

Supplementary information

VISTA is an acidic pH-selective ligand for PSGL-1

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Table 1 Data collection and refinement statistics

	VISTA + VISTA.18
Data collection	
Space group	I2 ₁ 2 ₁ 2 ₁
Cell dimensions	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	66.17, 125.86, 192.04
α , β , γ (°)	90.0, 90.0, 90.0
Resolution (Å)	1.61–96.02 (1.61–1.81)*
<i>R</i> _{sym} or <i>R</i> _{merge}	0.049 (0.724)
<i>I</i> / σI	18.75 (2.17)
<i>CC</i> _{1/2}	1.00 (0.743)
Completeness (%)	88.6 (73.9)
Redundancy	6.46 (5.57)
Refinement	
Resolution (Å)	1.61–96.02 (1.61–1.73)
No. reflections	55883 (1063)
<i>R</i> _{work} / <i>R</i> _{free}	18.2 / 22.4 (24.3 / 25.8)
No. atoms	
Protein	4281
Ligand/ion	84
Water	758
<i>B</i> -factors	
Protein	33.97
Ligand/ion	82.40
Water	42.13
R.m.s. deviations	
Bond lengths (Å)	0.008
Bond angles (°)	1.07
Ramachandran statistics (%)	
Residues in most favored regions	97.11
Residues in additionally allowed regions	2.71

*Values in parentheses are for highest-resolution shell.