|  |
| --- |
|  **Table 1** Data-collection and [refinement statistics](http://reference.iucr.org/dictionary/Statistics) |
|  Values in parentheses are for the outer shell. |
|  **Data Collection**  | **LtgA**  |  |  |  |  |
|  |  |  |  |  |  |
|  Data collection |
|    Wavelength (Å) | 0.9795 |  |  |  |  |
|    Resolution range (Å) | 49.84-1.98 (2.067-1.995) |  |  |  |  |
|    Space group | *P212121* |  |  |  |  |
|    Unit-cell parameters |
|     *a* (Å) | 66.82 |  |  |  |  |
|     *b* (Å) | 72.25 |  |  |  |  |
|     *c* (Å) | 122.31 |  |  |  |  |
|      (°), (°), (°) | 90 |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|    Total reflections | 299848 |  |  |  |  |
|    Unique reflections | 40499 |  |  |  |  |
|    Multiplicity | 7.4 (7.4) |  |  |  |  |
|    Completeness (%) | 98.63 (94.17) |  |  |  |  |
|    Mean *I*/(*I*) | 16.40 (1.47) |  |  |  |  |
|   Wilson *B* factor (Å2) | 43.22 |  |  |  |  |
|    *R*merge[#](http://onlinelibrary.wiley.com/iucr/doi/10.1107/S1399004714000911/mn5048bdy.html#TFN1) | 0.055 (0.063) |  |  |  |  |
|  Refinement |
|    *R* factor[+](http://onlinelibrary.wiley.com/iucr/doi/10.1107/S1399004714000911/mn5048bdy.html#TFN2) | 0.1929(0.3192) |  |  |  |  |
|    *R*free | 0.2464(0.3645) |  |  |  |  |
|    No. of atoms | 4661 |  |  |  |  |
|    No. of waters | 271 |  |  |  |  |
|    No. of protein residues | 563 |  |  |  |  |
|    R.m.s.d., bonds (Å) | 0.007 |  |  |  |  |
|    R.m.s.d., angles (°) | 0.96 |  |  |  |  |
|    Ramachandran favored (%) | 98 |  |  |  |  |
|    Ramachandran outliers (%) | 0 |  |  |  |  |
|    *B* factors (Å2) |
|     Average | 51.00 |  |  |  |  |
|     Macromolecules | 50.80 |  |  |  |  |
|     Ligand  Solvent All-atom clash score  | -------54.602.09 |  |  |  |  |
|   |  |  |  |  |  |
|  |

†*R*merge = ΣhklΣi∣*I*i(*hkl*) −〈*I* (*hkl*)〉∣/ΣhklΣI *I* (*hkl*)

‡*R*factor = Σhkl |∣*F* obs − *F* calc∣|/Σhkl |*F* obs|

*\*R*free was computed identically except that all reflections belonged to a test set consisting of a 10% random selection of the data.