

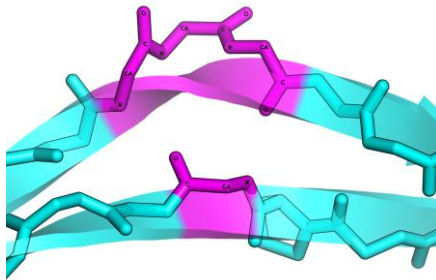
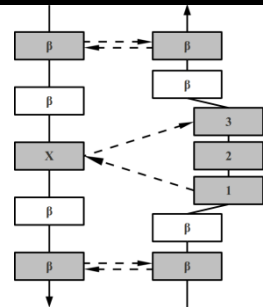
Table I. *β -bulge type definition.* In the hydrogen bonding patterns diagram, directional arrows represent oriented β -strands, squares represent residues in β -strands, oval represent residues out of β -strands, and same colour residues have their side chains pointing in the same direction. As all β -bulge types (except Bent) could be divided in sub-categories, only the most representative hydrogen bonding pattern of the classes have been presented (*See Chan, Hutchinson, Harris and Thornton (Prot Sci, 1993), for frequencies and details on sub-types.*)

β -bulge type	(A)ntiparallel / (P)arallel	Hydrogen bonding patterns	3D conformation examples	Characteristics
CLASSIC	AC			<p>The conformation of residue 1 is nearly α_R-helical.</p> <p>Residues 2 and X are close to the extended β conformation.</p> <p>All three residues have their side chains pointing in the same direction.</p>
	PC			<p>In parallel β-strands, the position 2 adopts the α_R-helical conformation and position 1 and X are in β conformation. In this case, the side chains of residues 1 and 2 point to opposite directions</p>
G1	AG			<p>Residue 1 is often a Glycine with dihedral angles in α_L region.</p> <p>The hydrogen-bonding pattern is similar to</p>

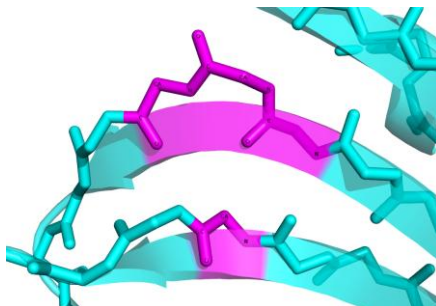
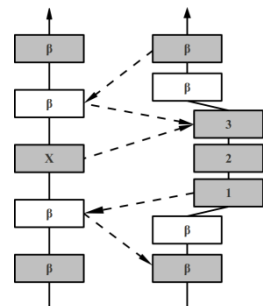
				that of the Classic β -bulges, except that residue 1 is always at the beginning of the β -strand (or at the end of a loop).
				The G1 β -bulge occurs only between anti parallel β -strands.
W I D E	AW			Wide β -bulge occurs between the widely spaced pairs of hydrogen bonds. As the residues 1 and 2 are not involved in any main-chain bonding they can adopt many different conformations.
	PW			
B E N T	AB			In anti-parallel case the residues conformations are either α_L - α_R or α_R - α_L .
	PB			In parallel case the conformation of both residues is α_R ;

S
P
E
C
I
A
L

AS



PS



Special β -bulges are very similar to the classic type, but with more than two inserted residues in the bulged strand.