

Table 2. Crystallographic data statistics

	Native (oligomannose)	Native (complex-sugar)	SeMet λ.peak (oligomannose)
Data Collection			
Space group	<i>P</i> 4 ₁ 2 ₁ 2	<i>P</i> 4 ₁ 2 ₁ 2	<i>P</i> 4 ₁ 2 ₁ 2
Unit cell <i>a=b, c</i> (Å)	134.09, 100.75	134.55, 99.24	134.27, 99.99
Wavelength (Å)	0.9780	1.0000	0.9790
Resolution (Å)	30-2.6 (2.69-2.6)	30-3.0 (3.11-3.0)	30-2.65 (2.74-2.65)
<i>R</i> _{sym} *	0.080 (0.644)	0.094 (0.388)	0.095 (0.636)
<i>I</i> / <i>σI</i>	11.6 (4.3)	9.4 (5.11)	10.9 (4.34)
Completeness (%)	99.2 (99.9)	99.6 (98.1)	100 (100)
Redundancy	12.1 (12.2)	7.0 (6.4)	6.7 (6.7)
Refinement			
Resolution (Å)	30-2.6	30-3.0	
No. reflections	28,599	18,688	
<i>R</i> _{work} / <i>R</i> _{free} †	0.225 / 0.248	0.227 / 0.271	
No. atoms			
Protein	3,277	3,242	
Ligand/ion	42	28	
Water	73	0	
B-factors (Å ²)			
Protein	51.87	58.74	
Ligand/ion	94.19	88.83	
Water	38.48	-	
R.m.s deviations			
Bond lengths (Å)	0.0066	0.0077	
Bond angles (°)	1.3697	1.4622	
Ramachandran plot			
Most favored	290	286	
Additional allowed	63	60	
Generously allowed	7	10	
Disallowed	0	1 (Q311)	

Highest-resolution shell is shown in parentheses.

* $R_{\text{sym}} = \sum |I_i - \langle I_i \rangle| / \sum I_i$, where I_i is the observed intensity and $\langle I_i \rangle$ is the average intensity obtained from multiple observations of symmetry-related reflections.

† $R_{\text{work}} = \sum_{hkl} ||F_{\text{obs}}| - |F_{\text{calc}}|| / \sum_{hkl} |F_{\text{obs}}|$. 7% of the reflections were excluded for R_{free} calculation.