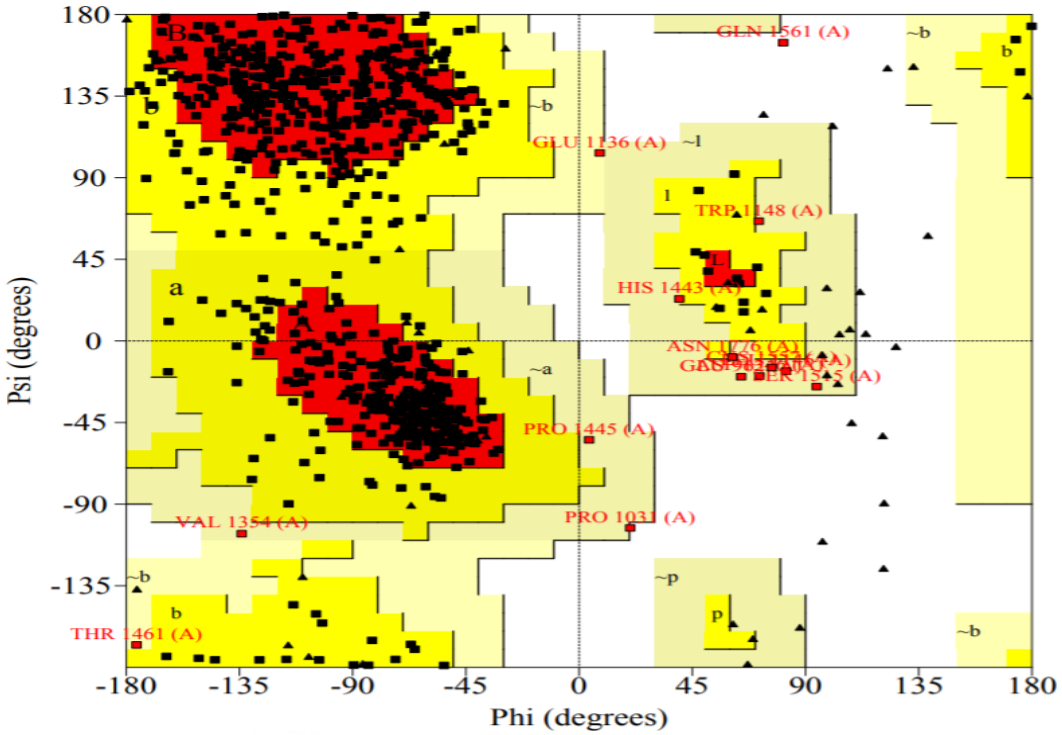
Supporting Information: 'A Search for Novel Antidiabetic Agents Using Ligand-Based Drug Design and Molecular Docking Studies Employing Human Intestinal Maltase-Glucoamylase as Model Enzyme'

Table 6. H-Bond interactions and other amino acid residues of the lead, designed compounds and acarbose against MGAM-C protein

Compounds	*H-bond*	*Carbon-H bond*	*π-Sulfur*	*Alkyl*	*π- Alkyl*	*π-π T-shaped*	*Halogen*	*π-π Stacked*	*π-Donor H-bond*
Lead compound	Tyr1251 Trp1369 Thr1586	-	-	-	-	-	Asp1562	Trp1355	Gln1561
C1	Trp1369 Ile1587	-	Trp1355 Phe1560	Ile1587.	Phe1560	Tyr1251 Phe1559	Asp1562	-	-
C2	Tyr1251 Trp1355	Gly1365 Gly1365	Phe1560	Ile1587.	Trp1355Trp1369 Ile1587.	Trp1355 Phe1559	-	-	-
C3	Thr1586	-	Phe1560	-	Trp1369	Tyr1251 Trp1355 Phe1559	-	-	-
C4	Gln1372 Arg1377 Thr1586	Gly1365	Phe1559 Phe1560	Val1363	Trp1355Trp1369	Tyr1251Trp1355 Phe1559	-	-	-
Acarbose	Lys1460 Asp1357 Gln1372 Tyr1251 Asp1157 Asp1526	Pro1159 Asp1357	-	-	Trp1369	-	-	-	-



Residues in most favoured regions [A,B,L]	613	79.9%
Residues in additional allowed regions [a,b,l,p]	142	18.5%
Residues in generously allowed regions [~a,~b,~l,~p]	11	1.4%
Residues in disallowed regions	1	0.1%
Number of non-glycine and non-proline residues	767	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	64	
Number of proline residues	57	
Total number of residues	890	

Figure 5. General structural evaluation of the MGAM-C with/without the design compounds