

Supplemental information

Analysis of the diverse antigenic landscape of the malaria protein RH5 identifies a potent vaccine-induced human public antibody clonotype

Jordan R. Barrett, Dimitra Pipini, Nathan D. Wright, Andrew J.R. Cooper, Giacomo Gorini, Doris Quinkert, Amelia M. Lias, Hannah Davies, Cassandra A. Rigby, Maya Aleshnick, Barnabas G. Williams, William J. Bradshaw, Neil G. Paterson, Thomas Martinson, Payton Kirtley, Luc Picard, Christine D. Wiggins, Francesca R. Donnellan, Lloyd D.W. King, Lawrence T. Wang, Jonathan F. Popplewell, Sarah E. Silk, Jed de Ruiter Swain, Katherine Skinner, Vinayaka Kotraiah, Amy R. Noe, Randall S. MacGill, C. Richter King, Ashley J. Birkett, Lorraine A. Soisson, Angela M. Minassian, Douglas A. Lauffenburger, Kazutoyo Miura, Carole A. Long, Brandon K. Wilder, Lizbé Koekemoer, Joshua Tan, Carolyn M. Nielsen, Kirsty McHugh, and Simon J. Draper

SUPPLEMENTAL TABLE

Table S1. Diffraction data collection and refinement statistics; related to Figures 4 and 6.

| | RH5ΔNL:R5.034 | RH5ΔNL:R5.251 |
|----------------------------------|---------------------------|----------------------------|
| PDB code | 8QKS | 8QKR |
| DATA COLLECTION | | |
| Wavelength (Å) | 0.99987 | 0.976 |
| Space group | P 1 2 1 | P 1 |
| Cell dimensions | | |
| a, b, c (Å) | 82.26, 376.79, 226.82, | 70.51, 92.58, 92.83, |
| α, β, γ (°) | 90.00, 90.06, 90.00 | 60.69, 72.11, 79.75 |
| Resolution range | 65.60 - 3.99 (3.99 -3.99) | 59.53 - 2.00 (3.23 – 3.23) |
| Total observation | 779 885 (30 383) | 111 799 (5 486) |
| Unique reflections | 115 245 (5 241) | 30 110 (1 432) |
| R pim (%) | 0.176 (2.963) | 0.21 (1.17) |
| R merge (%) | 0.422 (6.530) | 0.35 (1.98) |
| R meas (%) | 0.458 (7.198) | 0.41 (2.30) |
| CC_{1/2} | 0.993 (0.220) | 3.1 (0.4) |
| I / σ(I) | 2.7 (0.1) | 98.6 (90.3) |
| Completeness (%) | 99.0 (90.0) | 3.7 (3.8) |
| Multiplicity | 6.8 (5.8) | 52.670 |
| Wilson B-factor | 120.1 | 67.9 |
| REFINEMENT | | |
| Reflections in refinement | 115131 | 131374 |
| Reflections in free set | 1918 | 6552 |
| R_{work} | 0.446 | 0.254 |
| R_{free} | 0.465 | 0.327 |
| RMSD bonds | 0.0073 | 0.0039 |
| RMSD angles | 1.910 | 1.314 |
| Ramachandran favoured (%) | 85.3 | 82.8 |
| Ramachandran allowed (%) | 11.2 | 12.9 |
| Ramachandran outliers (%) | 3.5 | 4.4 |
| Rotamer outliers | 10 | 7.9 |
| Clash score | 4.8 | 19.6 |
| MolProbity score | 2.66 | 3.17 |