

Supplementary Table 1. Crystallographic data collection and refinement statistics.

Protein	441D6 Fab
PDB accession code	5TR8
Data collection	
Space group	C2
Cell constants	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	98.5, 83.3, 83.2
<i>a</i> , <i>b</i> , <i>g</i> (°)	90.0, 105.7, 90.0
Wavelength (Å)	1.00
Resolution (Å)	50.0-2.0 (2.07-2.00)
<i>R</i> _{merge}	11.6 (73.1)
<i>I</i> / <i>sI</i>	7.6 (1.5)
Completeness (%)	98.5 (94.4)
Redundancy	3.1 (2.3)
Refinement	
Resolution (Å)	24.6-2.01 (2.06-2.01)
Unique reflections	41926 (2138)
<i>R</i> _{work} / <i>R</i> _{free} (%)	17.8/19.9
No. atoms	
Protein	3330
Ligand/ion	10
Water	237
<i>B</i> -factors (Å ²)	
Protein	52.2
Ligand/ion	68.0
Water	58.1
R.m.s. deviations	
Bond lengths (Å)	0.007
Bond angles (°)	1.011
Ramachandran	
Most favored regions (%)	97.4
Additional allowed regions (%)	2.6
Disallowed regions (%)	0.0

Values in parentheses are for highest-resolution shell. The structure has been deposited in the PDB.