

Supporting information

Exploring the structure-activity relationship and interaction mechanism of flavonoids and α -glucosidase based on experimental analysis and molecular docking studies

Hongjin Tang,^{a,#,*} Lin Huang,^{b,#} Chunyong Sun,^c Dongsheng Zhao^{c,*}

^a *College of Biological and Chemical Engineering, Anhui Polytechnic University, Wuhu 241000, P. R. China*

^b *Affiliated Yijishan Hospital of Wannan Medical College, Wuhu 241001, P. R. China*

^c *College of Pharmacy, Shandong University of Traditional Chinese Medicine, Jinan 250355, P. R. China*

These two authors contributed equally to this work.

* Corresponding author.

E-mail address: tanghongjin@126.com, tanghongjin@ahpu.edu.cn (H.-J. Tang);
dongshengpw2008@163.com (D.-S. Zhao)

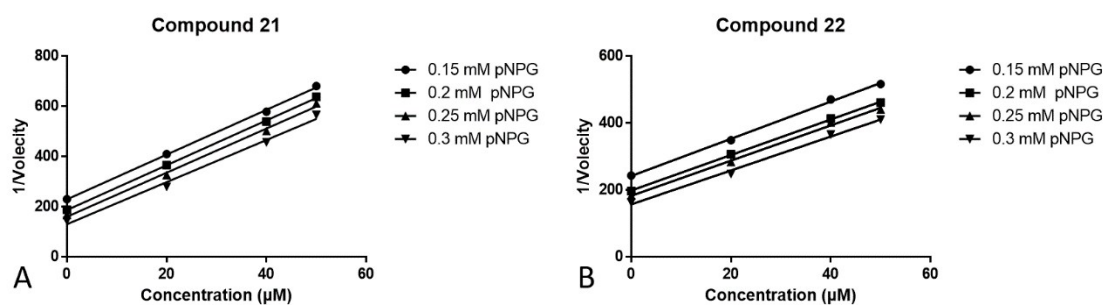


Figure S1 Dixon plots of compounds **21** (A) and **22** (B). The substrate pNPG concentrations were 0.15, 0.2, 0.25 and 0.3 mM.

Table S1. The results of the BLAST search performed on the FASTA sequence of the AG protein (GenBank: CAA00532.1)

Accession	Resolution	Query Cover	Percent Identity
3AXH_A	1.8 Å	99%	72.34%
3AJ7_A	1.3 Å	99%	71.89%
3A47_A	1.59 Å	99%	71.89%
3A4A_A	1.6 Å	99%	71.89%



Figure S2 The three-dimensional homology model of AG superimposed with the templates. The cartoon representation is with the following color: cyan (AG), purple (3AXH), yellow (3A47), brown (3A4A) and blue (3AJ7).

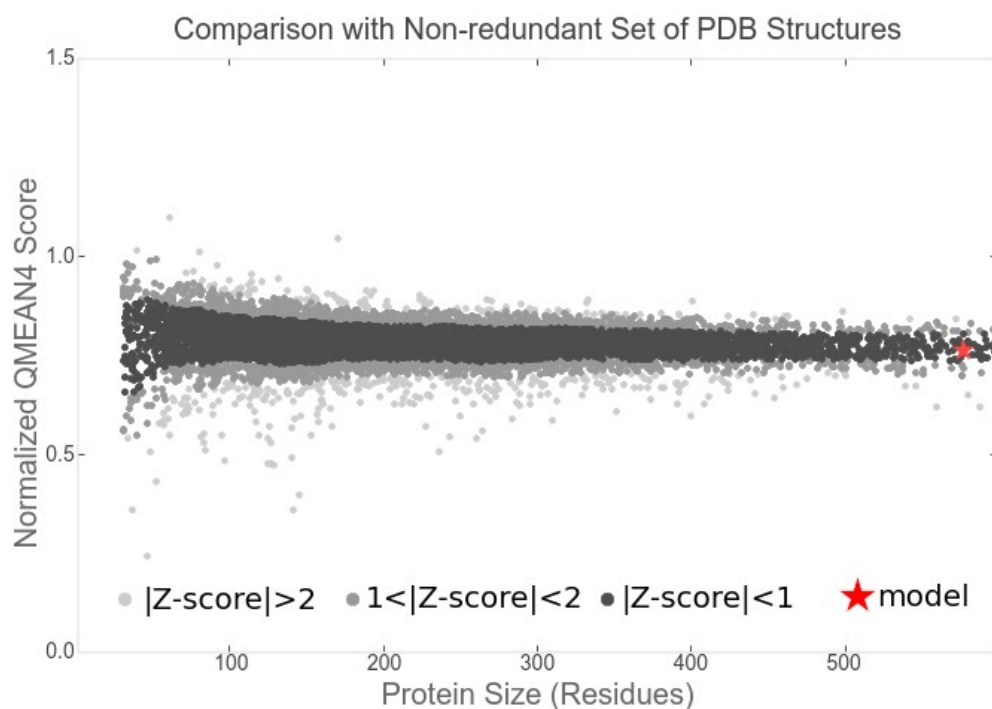


Figure S3 The overall quality of the homology model of AG in comparison with non-redundant PDB structures assessed by Swiss-Model structure assessment. Higher values of the QMEAN4 score indicate that the model is of comparable quality to experimental structures of similar size. An explanation of the QMEAN4 score is provided here: <https://swissmodel.expasy.org/qmean/help>

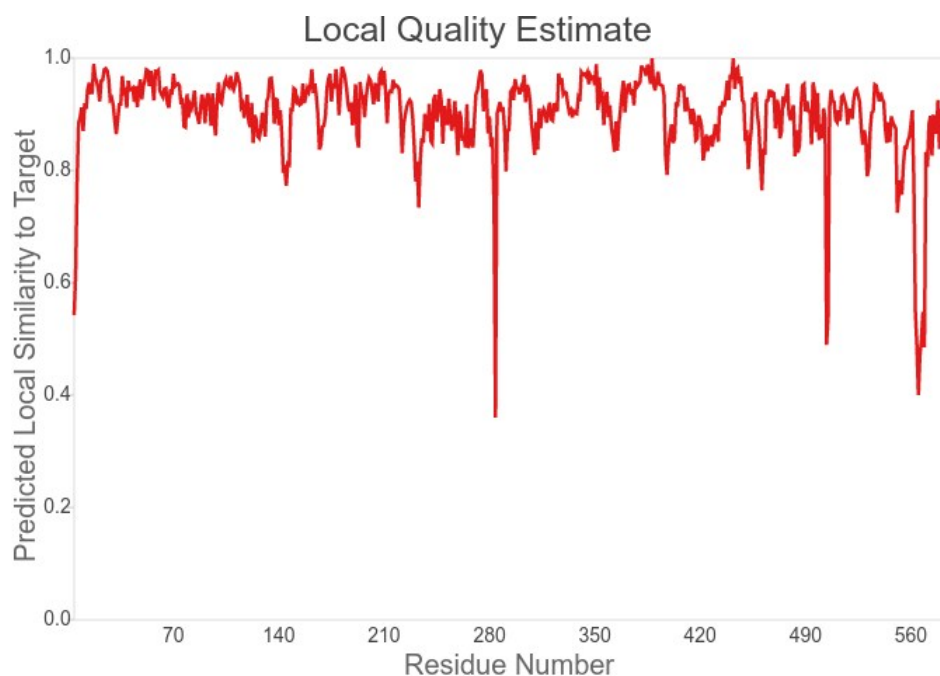


Figure S4 The per-residue quality estimate of the homology model of AG assessed by Swiss-Model structure assessment. Typically, residues showing a score below 0.6 are expected to be of low quality. An explanation of the Local Quality Estimate is provided here: <https://swissmodel.expasy.org/docs/examples>

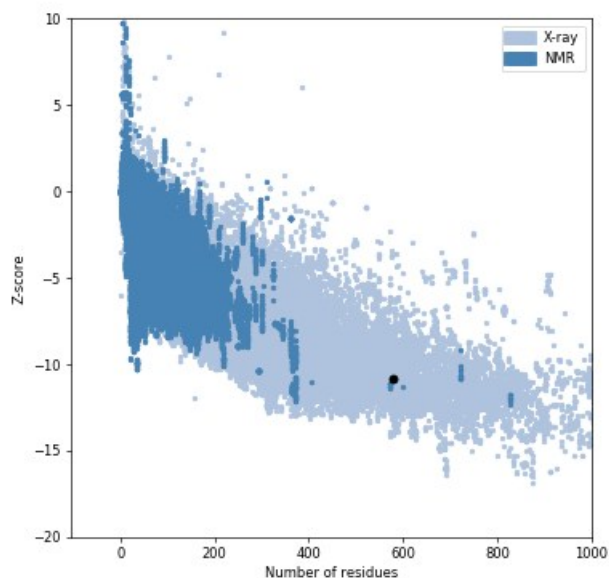


Figure S5 The overall quality estimate of the homology model of AG assessed by ProSa-web. The result of this evaluation is comparable between ProSa-web and Swiss-Model structure assessment shown in Figure S4.

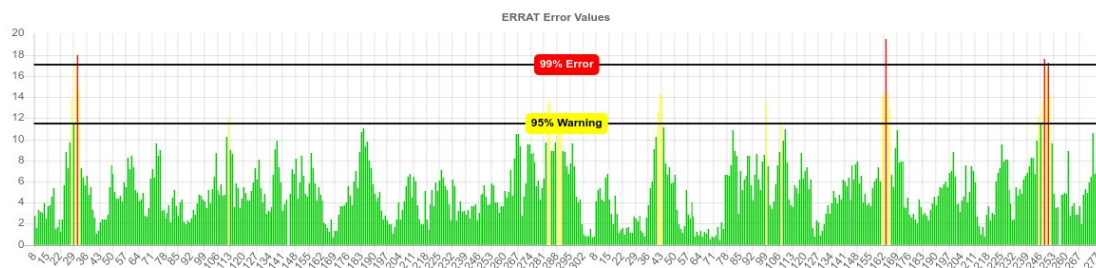


Figure S6 ERRAT results of the homology model of AG assessed by SAVES v5.0. The quality factor the model is 95.4306 (Good). Explanation: <https://servicesn.mbi.ucla.edu/ERRAT/help>

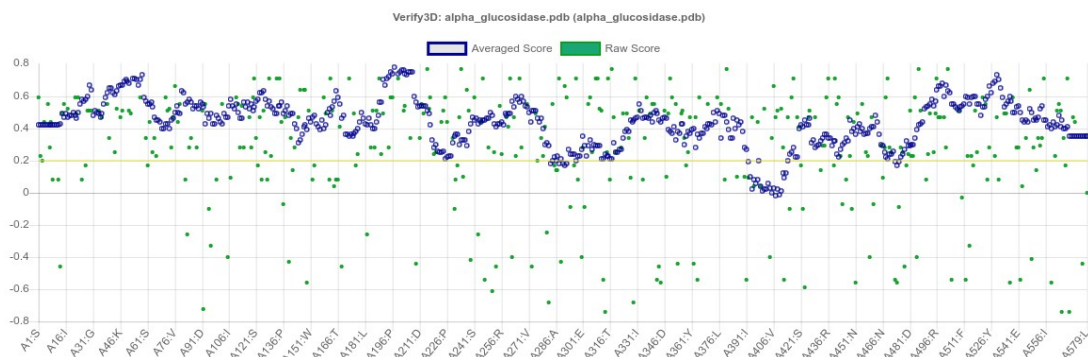


Figure S7 Verify 3D results of the homology model of AG assessed by SAVES v5.0. 94.99% of the residues have averaged 3D-1D score ≥ 0.2 (Pass) and at least 80% of the amino acids have scored ≥ 0.2 in the 3D/1D profile.

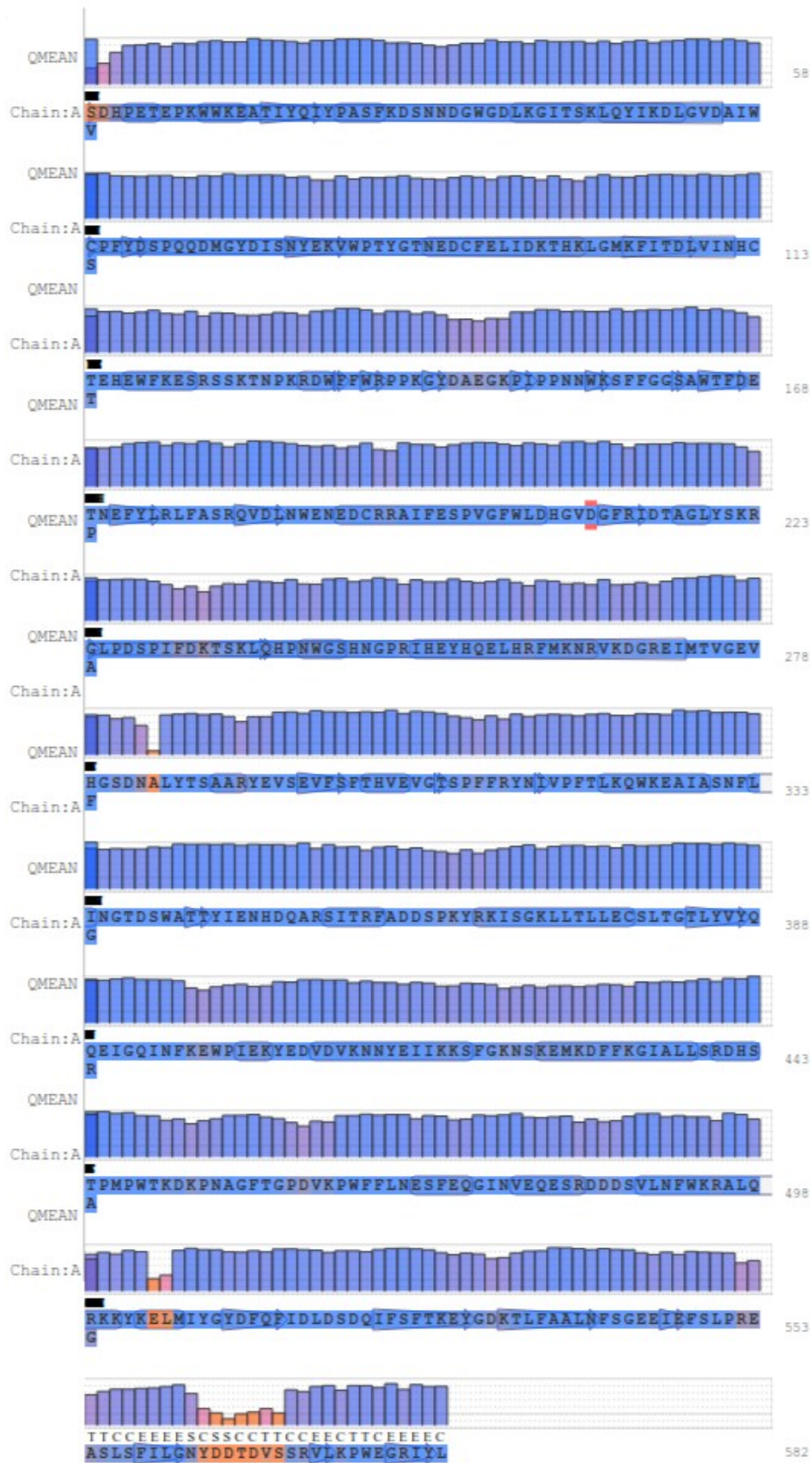


Figure S8 The secondary structure assignment of the homology model of AG.