

Alteromonas haloplanctis (psychrophilic) α -amylase

Diffraction data and refinement statistics for the ternary complexes of AHA/Tris with acarbose (pseudo tetra-saccharide and component II (pseudo tri-saccharide))

PDBCODE: 1G94 (complex with acarbose) 1G9H (complex with comp. II)

	acarbose	comp. II
Space group	C222 ₁	C222 ₁
Cell dimensions, Å	a=71.01	a=71.33
	b=139.96	b=138.68
	c=115.89	c=114.81
Measurements, <i>n</i>	110412	72535
Unique reflections	45586	43621
Resolution, Å	1.74	1.80
Completeness, %	76.6	82.2
Compl. outermost shell, %	34.8	54.2
R _{merge} , %	5.6	6.2
I/ σ (I) > 2, %	92.8	91.7
I/ σ (I) > 2 outermost shell, %	80.1	89.1
R _{factor} , %	15.64	16.80
R _{free} , %	18.73	20.09
rms deviation from ideal bond length, Å	0.007	0.008
rms deviation from ideal bond angle, °	1.66	1.60
Amino acid residues, <i>n</i>	448	448
Calcium ions	1	1
Chloride ions	1	1
Water molecules	285	274

An article describing a part of these data is submitted (Authors: N. Aghajari, M. Roth & R. Haser)

A second one is in preparation.