**Figure 2 – source data.**

**Data collection and refinement statistics of Rh5 and Rh5\_KI.**

|  |  |  |
| --- | --- | --- |
|  | Native | KI Derivative |
| **Data collection** |  |  |
| Space group | P212121 | P212121 |
| Cell dimensions |  |  |
| *a*, *b*, *c* (Å) | 53.98, 86.26, 114.83 |  |
| Resolution (Å) | 50-2.18 (2.21-2.18) | 50-3.46(3.74-3.46) |
| *R*merge (%) | 35.2 (530.8) | 32 (100.9) |
| *<I* / *I>* | 5.44 (0.52**)** | 7.87 (3.47) |
| Completeness (%) | 99.9 (99.9) | 100 (100) |
| Redundancy | 7.2 (7.3) | 4.8 (4.3) |
| *CC*1/2\* | 99.3 (16.4) | 97.6 (76.5) |
| **Ano**  Centric phasing power#  Acentric phasing power  Number of sites  **Refinement** | **-** | 0.956 (1.020)  0.57  0.73  3 |
| Resolution (Å) | 45.76-2.18 (2.26-2.18) |
| No. reflections | 28698/1454 |
| *R*work / *R*free | 20.0/24.5 (27.1/29.0) |
| No. atoms |  |
| Protein  Carbohydrate | 2822  14 |
| Ligand/ion | 5 |
| Water | 82 |
| *B*-factors (Å)2 |  |
| Protein  Carbohydrate | 58.9  67.9 |
| Ligand/ion | 67.9 |
| Water | 43.7 |
| R.m.s. deviations |  |  |
| Bond lengths (Å) | 0.009 |
| Bond angles ()  Ramachandran plot ( % )  Most favoured  Allowed  Outlier | 1.06  97.0  2.7  0.3 |  |

\* *CC*(1/2) = Pearson correlation coefficient between independently merged halves of the data set ([1](#_ENREF_1)). Highest resolution shell *CC*(1/2) values are significant at the *p* = 0.001 level.

#SIR resolution range (Å): 3.61 – 11.16

1. Karplus PA & Diederichs K (2012) Linking crystallographic model and data quality. *Science* 336(6084):1030-1033.