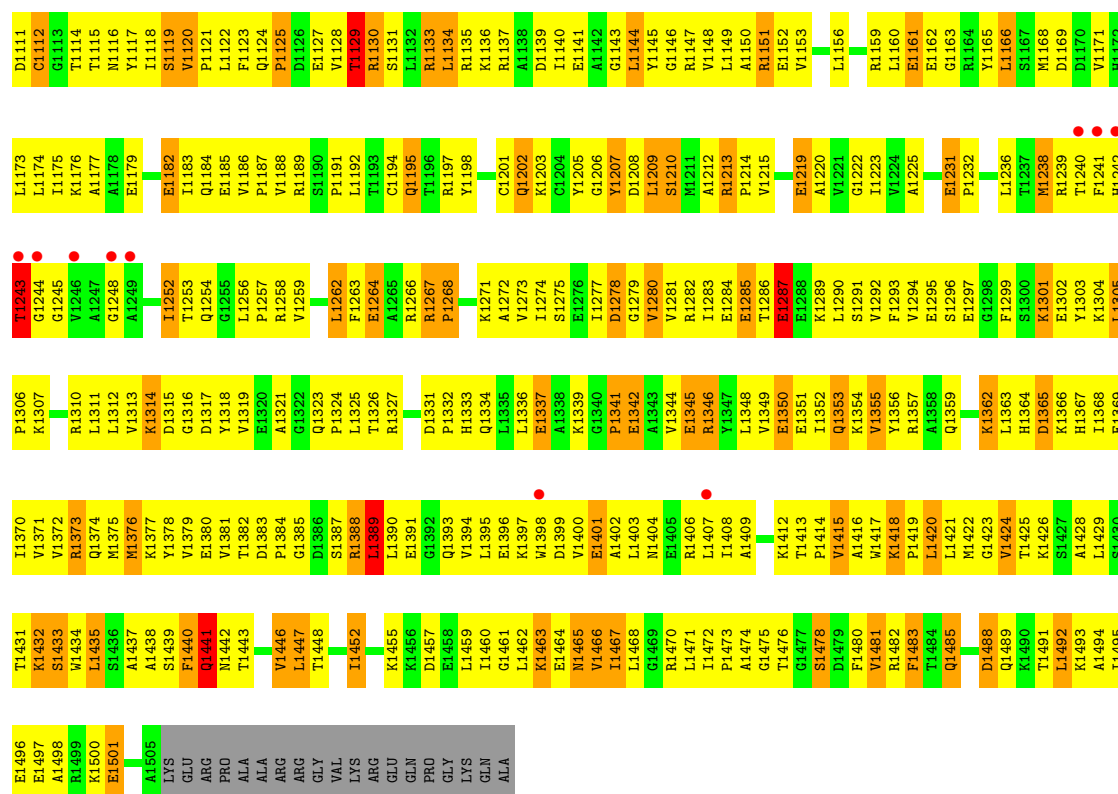


• Molecule 3: DNA-directed RNA polymerase beta' chain

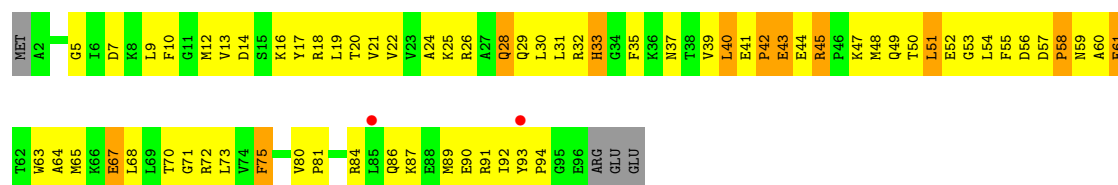




|       |       |      |      |      |      |      |      |      |      |      |     |     |      |      |      |
|-------|-------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|
| M1045 | L983  | N909 | Y841 | L778 | A715 | A649 | D583 | P521 | I461 | V395 | GLU | PHE | L191 | V126 | Y63  |
| Q1046 | T984  | S910 | V842 | A779 | F716 | L650 | M684 | P522 | Q462 | V396 | THR | LEU | L192 | L127 | K64  |
| K1047 | D985  | L311 | F843 | K780 | Q717 | E651 | G585 | D523 | Q463 | K397 | VAL | VAL | P193 | Y128 | R65  |
| P1048 | R986  | K912 | A844 | P781 | P718 | L652 | R586 | L524 | L464 | A386 | LEU | LEU | K66  | F129 | Q66  |
| S1049 | E987  |      | J845 | S782 | W719 | F653 | R587 | R525 | L465 | K399 | LEU | ARG | S130 | S130 | F68  |
| G1050 | R988  | V915 | K846 | R783 | L720 | K654 | P526 | P526 | K466 | V400 | THR | ARG | V195 | K131 | R67  |
| E1051 | Y989  | Y916 |      | D784 |      | P655 | P590 | N527 | E467 | Y401 | LEU | GLU | V196 | Y132 |      |
| T1052 | D990  | Q917 | L850 | I785 | Q723 | P656 | V591 | V528 | L468 | P402 | ASP | ASP | S197 | I133 | K71  |
| F1053 | A991  | A918 | L851 | I786 | Q724 | L657 | T592 | Q529 | D469 | F403 | LEU | LEU | S198 | V134 | W72  |
|       | I992  | F919 | A852 | I787 | S725 | L658 | N593 | V530 | L470 | E404 | PRO | PRO | C73  | D136 | C73  |
| P1056 | L993  | L920 | V853 | Q788 | I726 | K659 | P594 |      | E471 |      | VAL | VAL | D200 | D136 | E74  |
| V1057 | Q994  | R921 |      | L789 | Q727 | K660 |      | G533 | A472 |      | ALA | ALA | G201 | P137 | R75  |
| L1058 | L995  | L922 | I857 | W790 | I728 | M661 |      | B534 | L473 |      | GLU | THR | V202 | K138 | C76  |
| S1059 | W996  | G923 | V858 | I791 | H729 | E662 | D597 | F585 | E474 |      | PRO | THR | A203 | G139 | G77  |
| T1060 | T997  | M924 | D859 | I792 | P730 | E663 | R998 |      | K475 |      | LYS | PHE | L204 | A140 | G79  |
| F1061 | E998  | K925 | L860 | Q793 | L731 |      | P599 |      | E476 |      | ASP | LEU | Y205 | E141 | W78  |
| E1062 | T999  | K926 | Q861 | Q794 | W732 |      |      |      | L477 |      | THR | PRO | R206 | L142 | E79  |
| E1063 | T999  | T927 | V862 | Q795 | C732 | A667 | S602 | D539 | L478 |      | ARG | VAL | F207 | N143 | T80  |
| K1064 | E1001 | A928 | V863 | R796 | E734 | P668 | L603 | N541 | E479 |      | VAL | GLY | R208 | G144 | X82  |
| L1065 | K1002 |      | R854 | R797 | A735 | P669 | T804 | D542 | E480 |      | GLN | MET | R209 | V145 | S83  |
| T1066 | V1003 | L931 | T865 | K798 | F736 | V670 | D805 | L543 | M481 |      | PRO | THR | R210 | P146 | R84  |
| V1067 | T1004 | D932 | V866 | K799 | N737 | K671 | I606 | L544 | K482 |      | HIS | PRO | V211 | V147 | V85  |
| L1068 | Q1005 | A933 | R867 | K800 | Q744 | A672 | L607 | R545 | H483 |      | LEU | LEU | R212 | E148 | R86  |
| E1069 | A1006 | L934 | R877 | G801 | Q745 | A673 | S808 | R546 | P484 |      | ASN | VAL | K149 | K149 | R87  |
| Y1070 | I1007 | K935 | R877 | T808 | F746 | K674 | G609 | L547 | S485 |      | VAL | VAL | E214 | R150 | X88  |
| F1071 | F1008 | Y936 | R872 | G803 | D741 | R675 | K610 | L548 | R486 |      | VAL | HIS | Y215 | Q151 | R89  |
| I1072 | K1009 | Y937 | L873 | L804 | Q742 | R676 | Q611 | R549 | A487 |      | GLY | GLY | V216 | L152 |      |
| T1073 | S1010 | G938 | E874 | E805 | D743 | L677 | G612 | R550 | R488 |      | PRO | GLU | K217 | L153 |      |
| S1074 | F1011 | F939 | T875 | F806 | Q744 | E678 | R613 | N551 | R489 |      | GLY | ILE | E219 | T154 |      |
|       | E1012 |      | R876 | A807 | M745 | R679 | R614 | N552 | A490 |      | GLY | VAL | E219 |      |      |
| A1077 | E1013 | S945 | R877 | T808 | F746 | K674 | R615 | R553 | K491 |      | ALA | GLY | E219 |      |      |
| R1078 | N1014 | Q946 | R878 | P809 | V747 | R681 | Q616 | L584 | A492 |      | ARG | LYS | V231 | E157 |      |
| K1079 |       | I947 | R879 | E910 | H743 | D682 | L619 | K555 | R493 |      | VAL | GLY | V231 | Y158 |      |
| D1083 | N1018 | T948 | L880 | E911 | V749 | P683 |      | K556 | K494 |      | GLU | GLN | P238 | E160 |      |
| T1084 | I1020 | G950 | F882 | L813 | P750 |      |      | L557 | R495 |      | ALA | PRO | E161 | L161 |      |
| R1087 | Y1021 | I951 | A883 | A814 |      |      |      | A559 | E497 |      | ALA | LEU | L242 | R162 |      |
|       | V1022 | D952 | R884 |      |      |      |      | Q560 | V435 |      | ALA | ALA | A243 |      |      |
| D1090 | A1024 | D953 | T885 | E917 | F754 | V687 | D624 | G561 | V499 |      | GLU | ALA | P246 | K165 |      |
| S1091 | Q1025 | V955 | V886 | A755 | Q756 | D688 | S826 | G527 | V499 |      | ALA | ALA | E247 | Q166 |      |
| Y1092 | S1026 | I956 | A887 | A756 | Q757 | E693 | R628 | A562 | R500 |      | LYS | LYS | E248 | E167 |      |
| L1093 | G1027 | P957 | E888 | A759 | E758 | V694 | S629 | P563 | A501 |      | GLY | GLY | P248 | T168 |      |
| L1094 | A1028 | E958 | A889 | A822 | R760 | T695 | I631 | I565 | F502 |      | LEU | LEU | P248 | Y169 |      |
| T1095 | R1029 | E959 | V890 | L823 | I761 | H696 | V632 | I566 | L503 |      | LEU | LEU | P251 | D107 |      |
| R1096 | G1030 | K960 | D892 | N824 | Q762 |      | V633 | I567 | D504 |      | ARG | MET | P251 | L171 |      |
| L1098 | P1032 | E993 | K894 | I827 | A766 | L701 | P635 | E570 | P509 |      | PRO | PRO | ALA  | P172 |      |
| T1099 | Q1034 | V895 | K828 | V829 | S765 | L702 | K637 | K571 | E381 |      | ARG | GLN | GLY  | P173 |      |
| D1100 | Q1034 | E965 | A896 | V829 | H767 | W703 | K638 | B572 | E382 |      | VAL | VAL | GLY  | D176 |      |
| V1101 | T1035 |      | V897 | A830 | W768 | R704 | L839 | B573 | E382 |      | ARG | VAL | VAL  | A177 |      |
| H1102 | H1036 | D968 | E898 | G831 | L769 | A705 | L639 | M573 | V385 |      | ALA | ALA | VAL  | L115 |      |
| H1103 | Q1037 | R969 | L899 | R832 | L770 | P706 | M512 | L574 | H386 |      | ALA | ALA | VAL  | D117 |      |
| L1104 | L1038 | K970 | E899 | R832 | S771 | T707 | M513 | Q575 | L387 |      | GLN | GLN | LEU  | V179 |      |
| L1105 | G1039 | L971 | Q901 | E833 | Q772 | L708 | L514 | E576 | H388 |      | VAL | VAL | LYS  | D181 |      |
| V1106 | G1040 | L972 | L902 | T834 | A773 | H709 | A577 | A516 | E389 |      | GLU | GLU | GLY  | E182 |      |
| V1107 | L1041 |      | L902 | S835 | A773 | R710 | L644 | V578 | P390 |      | ALA | ALA | LEU  | E183 |      |
| R1108 | R1042 | Q976 | Q906 | V836 | S774 | R710 | P645 | D579 | A391 |      | GLU | GLU | GLY  | E184 |      |
| E1109 | G1043 | E907 | E907 | R837 | G775 |      | K646 | A580 | P518 |      | GLU | GLU | GLY  | V185 |      |
| A1110 | L1044 | F982 | K908 | R838 | E776 | I713 | R647 | L581 | E459 |      | GLY | GLY | ALA  | E124 |      |
|       |       |      |      |      | P777 | Q714 | M648 | L592 | L520 |      |     |     |      | K187 | Q125 |



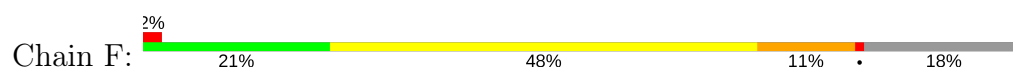
• Molecule 4: RNA polymerase omega chain



• Molecule 4: RNA polymerase omega chain



• Molecule 5: RNA polymerase sigma factor rpoD







## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 32   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 239.50Å 239.50Å 253.10Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)  | 25.00 – 2.50<br>24.85 – 2.50                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (25.00-2.50)<br>91.2 (24.85-2.50)              | Depositor<br>EDS |
| $R_{merge}$   | 0.07   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.13 (at 2.50Å)  | Xtriage          |
| Refinement program  | CNS 1.1  | Depositor        |
| R, $R_{free}$   | 0.225 , 0.257<br>0.223 , 0.255                                 | Depositor<br>DCC |
| $R_{free}$ test set   | 29386 reflections (6.10%)                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.1   | Xtriage          |
| Anisotropy  | 0.178  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 77.0  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$    | Xtriage          |
| Estimated twinning fraction   | 0.499 for -h,-k,l<br>0.085 for h,-h-k,-l<br>0.085 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.92   | EDS              |
| Total number of atoms   | 61089  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 67.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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, RBT, MG

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.79         | 1/1838 (0.1%)  | 0.86        | 2/2498 (0.1%)   |
| 1   | B     | 0.73         | 0/1838         | 0.82        | 3/2498 (0.1%)   |
| 1   | K     | 0.75         | 0/1838         | 0.84        | 2/2498 (0.1%)   |
| 1   | L     | 0.71         | 1/1838 (0.1%)  | 0.78        | 0/2498          |
| 2   | C     | 0.81         | 0/8997         | 0.88        | 6/12164 (0.0%)  |
| 2   | M     | 0.79         | 0/8997         | 0.88        | 8/12164 (0.1%)  |
| 3   | D     | 0.82         | 0/10975        | 0.93        | 22/14836 (0.1%) |
| 3   | N     | 0.80         | 0/10975        | 0.91        | 14/14836 (0.1%) |
| 4   | E     | 0.82         | 0/783          | 0.98        | 1/1054 (0.1%)   |
| 4   | O     | 0.84         | 0/783          | 0.96        | 1/1054 (0.1%)   |
| 5   | F     | 0.73         | 0/2812         | 0.82        | 2/3781 (0.1%)   |
| 5   | P     | 0.71         | 0/2812         | 0.80        | 1/3781 (0.0%)   |
| All | All   | 0.79         | 2/54486 (0.0%) | 0.88        | 62/73662 (0.1%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 48  | ILE  | C-N   | 5.18  | 1.44        | 1.34     |
| 1   | L     | 172 | SER  | N-CA  | -5.06 | 1.36        | 1.46     |

The worst 5 of 62 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 138  | LEU  | CA-CB-CG | 8.26  | 134.29      | 115.30   |
| 3   | D     | 199  | LEU  | CA-CB-CG | -8.08 | 96.72       | 115.30   |
| 3   | N     | 199  | LEU  | CA-CB-CG | -7.83 | 97.28       | 115.30   |
| 3   | N     | 1389 | LEU  | CA-CB-CG | 7.33  | 132.15      | 115.30   |
| 5   | F     | 361  | LEU  | CA-CB-CG | 7.04  | 131.49      | 115.30   |

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   | A     | 1806  | 0        | 1861     | 231     | 0            |
| 1   | B     | 1806  | 0        | 1861     | 211     | 0            |
| 1   | K     | 1806  | 0        | 1861     | 199     | 0            |
| 1   | L     | 1806  | 0        | 1861     | 202     | 0            |
| 2   | C     | 8829  | 0        | 8933     | 1201    | 0            |
| 2   | M     | 8829  | 0        | 8933     | 1179    | 0            |
| 3   | D     | 10797 | 0        | 10873    | 1404    | 0            |
| 3   | N     | 10797 | 0        | 10873    | 1285    | 0            |
| 4   | E     | 769   | 0        | 775      | 92      | 0            |
| 4   | O     | 769   | 0        | 775      | 99      | 0            |
| 5   | F     | 2771  | 0        | 2844     | 340     | 0            |
| 5   | P     | 2771  | 0        | 2844     | 315     | 0            |
| 6   | A     | 31    | 0        | 0        | 0       | 0            |
| 6   | B     | 23    | 0        | 0        | 0       | 0            |
| 6   | C     | 81    | 0        | 0        | 0       | 0            |
| 6   | D     | 137   | 0        | 0        | 0       | 0            |
| 6   | E     | 10    | 0        | 0        | 0       | 0            |
| 6   | F     | 31    | 0        | 0        | 0       | 0            |
| 6   | K     | 21    | 0        | 0        | 0       | 0            |
| 6   | L     | 25    | 0        | 0        | 0       | 0            |
| 6   | M     | 69    | 0        | 0        | 0       | 0            |
| 6   | N     | 108   | 0        | 0        | 0       | 0            |
| 6   | O     | 6     | 0        | 0        | 0       | 0            |
| 6   | P     | 20    | 0        | 0        | 0       | 0            |
| 7   | C     | 61    | 0        | 61       | 3       | 0            |
| 7   | M     | 61    | 0        | 61       | 3       | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | N     | 2     | 0        | 0        | 0       | 0            |
| 9   | A     | 253   | 0        | 0        | 49      | 0            |
| 9   | B     | 307   | 0        | 0        | 49      | 0            |
| 9   | C     | 1000  | 0        | 0        | 202     | 0            |
| 9   | D     | 1418  | 0        | 0        | 282     | 0            |
| 9   | E     | 112   | 0        | 0        | 22      | 0            |
| 9   | F     | 456   | 0        | 0        | 98      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | K     | 213   | 0        | 0        | 34      | 0            |
| 9   | L     | 237   | 0        | 0        | 58      | 0            |
| 9   | M     | 998   | 0        | 0        | 255     | 0            |
| 9   | N     | 1357  | 0        | 0        | 240     | 0            |
| 9   | O     | 117   | 0        | 0        | 26      | 0            |
| 9   | P     | 377   | 0        | 0        | 75      | 0            |
| All | All   | 61089 | 0        | 54416    | 6365    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

The worst 5 of 6365 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:A:42:ARG:HH12   | 2:C:857:ASP:HB3  | 1.08                     | 1.12              |
| 2:M:1054:THR:HG21 | 2:M:1079:PRO:HB3 | 1.27                     | 1.11              |
| 3:N:1045:MET:HG2  | 3:N:1073:SER:HA  | 1.35                     | 1.08              |
| 2:C:630:ARG:HH21  | 2:C:705:ILE:HG22 | 1.18                     | 1.07              |
| 3:N:52:PRO:HB2    | 3:N:80:VAL:HG13  | 1.34                     | 1.06              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|------------------|-----------|-----------|----------|-------------|----|
| 1   | A     | 227/315 (72%)    | 204 (90%) | 19 (8%)   | 4 (2%)   | 10          | 17 |
| 1   | B     | 227/315 (72%)    | 201 (88%) | 21 (9%)   | 5 (2%)   | 8           | 12 |
| 1   | K     | 227/315 (72%)    | 204 (90%) | 19 (8%)   | 4 (2%)   | 10          | 17 |
| 1   | L     | 227/315 (72%)    | 205 (90%) | 18 (8%)   | 4 (2%)   | 10          | 17 |
| 2   | C     | 1117/1119 (100%) | 911 (82%) | 153 (14%) | 53 (5%)  | 3           | 3  |

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| Mol | Chain | Analysed         | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|------------------|------------|-----------|----------|-------------|---|
| 2   | M     | 1117/1119 (100%) | 904 (81%)  | 168 (15%) | 45 (4%)  | 3           | 4 |
| 3   | D     | 1388/1524 (91%)  | 1112 (80%) | 202 (15%) | 74 (5%)  | 2           | 2 |
| 3   | N     | 1388/1524 (91%)  | 1118 (80%) | 195 (14%) | 75 (5%)  | 2           | 2 |
| 4   | E     | 93/99 (94%)      | 74 (80%)   | 15 (16%)  | 4 (4%)   | 3           | 3 |
| 4   | O     | 93/99 (94%)      | 76 (82%)   | 13 (14%)  | 4 (4%)   | 3           | 3 |
| 5   | F     | 341/423 (81%)    | 286 (84%)  | 40 (12%)  | 15 (4%)  | 3           | 3 |
| 5   | P     | 341/423 (81%)    | 290 (85%)  | 37 (11%)  | 14 (4%)  | 3           | 4 |
| All | All   | 6786/7590 (89%)  | 5585 (82%) | 900 (13%) | 301 (4%) | 3           | 3 |

5 of 301 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | GLU  |
| 1   | B     | 29  | GLU  |
| 1   | B     | 48  | ILE  |
| 2   | C     | 152 | PRO  |
| 2   | C     | 156 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric | Outliers  | Percentiles |   |
|-----|-------|-----------------|-----------|-----------|-------------|---|
| 1   | A     | 202/273 (74%)   | 148 (73%) | 54 (27%)  | 0           | 0 |
| 1   | B     | 202/273 (74%)   | 164 (81%) | 38 (19%)  | 2           | 3 |
| 1   | K     | 202/273 (74%)   | 144 (71%) | 58 (29%)  | 0           | 0 |
| 1   | L     | 202/273 (74%)   | 159 (79%) | 43 (21%)  | 1           | 2 |
| 2   | C     | 941/941 (100%)  | 738 (78%) | 203 (22%) | 1           | 2 |
| 2   | M     | 941/941 (100%)  | 737 (78%) | 204 (22%) | 1           | 2 |
| 3   | D     | 1123/1279 (88%) | 841 (75%) | 282 (25%) | 0           | 1 |
| 3   | N     | 1123/1279 (88%) | 865 (77%) | 258 (23%) | 1           | 1 |
| 4   | E     | 83/87 (95%)     | 67 (81%)  | 16 (19%)  | 1           | 3 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|-----------------|------------|------------|-------------|---|
| 4   | O     | 83/87 (95%)     | 61 (74%)   | 22 (26%)   | 0           | 1 |
| 5   | F     | 295/370 (80%)   | 235 (80%)  | 60 (20%)   | 1           | 2 |
| 5   | P     | 295/370 (80%)   | 247 (84%)  | 48 (16%)   | 3           | 5 |
| All | All   | 5692/6446 (88%) | 4406 (77%) | 1286 (23%) | 1           | 1 |

5 of 1286 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | E     | 33   | HIS  |
| 1   | L     | 29   | GLU  |
| 3   | N     | 1396 | GLU  |
| 5   | F     | 87   | GLU  |
| 1   | K     | 2    | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 174 such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | F     | 277  | GLN  |
| 1   | L     | 212  | ASN  |
| 3   | N     | 1374 | GLN  |
| 1   | K     | 63   | HIS  |
| 1   | K     | 227  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 568 ligands modelled in this entry, 566 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$ |
| 7   | RBT  | C     | 8001 | 6    | 60,66,66     | 2.78 | 22 (36%)    | 86,101,101  | 1.68 | 15 (17%)    |
| 7   | RBT  | M     | 8002 | -    | 60,66,66     | 2.73 | 22 (36%)    | 86,101,101  | 1.67 | 13 (15%)    |

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   |
|-----|------|-------|------|------|---------|--------------|---------|
| 7   | RBT  | C     | 8001 | 6    | -       | 0/59/116/116 | 0/2/6/6 |
| 7   | RBT  | M     | 8002 | -    | -       | 0/59/116/116 | 0/2/6/6 |

The worst 5 of 44 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | M     | 8002 | RBT  | O2-C8   | -3.58 | 1.28        | 1.37     |
| 7   | C     | 8001 | RBT  | O2-C8   | -2.73 | 1.30        | 1.37     |
| 7   | C     | 8001 | RBT  | C3-C4   | -2.12 | 1.42        | 1.48     |
| 7   | M     | 8002 | RBT  | O7-C35  | 2.01  | 1.39        | 1.35     |
| 7   | C     | 8001 | RBT  | C32-C22 | 2.09  | 1.58        | 1.53     |

The worst 5 of 28 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | C     | 8001 | RBT  | O3-C6-C5    | -3.79 | 111.08      | 114.25   |
| 7   | M     | 8002 | RBT  | O3-C6-C5    | -3.73 | 111.13      | 114.25   |
| 7   | C     | 8001 | RBT  | C9-C10-C5   | -2.89 | 116.06      | 119.96   |
| 7   | M     | 8002 | RBT  | C31-C20-C19 | -2.81 | 102.95      | 110.07   |
| 7   | M     | 8002 | RBT  | C9-C10-C5   | -2.78 | 116.21      | 119.96   |

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 |
|-----|-------|------|------|---------|--------------|
| 7   | C     | 8001 | RBT  | 3       | 0            |
| 7   | M     | 8002 | RBT  | 3       | 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   | A     | 229/315 (72%)    | -0.40  | 1 (0%) 92 92   | 29, 60, 84, 110       | 0       |
| 1   | B     | 229/315 (72%)    | -0.13  | 13 (5%) 24 25  | 44, 89, 114, 118      | 0       |
| 1   | K     | 229/315 (72%)    | -0.40  | 2 (0%) 84 85   | 33, 58, 89, 120       | 0       |
| 1   | L     | 229/315 (72%)    | -0.25  | 8 (3%) 44 47   | 49, 89, 109, 119      | 0       |
| 2   | C     | 1119/1119 (100%) | -0.39  | 10 (0%) 84 85  | 14, 74, 102, 117      | 0       |
| 2   | M     | 1119/1119 (100%) | -0.39  | 12 (1%) 80 81  | 19, 71, 103, 119      | 0       |
| 3   | D     | 1392/1524 (91%)  | -0.36  | 17 (1%) 79 80  | 19, 62, 107, 125      | 0       |
| 3   | N     | 1392/1524 (91%)  | -0.36  | 24 (1%) 70 72  | 23, 65, 107, 131      | 0       |
| 4   | E     | 95/99 (95%)      | -0.40  | 2 (2%) 64 66   | 41, 77, 107, 120      | 0       |
| 4   | O     | 95/99 (95%)      | -0.44  | 1 (1%) 80 81   | 33, 72, 94, 103       | 0       |
| 5   | F     | 345/423 (81%)    | -0.39  | 7 (2%) 65 67   | 46, 81, 104, 118      | 0       |
| 5   | P     | 345/423 (81%)    | -0.30  | 8 (2%) 61 63   | 53, 81, 108, 123      | 0       |
| All | All   | 6818/7590 (89%)  | -0.36  | 105 (1%) 74 75 | 14, 70, 105, 131      | 0       |

The worst 5 of 105 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | P     | 145  | PRO  | 5.8  |
| 3   | N     | 1243 | THR  | 5.8  |
| 2   | M     | 269  | LEU  | 5.2  |
| 3   | D     | 1244 | GLY  | 4.8  |
| 3   | D     | 1240 | THR  | 4.8  |

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

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

## 6.3 Carbohydrates [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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 7   | RBT  | C     | 8001 | 61/61 | 0.97 | 0.19 | 2.48  | 25,37,42,48                 | 0     |
| 6   | MG   | C     | 9121 | 1/1   | 0.99 | 0.15 | 1.83  | 43,43,43,43                 | 0     |
| 7   | RBT  | M     | 8002 | 61/61 | 0.96 | 0.18 | 1.80  | 28,39,48,54                 | 0     |
| 6   | MG   | K     | 9214 | 1/1   | 0.98 | 0.20 | 1.47  | 31,31,31,31                 | 0     |
| 8   | ZN   | D     | 7112 | 1/1   | 0.99 | 0.13 | 1.30  | 72,72,72,72                 | 0     |
| 6   | MG   | A     | 9001 | 1/1   | 0.98 | 0.18 | 1.15  | 26,26,26,26                 | 0     |
| 6   | MG   | D     | 9002 | 1/1   | 0.98 | 0.16 | 0.85  | 29,29,29,29                 | 0     |
| 8   | ZN   | N     | 7113 | 1/1   | 0.99 | 0.11 | 0.16  | 79,79,79,79                 | 0     |
| 6   | MG   | N     | 9218 | 1/1   | 0.99 | 0.12 | 0.05  | 32,32,32,32                 | 0     |
| 8   | ZN   | N     | 7059 | 1/1   | 1.00 | 0.12 | 0.04  | 83,83,83,83                 | 0     |
| 6   | MG   | D     | 9008 | 1/1   | 0.99 | 0.13 | -0.04 | 37,37,37,37                 | 0     |
| 6   | MG   | M     | 9220 | 1/1   | 0.96 | 0.13 | -0.11 | 45,45,45,45                 | 0     |
| 6   | MG   | D     | 9015 | 1/1   | 0.98 | 0.12 | -0.28 | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9042 | 1/1   | 0.97 | 0.12 | -0.32 | 47,47,47,47                 | 0     |
| 6   | MG   | F     | 9421 | 1/1   | 1.00 | 0.13 | -0.32 | 30,30,30,30                 | 0     |
| 6   | MG   | D     | 9021 | 1/1   | 0.99 | 0.12 | -0.44 | 34,34,34,34                 | 0     |
| 6   | MG   | K     | 9265 | 1/1   | 0.99 | 0.13 | -0.47 | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9123 | 1/1   | 0.98 | 0.14 | -0.52 | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9049 | 1/1   | 0.99 | 0.14 | -0.53 | 31,31,31,31                 | 0     |
| 6   | MG   | D     | 9036 | 1/1   | 0.98 | 0.13 | -0.56 | 41,41,41,41                 | 0     |
| 6   | MG   | C     | 9020 | 1/1   | 0.99 | 0.14 | -0.58 | 28,28,28,28                 | 0     |
| 6   | MG   | N     | 9215 | 1/1   | 0.99 | 0.10 | -0.83 | 40,40,40,40                 | 0     |
| 6   | MG   | N     | 9277 | 1/1   | 0.99 | 0.09 | -0.88 | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9172 | 1/1   | 0.98 | 0.10 | -0.88 | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9449 | 1/1   | 0.98 | 0.07 | -0.92 | 29,29,29,29                 | 0     |
| 6   | MG   | A     | 9024 | 1/1   | 0.99 | 0.10 | -0.94 | 29,29,29,29                 | 0     |
| 6   | MG   | D     | 9453 | 1/1   | 1.00 | 0.12 | -0.94 | 31,31,31,31                 | 0     |
| 6   | MG   | D     | 9069 | 1/1   | 1.00 | 0.12 | -0.94 | 32,32,32,32                 | 0     |
| 6   | MG   | C     | 9004 | 1/1   | 0.99 | 0.09 | -0.95 | 30,30,30,30                 | 0     |
| 6   | MG   | P     | 9275 | 1/1   | 0.99 | 0.09 | -0.99 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 6   | MG   | K     | 9487 | 1/1   | 0.99 | 0.12 | -1.04 | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9335 | 1/1   | 0.99 | 0.10 | -1.10 | 33,33,33,33                 | 0     |
| 6   | MG   | D     | 9026 | 1/1   | 0.97 | 0.12 | -1.14 | 37,37,37,37                 | 0     |
| 6   | MG   | M     | 9323 | 1/1   | 0.99 | 0.10 | -1.16 | 37,37,37,37                 | 0     |
| 6   | MG   | B     | 9163 | 1/1   | 0.92 | 0.06 | -1.21 | 44,44,44,44                 | 0     |
| 6   | MG   | C     | 9025 | 1/1   | 0.99 | 0.10 | -1.22 | 39,39,39,39                 | 0     |
| 6   | MG   | C     | 9161 | 1/1   | 0.99 | 0.07 | -1.25 | 40,40,40,40                 | 0     |
| 6   | MG   | F     | 9053 | 1/1   | 0.99 | 0.10 | -1.25 | 34,34,34,34                 | 0     |
| 6   | MG   | C     | 9005 | 1/1   | 0.99 | 0.08 | -1.25 | 31,31,31,31                 | 0     |
| 6   | MG   | M     | 9312 | 1/1   | 0.97 | 0.10 | -1.26 | 37,37,37,37                 | 0     |
| 6   | MG   | N     | 9526 | 1/1   | 0.98 | 0.10 | -1.26 | 30,30,30,30                 | 0     |
| 6   | MG   | P     | 9536 | 1/1   | 0.99 | 0.07 | -1.27 | 41,41,41,41                 | 0     |
| 6   | MG   | C     | 9398 | 1/1   | 0.95 | 0.10 | -1.31 | 44,44,44,44                 | 0     |
| 6   | MG   | C     | 9011 | 1/1   | 0.99 | 0.10 | -1.37 | 39,39,39,39                 | 0     |
| 6   | MG   | N     | 9221 | 1/1   | 0.99 | 0.10 | -1.39 | 30,30,30,30                 | 0     |
| 6   | MG   | C     | 9144 | 1/1   | 0.99 | 0.09 | -1.40 | 39,39,39,39                 | 0     |
| 6   | MG   | D     | 9441 | 1/1   | 0.98 | 0.10 | -1.41 | 46,46,46,46                 | 0     |
| 6   | MG   | N     | 9475 | 1/1   | 0.99 | 0.07 | -1.51 | 43,43,43,43                 | 0     |
| 6   | MG   | N     | 9226 | 1/1   | 0.99 | 0.07 | -1.53 | 30,30,30,30                 | 0     |
| 6   | MG   | N     | 9263 | 1/1   | 0.99 | 0.08 | -1.70 | 37,37,37,37                 | 0     |
| 6   | MG   | N     | 9280 | 1/1   | 0.99 | 0.09 | -1.73 | 34,34,34,34                 | 0     |
| 6   | MG   | L     | 9272 | 1/1   | 0.99 | 0.10 | -1.78 | 29,29,29,29                 | 0     |
| 6   | MG   | C     | 9046 | 1/1   | 0.99 | 0.09 | -1.80 | 31,31,31,31                 | 0     |
| 8   | ZN   | D     | 7058 | 1/1   | 0.95 | 0.07 | -1.81 | 100,100,100,100             | 0     |
| 6   | MG   | D     | 9181 | 1/1   | 0.99 | 0.06 | -1.83 | 36,36,36,36                 | 0     |
| 6   | MG   | B     | 9101 | 1/1   | 0.98 | 0.08 | -1.86 | 40,40,40,40                 | 0     |
| 6   | MG   | F     | 9465 | 1/1   | 0.99 | 0.06 | -1.88 | 36,36,36,36                 | 0     |
| 6   | MG   | M     | 9372 | 1/1   | 0.99 | 0.09 | -1.96 | 47,47,47,47                 | 0     |
| 6   | MG   | D     | 9105 | 1/1   | 0.99 | 0.07 | -1.96 | 48,48,48,48                 | 0     |
| 6   | MG   | K     | 9212 | 1/1   | 1.00 | 0.08 | -2.00 | 33,33,33,33                 | 0     |
| 6   | MG   | N     | 9207 | 1/1   | 0.98 | 0.10 | -2.11 | 30,30,30,30                 | 0     |
| 6   | MG   | D     | 9179 | 1/1   | 1.00 | 0.09 | -2.24 | 30,30,30,30                 | 0     |
| 6   | MG   | D     | 9037 | 1/1   | 1.00 | 0.08 | -2.28 | 31,31,31,31                 | 0     |
| 6   | MG   | C     | 9056 | 1/1   | 0.99 | 0.06 | -2.39 | 34,34,34,34                 | 0     |
| 6   | MG   | N     | 9509 | 1/1   | 0.99 | 0.11 | -2.45 | 31,31,31,31                 | 0     |
| 6   | MG   | C     | 9515 | 1/1   | 0.98 | 0.08 | -2.46 | 41,41,41,41                 | 0     |
| 6   | MG   | F     | 9407 | 1/1   | 0.99 | 0.07 | -2.54 | 32,32,32,32                 | 0     |
| 6   | MG   | D     | 9013 | 1/1   | 1.00 | 0.09 | -2.56 | 34,34,34,34                 | 0     |
| 6   | MG   | M     | 9478 | 1/1   | 0.98 | 0.06 | -2.56 | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9129 | 1/1   | 0.99 | 0.09 | -2.67 | 38,38,38,38                 | 0     |
| 6   | MG   | N     | 9248 | 1/1   | 0.99 | 0.06 | -2.78 | 47,47,47,47                 | 0     |
| 6   | MG   | F     | 9032 | 1/1   | 0.99 | 0.09 | -3.07 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 6   | MG   | C     | 9414 | 1/1   | 0.97 | 0.07 | -3.10 | 41,41,41,41                 | 0     |
| 6   | MG   | N     | 9531 | 1/1   | 1.00 | 0.10 | -3.10 | 38,38,38,38                 | 0     |
| 6   | MG   | D     | 9147 | 1/1   | 0.96 | 0.09 | -3.13 | 40,40,40,40                 | 0     |
| 6   | MG   | C     | 9431 | 1/1   | 0.99 | 0.06 | -3.14 | 42,42,42,42                 | 0     |
| 6   | MG   | C     | 9420 | 1/1   | 0.99 | 0.07 | -3.36 | 37,37,37,37                 | 0     |
| 6   | MG   | C     | 9047 | 1/1   | 0.97 | 0.06 | -3.48 | 47,47,47,47                 | 0     |
| 6   | MG   | D     | 9017 | 1/1   | 0.99 | 0.07 | -3.74 | 37,37,37,37                 | 0     |
| 6   | MG   | N     | 9349 | 1/1   | 0.96 | 0.06 | -3.81 | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9012 | 1/1   | 0.98 | 0.06 | -4.18 | 39,39,39,39                 | 0     |
| 6   | MG   | D     | 9120 | 1/1   | 0.99 | 0.07 | -4.76 | 34,34,34,34                 | 0     |
| 6   | MG   | D     | 9003 | 1/1   | 0.98 | 0.06 | -4.97 | 43,43,43,43                 | 0     |
| 6   | MG   | D     | 9451 | 1/1   | 0.98 | 0.09 | -5.59 | 37,37,37,37                 | 0     |
| 6   | MG   | K     | 9217 | 1/1   | 0.98 | 0.06 | -5.86 | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9282 | 1/1   | 0.99 | 0.06 | -6.71 | 38,38,38,38                 | 0     |
| 6   | MG   | D     | 9055 | 1/1   | 0.98 | 0.09 | -     | 51,51,51,51                 | 0     |
| 6   | MG   | F     | 9437 | 1/1   | 0.98 | 0.09 | -     | 47,47,47,47                 | 0     |
| 6   | MG   | D     | 9087 | 1/1   | 1.00 | 0.09 | -     | 27,27,27,27                 | 0     |
| 6   | MG   | C     | 9156 | 1/1   | 0.97 | 0.12 | -     | 43,43,43,43                 | 0     |
| 6   | MG   | N     | 9303 | 1/1   | 0.99 | 0.12 | -     | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9098 | 1/1   | 0.99 | 0.09 | -     | 52,52,52,52                 | 0     |
| 6   | MG   | L     | 9530 | 1/1   | 0.99 | 0.10 | -     | 58,58,58,58                 | 0     |
| 6   | MG   | D     | 9452 | 1/1   | 0.99 | 0.10 | -     | 32,32,32,32                 | 0     |
| 6   | MG   | K     | 9367 | 1/1   | 0.98 | 0.09 | -     | 38,38,38,38                 | 0     |
| 6   | MG   | C     | 9171 | 1/1   | 0.99 | 0.09 | -     | 33,33,33,33                 | 0     |
| 6   | MG   | D     | 9182 | 1/1   | 1.00 | 0.07 | -     | 46,46,46,46                 | 0     |
| 6   | MG   | D     | 9436 | 1/1   | 0.99 | 0.09 | -     | 46,46,46,46                 | 0     |
| 6   | MG   | A     | 9062 | 1/1   | 0.96 | 0.11 | -     | 45,45,45,45                 | 0     |
| 6   | MG   | N     | 9286 | 1/1   | 0.99 | 0.12 | -     | 46,46,46,46                 | 0     |
| 6   | MG   | N     | 9498 | 1/1   | 0.98 | 0.09 | -     | 45,45,45,45                 | 0     |
| 6   | MG   | A     | 9116 | 1/1   | 0.99 | 0.12 | -     | 47,47,47,47                 | 0     |
| 6   | MG   | C     | 9031 | 1/1   | 0.99 | 0.12 | -     | 43,43,43,43                 | 0     |
| 6   | MG   | N     | 9371 | 1/1   | 0.99 | 0.10 | -     | 30,30,30,30                 | 0     |
| 6   | MG   | F     | 9542 | 1/1   | 0.99 | 0.19 | -     | 50,50,50,50                 | 0     |
| 6   | MG   | L     | 9480 | 1/1   | 0.99 | 0.13 | -     | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9342 | 1/1   | 0.98 | 0.07 | -     | 48,48,48,48                 | 0     |
| 6   | MG   | M     | 9223 | 1/1   | 0.99 | 0.10 | -     | 48,48,48,48                 | 0     |
| 6   | MG   | A     | 9097 | 1/1   | 0.98 | 0.09 | -     | 41,41,41,41                 | 0     |
| 6   | MG   | A     | 9117 | 1/1   | 0.99 | 0.07 | -     | 32,32,32,32                 | 0     |
| 6   | MG   | K     | 9370 | 1/1   | 0.99 | 0.06 | -     | 46,46,46,46                 | 0     |
| 6   | MG   | K     | 9477 | 1/1   | 1.00 | 0.11 | -     | 38,38,38,38                 | 0     |
| 6   | MG   | D     | 9543 | 1/1   | 0.97 | 0.12 | -     | 46,46,46,46                 | 0     |
| 6   | MG   | M     | 9347 | 1/1   | 0.98 | 0.11 | -     | 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 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | C     | 9027 | 1/1   | 1.00 | 0.12 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | P     | 9304 | 1/1   | 0.97 | 0.10 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | M     | 9254 | 1/1   | 0.99 | 0.08 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | N     | 9301 | 1/1   | 0.98 | 0.08 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | D     | 9162 | 1/1   | 0.99 | 0.11 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | L     | 9278 | 1/1   | 1.00 | 0.08 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | E     | 9131 | 1/1   | 0.98 | 0.08 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | C     | 9086 | 1/1   | 0.99 | 0.10 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | D     | 9517 | 1/1   | 0.99 | 0.09 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | N     | 9297 | 1/1   | 0.98 | 0.13 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | D     | 9446 | 1/1   | 0.99 | 0.10 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | B     | 9092 | 1/1   | 0.98 | 0.11 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | A     | 9078 | 1/1   | 0.98 | 0.13 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | M     | 9340 | 1/1   | 0.99 | 0.10 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | M     | 9259 | 1/1   | 0.97 | 0.17 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | L     | 9330 | 1/1   | 0.99 | 0.09 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | C     | 9457 | 1/1   | 0.98 | 0.10 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | F     | 9054 | 1/1   | 0.99 | 0.07 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | C     | 9422 | 1/1   | 0.99 | 0.13 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | D     | 9155 | 1/1   | 0.96 | 0.12 | -    | 56,56,56,56                 | 0     |
| 6   | MG   | C     | 9455 | 1/1   | 0.97 | 0.12 | -    | 61,61,61,61                 | 0     |
| 6   | MG   | N     | 9244 | 1/1   | 0.97 | 0.08 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | M     | 9336 | 1/1   | 0.99 | 0.10 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | D     | 9463 | 1/1   | 0.99 | 0.11 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | A     | 9514 | 1/1   | 0.96 | 0.12 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | D     | 9122 | 1/1   | 0.99 | 0.10 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | K     | 9553 | 1/1   | 0.98 | 0.09 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | D     | 9077 | 1/1   | 0.99 | 0.10 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | N     | 9356 | 1/1   | 0.99 | 0.14 | -    | 29,29,29,29                 | 0     |
| 6   | MG   | E     | 9151 | 1/1   | 0.98 | 0.05 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | N     | 9327 | 1/1   | 0.97 | 0.11 | -    | 54,54,54,54                 | 0     |
| 6   | MG   | D     | 9174 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9393 | 1/1   | 0.99 | 0.13 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9095 | 1/1   | 0.97 | 0.06 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | F     | 9164 | 1/1   | 0.99 | 0.11 | -    | 29,29,29,29                 | 0     |
| 6   | MG   | A     | 9559 | 1/1   | 0.97 | 0.12 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | D     | 9112 | 1/1   | 0.98 | 0.13 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | D     | 9159 | 1/1   | 0.99 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9246 | 1/1   | 0.97 | 0.13 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | D     | 9100 | 1/1   | 0.99 | 0.07 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | M     | 9251 | 1/1   | 0.99 | 0.13 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | P     | 9502 | 1/1   | 0.99 | 0.07 | -    | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | N     | 9307 | 1/1   | 0.99 | 0.09 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | M     | 9481 | 1/1   | 0.99 | 0.09 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | C     | 9546 | 1/1   | 0.98 | 0.06 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | D     | 9203 | 1/1   | 0.99 | 0.09 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | C     | 9023 | 1/1   | 0.97 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | A     | 9139 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9456 | 1/1   | 0.99 | 0.07 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | K     | 9344 | 1/1   | 0.98 | 0.12 | -    | 55,55,55,55                 | 0     |
| 6   | MG   | C     | 9191 | 1/1   | 0.98 | 0.13 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | N     | 9534 | 1/1   | 0.98 | 0.09 | -    | 54,54,54,54                 | 0     |
| 6   | MG   | M     | 9472 | 1/1   | 0.99 | 0.06 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | D     | 9417 | 1/1   | 0.99 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | P     | 9296 | 1/1   | 0.99 | 0.07 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | M     | 9219 | 1/1   | 0.98 | 0.10 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | A     | 9050 | 1/1   | 0.97 | 0.10 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | A     | 9394 | 1/1   | 0.99 | 0.10 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | C     | 9141 | 1/1   | 0.98 | 0.12 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | C     | 9028 | 1/1   | 0.99 | 0.07 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | N     | 9499 | 1/1   | 0.98 | 0.08 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | M     | 9285 | 1/1   | 0.98 | 0.13 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | F     | 9045 | 1/1   | 0.99 | 0.10 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | D     | 9016 | 1/1   | 0.99 | 0.07 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | M     | 9540 | 1/1   | 0.98 | 0.16 | -    | 63,63,63,63                 | 0     |
| 6   | MG   | D     | 9110 | 1/1   | 0.98 | 0.13 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | N     | 9508 | 1/1   | 0.97 | 0.11 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | O     | 9231 | 1/1   | 1.00 | 0.15 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | L     | 9346 | 1/1   | 0.97 | 0.14 | -    | 52,52,52,52                 | 0     |
| 6   | MG   | L     | 9311 | 1/1   | 0.98 | 0.07 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | C     | 9083 | 1/1   | 0.98 | 0.11 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | F     | 9048 | 1/1   | 0.96 | 0.16 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | P     | 9353 | 1/1   | 0.99 | 0.11 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | D     | 9057 | 1/1   | 0.98 | 0.11 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | M     | 9216 | 1/1   | 0.99 | 0.12 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | B     | 9512 | 1/1   | 0.99 | 0.20 | -    | 53,53,53,53                 | 0     |
| 6   | MG   | D     | 9405 | 1/1   | 0.99 | 0.10 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | B     | 9427 | 1/1   | 0.98 | 0.11 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | C     | 9157 | 1/1   | 0.98 | 0.16 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | N     | 9266 | 1/1   | 0.98 | 0.08 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | K     | 9264 | 1/1   | 1.00 | 0.09 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | D     | 9403 | 1/1   | 0.99 | 0.16 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | P     | 9240 | 1/1   | 0.99 | 0.11 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | A     | 9440 | 1/1   | 0.99 | 0.10 | -    | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | D     | 9418 | 1/1   | 0.99 | 0.08 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | M     | 9224 | 1/1   | 0.99 | 0.06 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | C     | 9170 | 1/1   | 0.99 | 0.10 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | C     | 9185 | 1/1   | 0.99 | 0.18 | -    | 60,60,60,60                 | 0     |
| 6   | MG   | M     | 9380 | 1/1   | 1.00 | 0.08 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | N     | 9506 | 1/1   | 0.98 | 0.10 | -    | 56,56,56,56                 | 0     |
| 6   | MG   | D     | 9128 | 1/1   | 0.99 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9474 | 1/1   | 0.96 | 0.13 | -    | 56,56,56,56                 | 0     |
| 6   | MG   | N     | 9305 | 1/1   | 0.99 | 0.09 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | M     | 9255 | 1/1   | 0.96 | 0.13 | -    | 58,58,58,58                 | 0     |
| 6   | MG   | L     | 9234 | 1/1   | 0.99 | 0.07 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | N     | 9550 | 1/1   | 0.99 | 0.09 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | M     | 9267 | 1/1   | 0.96 | 0.12 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | N     | 9501 | 1/1   | 0.99 | 0.08 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | M     | 9382 | 1/1   | 0.99 | 0.09 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | N     | 9529 | 1/1   | 0.98 | 0.08 | -    | 55,55,55,55                 | 0     |
| 6   | MG   | D     | 9067 | 1/1   | 0.97 | 0.12 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | M     | 9227 | 1/1   | 0.98 | 0.10 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | C     | 9113 | 1/1   | 0.99 | 0.16 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | B     | 9434 | 1/1   | 0.99 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | B     | 9150 | 1/1   | 0.98 | 0.10 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | M     | 9366 | 1/1   | 0.99 | 0.10 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | M     | 9298 | 1/1   | 0.98 | 0.12 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | M     | 9318 | 1/1   | 0.99 | 0.14 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | M     | 9328 | 1/1   | 0.99 | 0.09 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | M     | 9210 | 1/1   | 0.99 | 0.13 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9549 | 1/1   | 0.98 | 0.11 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | N     | 9503 | 1/1   | 0.96 | 0.12 | -    | 52,52,52,52                 | 0     |
| 6   | MG   | M     | 9334 | 1/1   | 0.97 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | D     | 9562 | 1/1   | 0.99 | 0.17 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | N     | 9238 | 1/1   | 0.99 | 0.16 | -    | 29,29,29,29                 | 0     |
| 6   | MG   | C     | 9007 | 1/1   | 0.98 | 0.11 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | D     | 9094 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | M     | 9241 | 1/1   | 1.00 | 0.09 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9401 | 1/1   | 0.98 | 0.12 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | N     | 9533 | 1/1   | 0.99 | 0.12 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | D     | 9149 | 1/1   | 1.00 | 0.13 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | F     | 9089 | 1/1   | 0.99 | 0.10 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | M     | 9283 | 1/1   | 0.98 | 0.14 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | M     | 9361 | 1/1   | 0.99 | 0.10 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | D     | 9058 | 1/1   | 0.99 | 0.11 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | D     | 9202 | 1/1   | 0.98 | 0.18 | -    | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | L     | 9299 | 1/1   | 1.00 | 0.07 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9358 | 1/1   | 0.97 | 0.12 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | D     | 9445 | 1/1   | 0.98 | 0.13 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | N     | 9387 | 1/1   | 0.99 | 0.07 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | P     | 9558 | 1/1   | 0.98 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | N     | 9230 | 1/1   | 0.97 | 0.09 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | C     | 9444 | 1/1   | 0.99 | 0.09 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | B     | 9450 | 1/1   | 0.99 | 0.08 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | E     | 9467 | 1/1   | 0.97 | 0.12 | -    | 52,52,52,52                 | 0     |
| 6   | MG   | D     | 9075 | 1/1   | 0.99 | 0.11 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | M     | 9325 | 1/1   | 0.97 | 0.10 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | P     | 9541 | 1/1   | 0.98 | 0.10 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | N     | 9528 | 1/1   | 0.99 | 0.10 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | C     | 9201 | 1/1   | 0.99 | 0.08 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | N     | 9365 | 1/1   | 0.98 | 0.12 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | D     | 9143 | 1/1   | 1.00 | 0.14 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9521 | 1/1   | 0.99 | 0.12 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | D     | 9466 | 1/1   | 0.98 | 0.10 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | D     | 9168 | 1/1   | 0.98 | 0.06 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | F     | 9547 | 1/1   | 1.00 | 0.09 | -    | 52,52,52,52                 | 0     |
| 6   | MG   | N     | 9381 | 1/1   | 0.97 | 0.07 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9256 | 1/1   | 0.99 | 0.09 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | A     | 9430 | 1/1   | 0.97 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9314 | 1/1   | 0.98 | 0.11 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | F     | 9135 | 1/1   | 0.99 | 0.14 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | N     | 9379 | 1/1   | 0.99 | 0.06 | -    | 56,56,56,56                 | 0     |
| 6   | MG   | L     | 9300 | 1/1   | 0.99 | 0.07 | -    | 58,58,58,58                 | 0     |
| 6   | MG   | C     | 9088 | 1/1   | 0.99 | 0.12 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9235 | 1/1   | 0.95 | 0.12 | -    | 63,63,63,63                 | 0     |
| 6   | MG   | D     | 9038 | 1/1   | 0.99 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | M     | 9261 | 1/1   | 0.96 | 0.10 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | C     | 9462 | 1/1   | 0.99 | 0.12 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | N     | 9245 | 1/1   | 0.98 | 0.12 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | M     | 9377 | 1/1   | 0.98 | 0.12 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | M     | 9469 | 1/1   | 1.00 | 0.14 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | B     | 9391 | 1/1   | 0.99 | 0.12 | -    | 27,27,27,27                 | 0     |
| 6   | MG   | D     | 9052 | 1/1   | 0.99 | 0.09 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | F     | 9197 | 1/1   | 0.99 | 0.10 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | N     | 9295 | 1/1   | 0.98 | 0.05 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | B     | 9180 | 1/1   | 0.99 | 0.09 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | C     | 9029 | 1/1   | 0.99 | 0.12 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9273 | 1/1   | 0.99 | 0.17 | -    | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | N     | 9504 | 1/1   | 0.98 | 0.10 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | F     | 9435 | 1/1   | 0.99 | 0.08 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | N     | 9376 | 1/1   | 0.99 | 0.13 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | D     | 9158 | 1/1   | 0.99 | 0.08 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | N     | 9490 | 1/1   | 0.98 | 0.12 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | N     | 9320 | 1/1   | 0.99 | 0.11 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | D     | 9548 | 1/1   | 0.97 | 0.12 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | E     | 9186 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9154 | 1/1   | 0.99 | 0.12 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | O     | 9359 | 1/1   | 0.96 | 0.08 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | D     | 9169 | 1/1   | 0.99 | 0.12 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | L     | 9471 | 1/1   | 0.99 | 0.10 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | M     | 9384 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | P     | 9333 | 1/1   | 0.99 | 0.07 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | D     | 9189 | 1/1   | 0.99 | 0.10 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | D     | 9423 | 1/1   | 0.97 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | M     | 9287 | 1/1   | 0.99 | 0.08 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | P     | 9322 | 1/1   | 0.96 | 0.12 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | L     | 9505 | 1/1   | 0.98 | 0.10 | -    | 58,58,58,58                 | 0     |
| 6   | MG   | D     | 9510 | 1/1   | 1.00 | 0.12 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | D     | 9043 | 1/1   | 1.00 | 0.11 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | L     | 9258 | 1/1   | 0.94 | 0.10 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | N     | 9527 | 1/1   | 1.00 | 0.14 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | D     | 9424 | 1/1   | 0.98 | 0.14 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | B     | 9103 | 1/1   | 0.99 | 0.09 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | N     | 9313 | 1/1   | 0.98 | 0.09 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | C     | 9439 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9368 | 1/1   | 0.99 | 0.09 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | P     | 9326 | 1/1   | 0.99 | 0.08 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | M     | 9321 | 1/1   | 0.99 | 0.13 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | L     | 9260 | 1/1   | 0.99 | 0.09 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | D     | 9519 | 1/1   | 0.99 | 0.12 | -    | 55,55,55,55                 | 0     |
| 6   | MG   | A     | 9560 | 1/1   | 0.99 | 0.13 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | C     | 9044 | 1/1   | 0.99 | 0.08 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9084 | 1/1   | 0.96 | 0.10 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | M     | 9383 | 1/1   | 0.96 | 0.09 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | C     | 9196 | 1/1   | 0.99 | 0.13 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | C     | 9205 | 1/1   | 0.99 | 0.12 | -    | 53,53,53,53                 | 0     |
| 6   | MG   | F     | 9206 | 1/1   | 0.98 | 0.12 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | M     | 9331 | 1/1   | 1.00 | 0.08 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | C     | 9127 | 1/1   | 1.00 | 0.10 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | N     | 9242 | 1/1   | 0.98 | 0.12 | -    | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | A     | 9145 | 1/1   | 0.97 | 0.11 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | B     | 9146 | 1/1   | 0.99 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | E     | 9511 | 1/1   | 1.00 | 0.12 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | D     | 9397 | 1/1   | 0.98 | 0.12 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | N     | 9319 | 1/1   | 0.98 | 0.11 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | E     | 9115 | 1/1   | 0.99 | 0.08 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | C     | 9124 | 1/1   | 0.98 | 0.08 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | D     | 9175 | 1/1   | 0.99 | 0.09 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | F     | 9010 | 1/1   | 0.97 | 0.17 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | N     | 9486 | 1/1   | 0.97 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | P     | 9329 | 1/1   | 0.99 | 0.07 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | M     | 9233 | 1/1   | 0.98 | 0.15 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | D     | 9523 | 1/1   | 0.97 | 0.11 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | C     | 9415 | 1/1   | 0.99 | 0.11 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | B     | 9395 | 1/1   | 0.98 | 0.11 | -    | 56,56,56,56                 | 0     |
| 6   | MG   | N     | 9208 | 1/1   | 0.97 | 0.12 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9375 | 1/1   | 0.99 | 0.10 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | A     | 9178 | 1/1   | 0.99 | 0.09 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | P     | 9317 | 1/1   | 0.98 | 0.18 | -    | 53,53,53,53                 | 0     |
| 6   | MG   | A     | 9411 | 1/1   | 0.99 | 0.10 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | K     | 9257 | 1/1   | 0.96 | 0.12 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | D     | 9561 | 1/1   | 0.99 | 0.06 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | A     | 9194 | 1/1   | 0.99 | 0.09 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | D     | 9416 | 1/1   | 0.99 | 0.09 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | D     | 9136 | 1/1   | 0.99 | 0.10 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | D     | 9073 | 1/1   | 0.99 | 0.15 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | N     | 9289 | 1/1   | 0.99 | 0.09 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9225 | 1/1   | 0.99 | 0.08 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | D     | 9166 | 1/1   | 0.99 | 0.08 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | B     | 9389 | 1/1   | 0.98 | 0.10 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | N     | 9352 | 1/1   | 0.99 | 0.05 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | F     | 9072 | 1/1   | 0.99 | 0.07 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | A     | 9107 | 1/1   | 0.97 | 0.07 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | C     | 9074 | 1/1   | 0.99 | 0.13 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | O     | 9355 | 1/1   | 0.99 | 0.14 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | D     | 9443 | 1/1   | 0.99 | 0.07 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | C     | 9071 | 1/1   | 0.99 | 0.13 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | D     | 9039 | 1/1   | 0.98 | 0.11 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | B     | 9137 | 1/1   | 0.99 | 0.09 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9520 | 1/1   | 0.96 | 0.14 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | D     | 9059 | 1/1   | 0.98 | 0.10 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | E     | 9187 | 1/1   | 0.99 | 0.12 | -    | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | N     | 9491 | 1/1   | 1.00 | 0.11 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | A     | 9018 | 1/1   | 0.99 | 0.14 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | D     | 9065 | 1/1   | 0.99 | 0.14 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | D     | 9454 | 1/1   | 0.99 | 0.08 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | D     | 9518 | 1/1   | 0.97 | 0.11 | -    | 55,55,55,55                 | 0     |
| 6   | MG   | E     | 9438 | 1/1   | 0.99 | 0.10 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | P     | 9274 | 1/1   | 0.99 | 0.11 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | C     | 9106 | 1/1   | 1.00 | 0.09 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9447 | 1/1   | 0.98 | 0.10 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | K     | 9363 | 1/1   | 0.97 | 0.09 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | M     | 9364 | 1/1   | 0.94 | 0.08 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | C     | 9545 | 1/1   | 0.99 | 0.10 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | C     | 9428 | 1/1   | 0.99 | 0.12 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | C     | 9081 | 1/1   | 0.97 | 0.13 | -    | 52,52,52,52                 | 0     |
| 6   | MG   | D     | 9090 | 1/1   | 0.99 | 0.11 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | F     | 9035 | 1/1   | 0.99 | 0.10 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | F     | 9153 | 1/1   | 0.98 | 0.07 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | D     | 9544 | 1/1   | 0.99 | 0.11 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | L     | 9271 | 1/1   | 0.99 | 0.09 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | B     | 9033 | 1/1   | 0.99 | 0.10 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | F     | 9429 | 1/1   | 0.98 | 0.12 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | N     | 9316 | 1/1   | 0.99 | 0.09 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | N     | 9354 | 1/1   | 0.95 | 0.07 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | F     | 9030 | 1/1   | 1.00 | 0.11 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9476 | 1/1   | 0.99 | 0.06 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | D     | 9099 | 1/1   | 0.98 | 0.07 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | C     | 9063 | 1/1   | 0.98 | 0.10 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | D     | 9516 | 1/1   | 0.98 | 0.05 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | D     | 9140 | 1/1   | 0.98 | 0.13 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | N     | 9470 | 1/1   | 1.00 | 0.15 | -    | 27,27,27,27                 | 0     |
| 6   | MG   | C     | 9014 | 1/1   | 0.98 | 0.14 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | D     | 9119 | 1/1   | 0.99 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | N     | 9281 | 1/1   | 0.98 | 0.09 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | L     | 9249 | 1/1   | 0.97 | 0.07 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | A     | 9102 | 1/1   | 0.98 | 0.09 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | M     | 9268 | 1/1   | 0.99 | 0.11 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | M     | 9385 | 1/1   | 0.99 | 0.10 | -    | 29,29,29,29                 | 0     |
| 6   | MG   | C     | 9130 | 1/1   | 0.99 | 0.14 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | L     | 9345 | 1/1   | 0.99 | 0.12 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | D     | 9460 | 1/1   | 0.99 | 0.14 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | C     | 9190 | 1/1   | 0.96 | 0.07 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | F     | 9513 | 1/1   | 0.99 | 0.14 | -    | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | D     | 9096 | 1/1   | 0.97 | 0.14 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | N     | 9538 | 1/1   | 0.92 | 0.10 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | N     | 9291 | 1/1   | 0.99 | 0.15 | -    | 55,55,55,55                 | 0     |
| 6   | MG   | M     | 9348 | 1/1   | 0.97 | 0.11 | -    | 63,63,63,63                 | 0     |
| 6   | MG   | O     | 9209 | 1/1   | 0.97 | 0.11 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9060 | 1/1   | 0.99 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9310 | 1/1   | 0.98 | 0.08 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | D     | 9091 | 1/1   | 0.99 | 0.14 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | F     | 9525 | 1/1   | 0.99 | 0.08 | -    | 54,54,54,54                 | 0     |
| 6   | MG   | N     | 9555 | 1/1   | 0.97 | 0.11 | -    | 56,56,56,56                 | 0     |
| 6   | MG   | D     | 9425 | 1/1   | 0.99 | 0.09 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | C     | 9396 | 1/1   | 0.98 | 0.14 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | M     | 9290 | 1/1   | 0.98 | 0.12 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | N     | 9247 | 1/1   | 0.97 | 0.08 | -    | 29,29,29,29                 | 0     |
| 6   | MG   | N     | 9270 | 1/1   | 0.99 | 0.13 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | N     | 9308 | 1/1   | 1.00 | 0.12 | -    | 31,31,31,31                 | 0     |
| 6   | MG   | M     | 9489 | 1/1   | 0.99 | 0.09 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | O     | 9337 | 1/1   | 1.00 | 0.08 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | A     | 9126 | 1/1   | 0.99 | 0.10 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | N     | 9324 | 1/1   | 0.99 | 0.08 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | N     | 9468 | 1/1   | 1.00 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9524 | 1/1   | 0.99 | 0.08 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | D     | 9125 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | A     | 9200 | 1/1   | 0.99 | 0.10 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | N     | 9360 | 1/1   | 1.00 | 0.05 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | N     | 9262 | 1/1   | 0.98 | 0.14 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | C     | 9193 | 1/1   | 0.99 | 0.09 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | M     | 9373 | 1/1   | 0.99 | 0.12 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | D     | 9432 | 1/1   | 0.98 | 0.10 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | E     | 9402 | 1/1   | 0.99 | 0.12 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | M     | 9497 | 1/1   | 0.99 | 0.12 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | L     | 9479 | 1/1   | 0.99 | 0.10 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | M     | 9211 | 1/1   | 0.98 | 0.10 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | D     | 9019 | 1/1   | 0.98 | 0.15 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9068 | 1/1   | 0.95 | 0.12 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | F     | 9133 | 1/1   | 0.99 | 0.10 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | D     | 9111 | 1/1   | 0.96 | 0.09 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | K     | 9493 | 1/1   | 0.99 | 0.09 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | D     | 9066 | 1/1   | 0.97 | 0.11 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | F     | 9410 | 1/1   | 0.94 | 0.12 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | M     | 9276 | 1/1   | 0.98 | 0.14 | -    | 54,54,54,54                 | 0     |
| 6   | MG   | B     | 9199 | 1/1   | 0.95 | 0.10 | -    | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | B     | 9419 | 1/1   | 0.98 | 0.11 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | B     | 9079 | 1/1   | 0.98 | 0.11 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | M     | 9485 | 1/1   | 0.98 | 0.06 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | D     | 9041 | 1/1   | 0.98 | 0.10 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | D     | 9070 | 1/1   | 0.99 | 0.10 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | N     | 9228 | 1/1   | 0.98 | 0.08 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | C     | 9408 | 1/1   | 0.99 | 0.12 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | K     | 9492 | 1/1   | 0.99 | 0.10 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | A     | 9173 | 1/1   | 0.99 | 0.10 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | N     | 9343 | 1/1   | 0.99 | 0.09 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | N     | 9237 | 1/1   | 0.99 | 0.14 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | L     | 9483 | 1/1   | 0.97 | 0.15 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | B     | 9442 | 1/1   | 0.99 | 0.12 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | M     | 9293 | 1/1   | 0.98 | 0.11 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | N     | 9386 | 1/1   | 0.99 | 0.08 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | A     | 9522 | 1/1   | 0.98 | 0.11 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | L     | 9374 | 1/1   | 0.99 | 0.09 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | D     | 9459 | 1/1   | 0.99 | 0.10 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | D     | 9009 | 1/1   | 0.98 | 0.12 | -    | 53,53,53,53                 | 0     |
| 6   | MG   | D     | 9082 | 1/1   | 0.99 | 0.11 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | P     | 9284 | 1/1   | 0.97 | 0.10 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | C     | 9177 | 1/1   | 0.96 | 0.09 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | M     | 9557 | 1/1   | 0.98 | 0.09 | -    | 54,54,54,54                 | 0     |
| 6   | MG   | N     | 9554 | 1/1   | 0.97 | 0.11 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | C     | 9458 | 1/1   | 0.98 | 0.09 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | N     | 9253 | 1/1   | 0.96 | 0.08 | -    | 39,39,39,39                 | 0     |
| 6   | MG   | L     | 9213 | 1/1   | 0.98 | 0.23 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | N     | 9357 | 1/1   | 0.99 | 0.09 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | C     | 9076 | 1/1   | 0.98 | 0.11 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9152 | 1/1   | 0.97 | 0.11 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | D     | 9142 | 1/1   | 0.99 | 0.11 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | M     | 9252 | 1/1   | 0.99 | 0.12 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9104 | 1/1   | 0.98 | 0.09 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | D     | 9433 | 1/1   | 0.99 | 0.12 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | D     | 9051 | 1/1   | 0.99 | 0.07 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | N     | 9315 | 1/1   | 0.98 | 0.11 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | L     | 9532 | 1/1   | 0.98 | 0.08 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | A     | 9413 | 1/1   | 0.96 | 0.10 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | D     | 9132 | 1/1   | 0.99 | 0.10 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | K     | 9507 | 1/1   | 0.99 | 0.14 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | N     | 9341 | 1/1   | 0.98 | 0.13 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | M     | 9473 | 1/1   | 0.97 | 0.11 | -    | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | D     | 9006 | 1/1   | 1.00 | 0.14 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | P     | 9239 | 1/1   | 1.00 | 0.11 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | D     | 9034 | 1/1   | 0.98 | 0.16 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | O     | 9362 | 1/1   | 0.98 | 0.04 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | K     | 9496 | 1/1   | 0.99 | 0.09 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | N     | 9294 | 1/1   | 0.99 | 0.07 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | B     | 9148 | 1/1   | 0.98 | 0.15 | -    | 54,54,54,54                 | 0     |
| 6   | MG   | M     | 9369 | 1/1   | 0.99 | 0.09 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | N     | 9302 | 1/1   | 1.00 | 0.14 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | M     | 9222 | 1/1   | 0.99 | 0.09 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | L     | 9236 | 1/1   | 0.99 | 0.08 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | C     | 9204 | 1/1   | 0.99 | 0.12 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | C     | 9160 | 1/1   | 1.00 | 0.12 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | N     | 9551 | 1/1   | 0.97 | 0.08 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | D     | 9138 | 1/1   | 0.99 | 0.12 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | N     | 9338 | 1/1   | 0.98 | 0.12 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | K     | 9279 | 1/1   | 0.99 | 0.11 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | P     | 9388 | 1/1   | 0.99 | 0.08 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | A     | 9404 | 1/1   | 1.00 | 0.16 | -    | 55,55,55,55                 | 0     |
| 6   | MG   | E     | 9184 | 1/1   | 0.97 | 0.16 | -    | 48,48,48,48                 | 0     |
| 6   | MG   | D     | 9134 | 1/1   | 0.99 | 0.10 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | K     | 9484 | 1/1   | 0.98 | 0.11 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | C     | 9183 | 1/1   | 0.98 | 0.16 | -    | 44,44,44,44                 | 0     |
| 6   | MG   | M     | 9535 | 1/1   | 0.99 | 0.12 | -    | 40,40,40,40                 | 0     |
| 6   | MG   | M     | 9332 | 1/1   | 0.97 | 0.13 | -    | 54,54,54,54                 | 0     |
| 6   | MG   | M     | 9537 | 1/1   | 0.99 | 0.13 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | D     | 9108 | 1/1   | 0.98 | 0.11 | -    | 51,51,51,51                 | 0     |
| 6   | MG   | D     | 9118 | 1/1   | 0.99 | 0.12 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | D     | 9085 | 1/1   | 0.99 | 0.10 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | F     | 9167 | 1/1   | 0.98 | 0.12 | -    | 59,59,59,59                 | 0     |
| 6   | MG   | M     | 9488 | 1/1   | 0.98 | 0.12 | -    | 42,42,42,42                 | 0     |
| 6   | MG   | K     | 9351 | 1/1   | 0.97 | 0.09 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | C     | 9390 | 1/1   | 1.00 | 0.12 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | B     | 9176 | 1/1   | 1.00 | 0.09 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | A     | 9109 | 1/1   | 0.98 | 0.09 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | D     | 9061 | 1/1   | 0.99 | 0.11 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | M     | 9350 | 1/1   | 0.98 | 0.09 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | D     | 9195 | 1/1   | 1.00 | 0.08 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | P     | 9269 | 1/1   | 0.99 | 0.09 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | L     | 9378 | 1/1   | 0.98 | 0.14 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | F     | 9448 | 1/1   | 0.98 | 0.10 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | N     | 9482 | 1/1   | 0.99 | 0.14 | -    | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 6   | MG   | D     | 9464 | 1/1   | 0.99 | 0.12 | -    | 38,38,38,38                 | 0     |
| 6   | MG   | C     | 9426 | 1/1   | 0.99 | 0.06 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | M     | 9500 | 1/1   | 0.99 | 0.09 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | P     | 9494 | 1/1   | 0.99 | 0.10 | -    | 50,50,50,50                 | 0     |
| 6   | MG   | N     | 9552 | 1/1   | 0.99 | 0.11 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | N     | 9292 | 1/1   | 0.98 | 0.16 | -    | 52,52,52,52                 | 0     |
| 6   | MG   | D     | 9114 | 1/1   | 0.99 | 0.10 | -    | 32,32,32,32                 | 0     |
| 6   | MG   | C     | 9198 | 1/1   | 0.99 | 0.11 | -    | 36,36,36,36                 | 0     |
| 6   | MG   | M     | 9309 | 1/1   | 0.98 | 0.15 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9406 | 1/1   | 0.98 | 0.10 | -    | 47,47,47,47                 | 0     |
| 6   | MG   | N     | 9539 | 1/1   | 0.97 | 0.10 | -    | 57,57,57,57                 | 0     |
| 6   | MG   | C     | 9192 | 1/1   | 0.97 | 0.10 | -    | 55,55,55,55                 | 0     |
| 6   | MG   | L     | 9556 | 1/1   | 0.98 | 0.09 | -    | 58,58,58,58                 | 0     |
| 6   | MG   | D     | 9392 | 1/1   | 0.99 | 0.09 | -    | 46,46,46,46                 | 0     |
| 6   | MG   | N     | 9250 | 1/1   | 0.95 | 0.16 | -    | 61,61,61,61                 | 0     |
| 6   | MG   | A     | 9412 | 1/1   | 0.99 | 0.12 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | B     | 9040 | 1/1   | 0.99 | 0.16 | -    | 29,29,29,29                 | 0     |
| 6   | MG   | M     | 9229 | 1/1   | 0.98 | 0.09 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | C     | 9399 | 1/1   | 0.96 | 0.10 | -    | 43,43,43,43                 | 0     |
| 6   | MG   | D     | 9093 | 1/1   | 0.99 | 0.11 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | N     | 9306 | 1/1   | 0.99 | 0.13 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | N     | 9339 | 1/1   | 0.99 | 0.11 | -    | 34,34,34,34                 | 0     |
| 6   | MG   | C     | 9400 | 1/1   | 0.99 | 0.12 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | D     | 9064 | 1/1   | 0.99 | 0.11 | -    | 41,41,41,41                 | 0     |
| 6   | MG   | D     | 9188 | 1/1   | 0.99 | 0.09 | -    | 37,37,37,37                 | 0     |
| 6   | MG   | K     | 9495 | 1/1   | 0.99 | 0.10 | -    | 35,35,35,35                 | 0     |
| 6   | MG   | M     | 9243 | 1/1   | 0.98 | 0.11 | -    | 45,45,45,45                 | 0     |
| 6   | MG   | F     | 9461 | 1/1   | 0.97 | 0.12 | -    | 52,52,52,52                 | 0     |
| 6   | MG   | F     | 9080 | 1/1   | 0.99 | 0.12 | -    | 30,30,30,30                 | 0     |
| 6   | MG   | N     | 9232 | 1/1   | 0.98 | 0.10 | -    | 33,33,33,33                 | 0     |
| 6   | MG   | C     | 9022 | 1/1   | 0.99 | 0.12 | -    | 28,28,28,28                 | 0     |
| 6   | MG   | A     | 9165 | 1/1   | 0.98 | 0.11 | -    | 65,65,65,65                 | 0     |
| 6   | MG   | C     | 9409 | 1/1   | 0.99 | 0.12 | -    | 49,49,49,49                 | 0     |
| 6   | MG   | N     | 9288 | 1/1   | 0.98 | 0.10 | -    | 33,33,33,33                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.