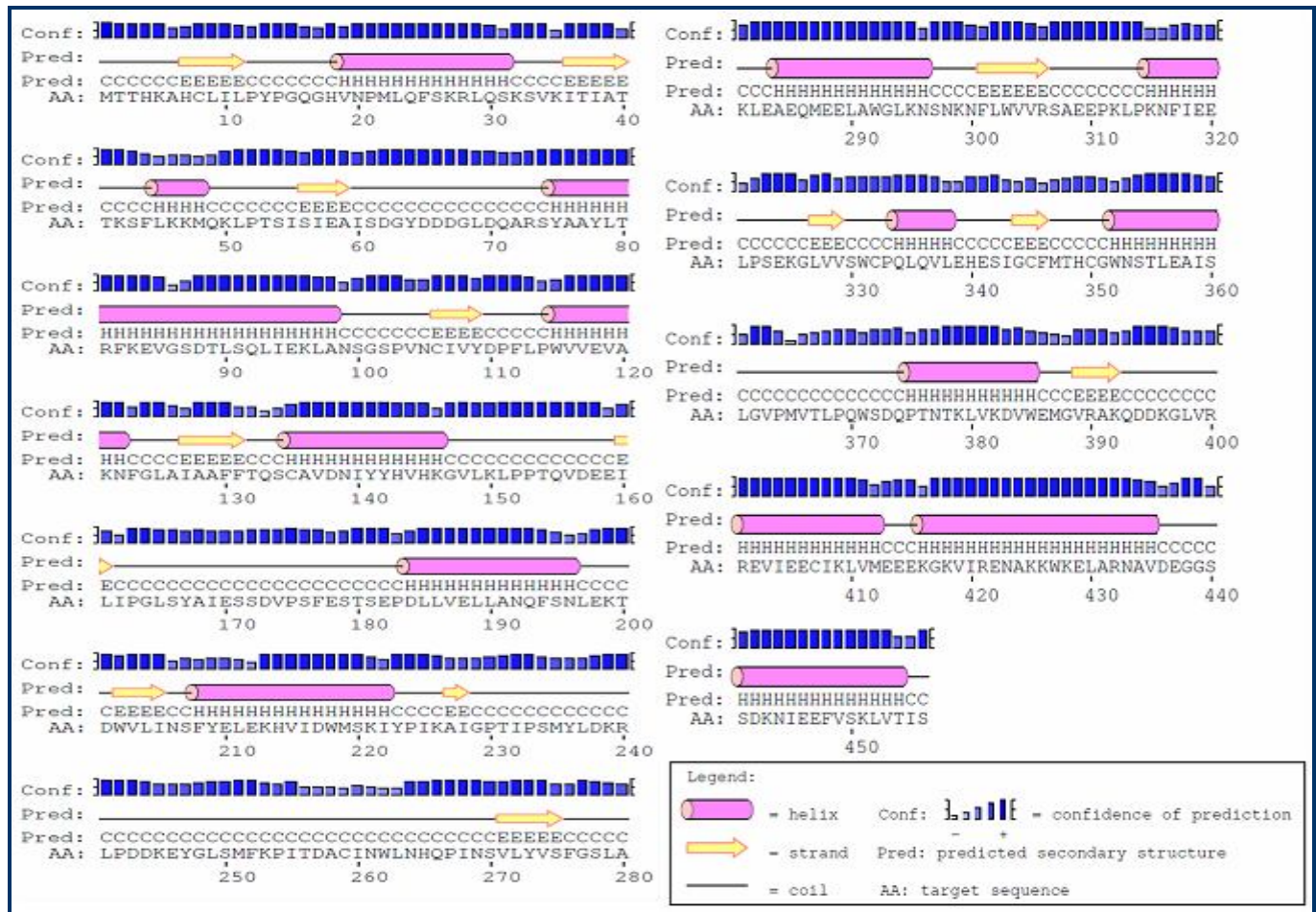# BIOINFORMATION

Supplementary material:

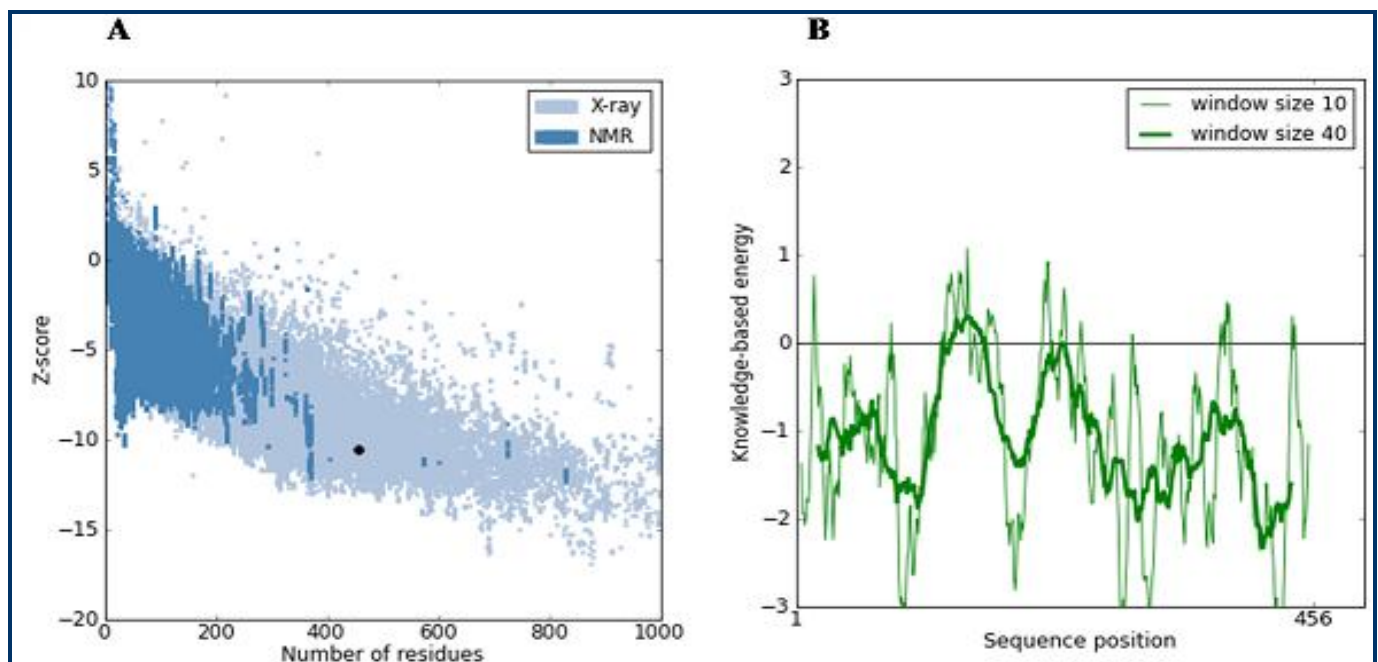**Figure S1:** Predicted secondary structure of WsFGT protein

Figure S2: (A) The plan of Z-Score shows spot of Z score's value of protein determined by NMR (represented in dark blue colour) and by X-ray (represented in light blue colour) using ProSAII program. The black dot represents Z-Score of the model; **(B)** Energy plot obtained from ProSAII.

Table 1: Ramachandran plot statistics for 3D model of WsFGT

Residues in quadrangles	Scattered residues	
	Number	**Percentage**
Most favoured regions [A, B, L]	373	91.6
Additional allowed regions [a,b,l,p]	34	8.4
Generously allowed regions [~a,~b,~l,~p]	0	0.0
Disallowed regions [XX]	0	0.0
Non-glycine and non-proline residues	407	100

Table 2: Tm scores and RMSD values of WsFGT models

PDB Template	Tm Score	RMSD
2PQ6 (*Medicago truncatula*)	0.90902	0.916 Å
2C1Z (*Vitis vinifera*)	0.92189	0.970 Å
3HBJ (*M. truncatula*)	0.91289	0.986 Å
2ACW (*M. truncatula*)	0.89778	1.006 Å
2VG8 (*Arabidopsis thaliana*)	0.88744	1.074 Å

Table 3: Docking statistics of WsFGT with substrates

Substrate	Interaction energy kcal/mol	No of Hydrogen bonds	Hydrogen bond length Å	Amino acid residues
UDP-Glucose	-10.9	12	2.1 - 3.4	His18, Asn20, Gln133, Lys245, Ser278, Gln334, His349, Asn353, Ser354, Glu357 and Trp371
Luteolin	-9.3	7	2.1 - 3.1	Tyr13, His18, Gln133, His349, Trp352 and Asn353
Apigenin	-9.2	7	2.1 - 3.4	Tyr13, His18, Gln133, His349, Trp352 and Asn353
Naringenin	-9.2	6	1.7 - 2.5	Tyr13, His18, Trp352, Asn353 and His349
Kaempferol	-9.2	8	2.5 - 3.3	Tyr13, His18, Gln133, His349, Trp352, Asn353 and Trp371
Diadzein	-8.4	5	2.2 - 3.3	Ser278, Ser354, 357 and Trp371
Genistein	-8.4	5	2.3 - 3.2	Trp352, Asn353, Glu357 and Trp371