

Table 1 Data collection and refinement statistics

	HRUclD ^{LD} (5NWP)	UclD ^{LD} (5VQ5)
Data collection		
Space group	P2 ₁	P2 ₁ 2 ₁ 2 ₁
Cell dimensions		
<i>a, b, c</i> (Å)	31.0, 91.9, 64.9	39.0, 58.6, 175.1
α, β, γ (°)	90.0, 96.5, 90.0	90.0, 90.0, 90.0
Resolution (Å) ^a	91.87 – 1.05 (1.11- 1.05)	55.60-1.6 (1.66- 1.60)
<i>R</i> _{merge} ^a	0.079 (0.336)	0.05 (0.43)
<i>I</i> / σ (<i>I</i>) ^a	11.9 (2.1)	17.68 (1.43)
<i>CC</i> _{1/2} ^a	99.6 (86.0)	0.998 (0.659)
Completeness (%) ^a	88.6 (43.8)	99.97 (99.98)
Redundancy ^a	5.0 (2.0)	2.0 (2.0)
Refinement		
Resolution (Å)	91.87 - 1.05	55.60 - 1.60
No. reflections	144393	108142
<i>R</i> _{work} / <i>R</i> _{free}	0.118 / 0.143	0.172 / 0.218
No. atoms	6890	3289
Protein	6223	2804
Iodide	/	6
Sulphate	1	/
Water	662	479
<i>B</i> factors		
Protein	10.7	22.4
Iodide	/	62.6
Sulphate	11.0	/
Water	23.9	36.2
R.m.s. deviations		
Bond lengths (Å)	0.028	0.002
Bond angles (°)	2.281	0.58

Number of crystals for each structure should be noted in footnote.

^a Values in parentheses are for highest-resolution shell.