

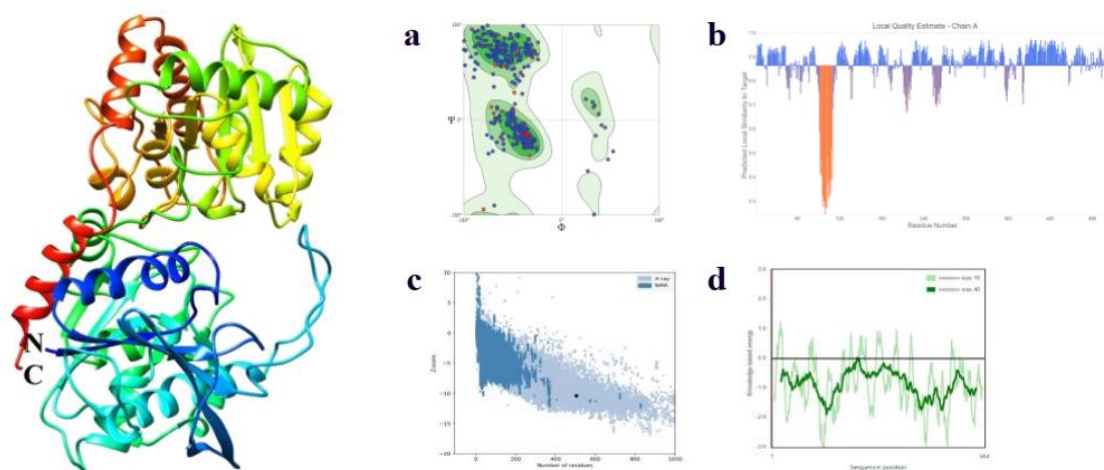
Molecular evolution of the granule-bound starch synthase in flowering plants

SUPPORT INFORMATION

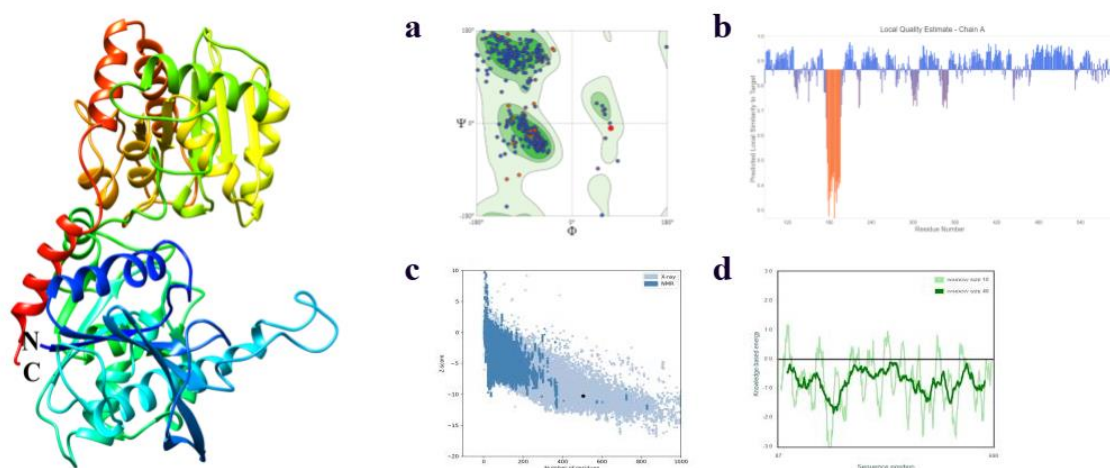
Support information 01. Swiss-Model webserver template search results; identity values (%), coverage (%), and resolution of the template structures. All template protein structures obtained from the Protein Data Bank were elucidated by X-ray.

GenBank accession code	Species	Enzyme	PDB accession codes (Templates)	Identity %	Coverage	Method	Resolution
NP_174566.1	<i>Arabidopsis thaliana</i>	GBS SI	3VUE.A GBSSI	69.45	0.86	X-RAY	2.7 Å
XP_027182769.1	<i>Coffea eugenioides</i>	GBS SI	3VUE.A GBSSI	70.78	0.86	X-RAY	2.7 Å
XP_027153219.1	<i>Coffea eugenioides</i>	GBS SII	4HLN.A GBSSI	50.82	0.62	X-RAY	2.7 Å
XP_028182166.1	<i>Glycine soja</i>	GBS SI	3VUE.A GBSSI	69.83	0.87	X-RAY	2.7 Å
XP_028195575.1	<i>Glycine soja</i>	GBS SII	4HLN.A GBSSI	52.47	0.63	X-RAY	2.7 Å
AHA51121.1	<i>Musa acuminata</i>	GBS SI	3VUE.A GBSSI	73.43	0.76	X-RAY	2.7 Å
AHA51125.1	<i>Musa acuminata</i>	GBS SII	4HLN.A GBSSI	50.53	0.62	X-RAY	2.7 Å
XP_006655754.2	<i>Oryza brachyantha</i>	GBS SI	3VUE.A GBSSI	95.45	0.87	X-RAY	2.7 Å
UBF46438.1	<i>Oryza brachyantha</i>	GBS SII	3VUE.A GBSSI	69.26	0.87	X-RAY	2.7 Å
XP_021822644.1	<i>Prunus avium</i>	GBS SI	3VUE.A GBSSI	70.97	0.85	X-RAY	2.7 Å
XP_021812457.1	<i>Prunus avium</i>	GBS SII	4HLN.A GBSSI	50.41	0.63	X-RAY	2.7 Å
XP_015162571.1	<i>Solanum tuberosum</i>	GBS SI	3VUE.A GBSSI	69.45	0.83	X-RAY	2.7 Å
NP_001274977.1	<i>Solanum tuberosum</i>	GBS SII	4HLN.A GBSSI	50.92	0.63	X-RAY	2.7 Å
ABP35819.1	<i>Sorghum bicolor</i>	GBS SII	3VUE.A GBSSI	69.39	0.87	X-RAY	2.7 Å
ABU98327.1	<i>Sorghum leiocladum</i>	GBS SI	3VUE.A GBSSI	88.99	0.87	X-RAY	2.7 Å

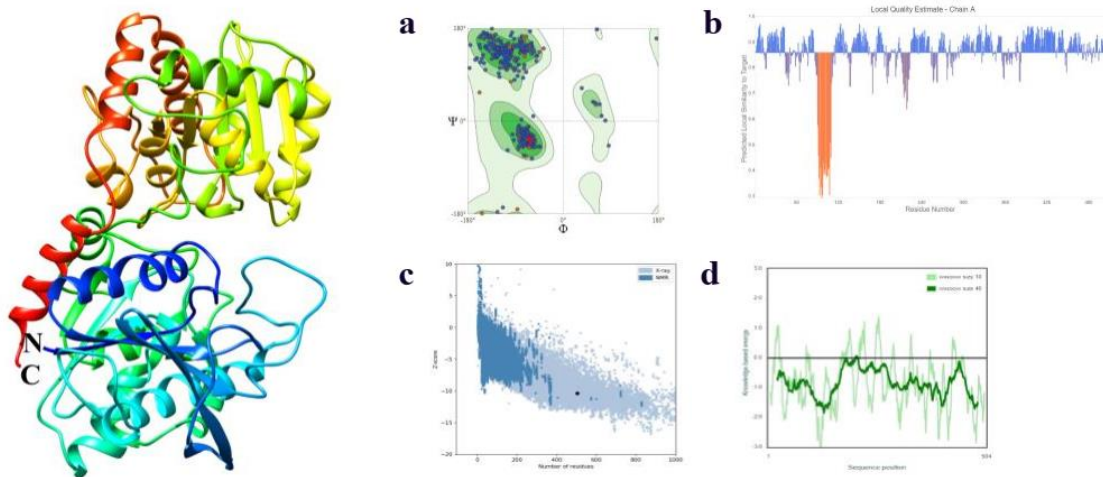
Support information 01. All theoretical models obtained through homology modeling on the swiss-model server and validation data for each model.



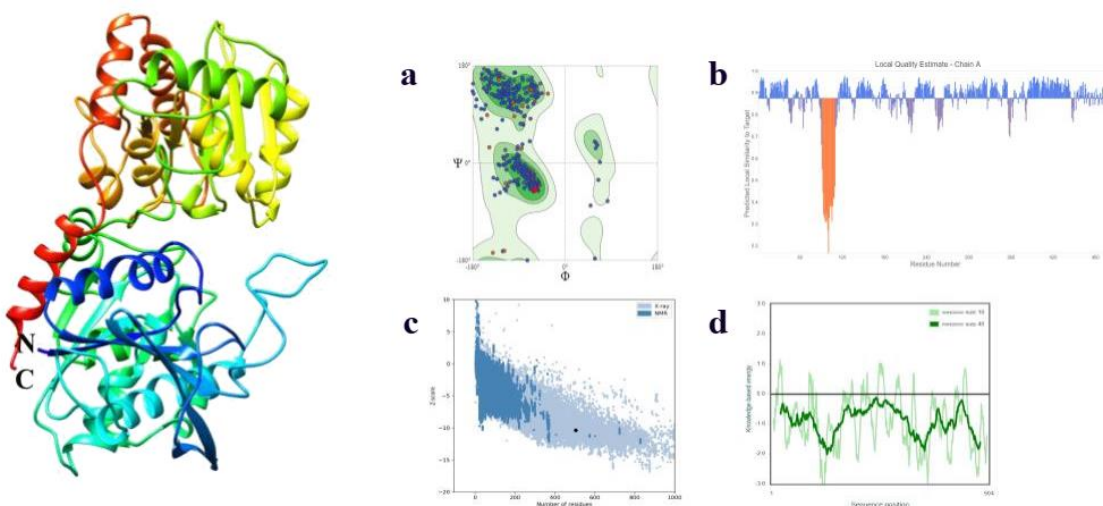
S1 Figure 1. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Arabidopsis thaliana*. (a) Stereochemical analysis, (b) QNEMAN composite score analysis, (c) Zscore, (d) Energy graph.



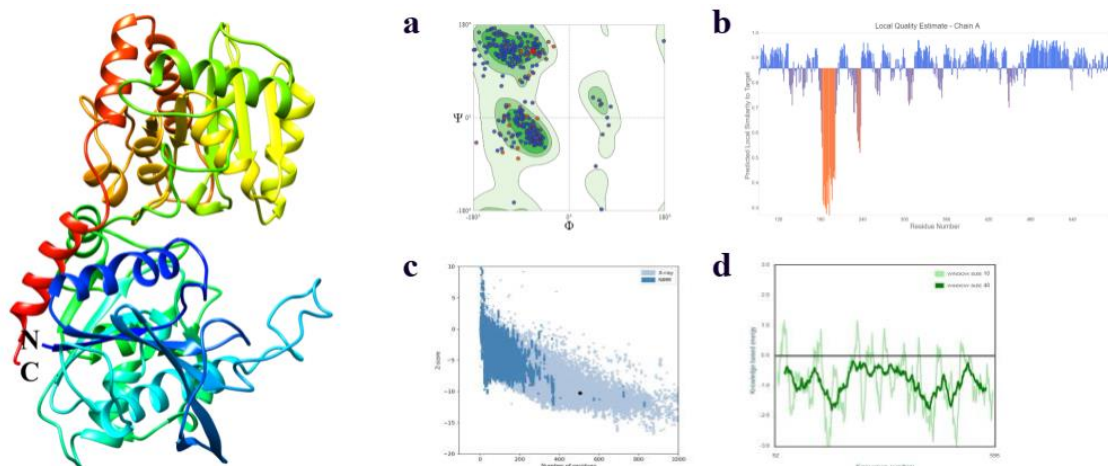
S1 Figure 2. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Coffea eugenioides*. (a) Stereochemical analysis, (b) QNEMAN composite score analysis, (c) Zscore, (d) Energy graph.



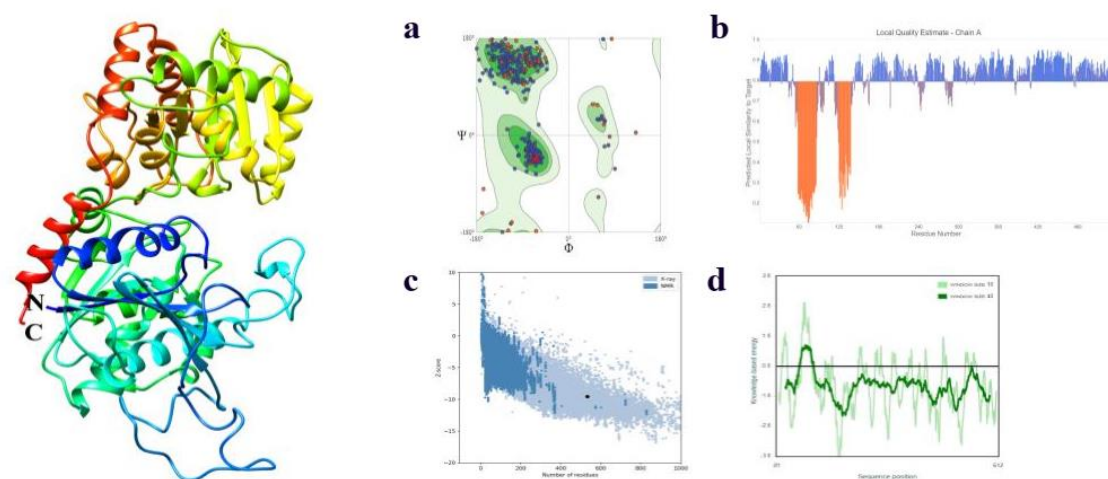
S1 Figure 3. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Glycine soja*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



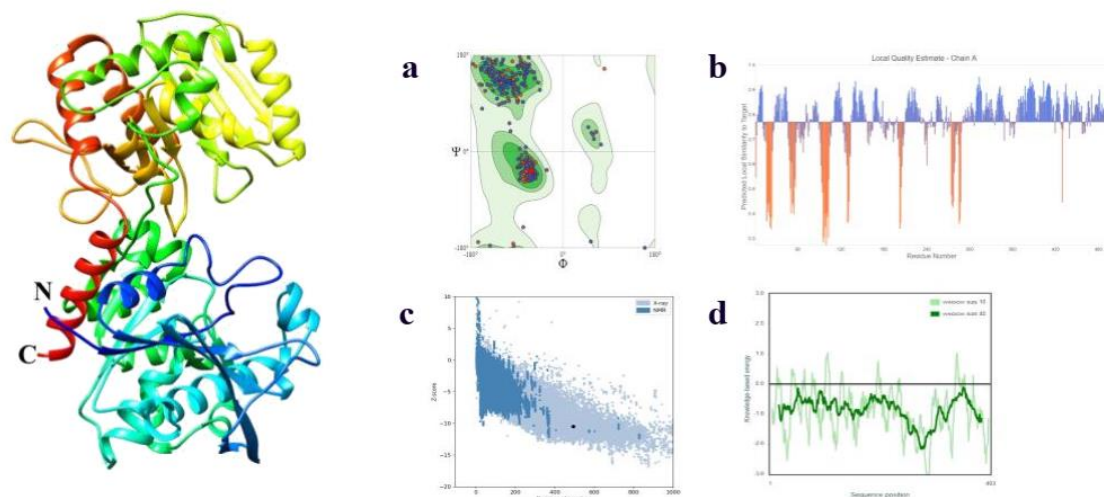
S1 Figure 4. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Musa acimunata*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



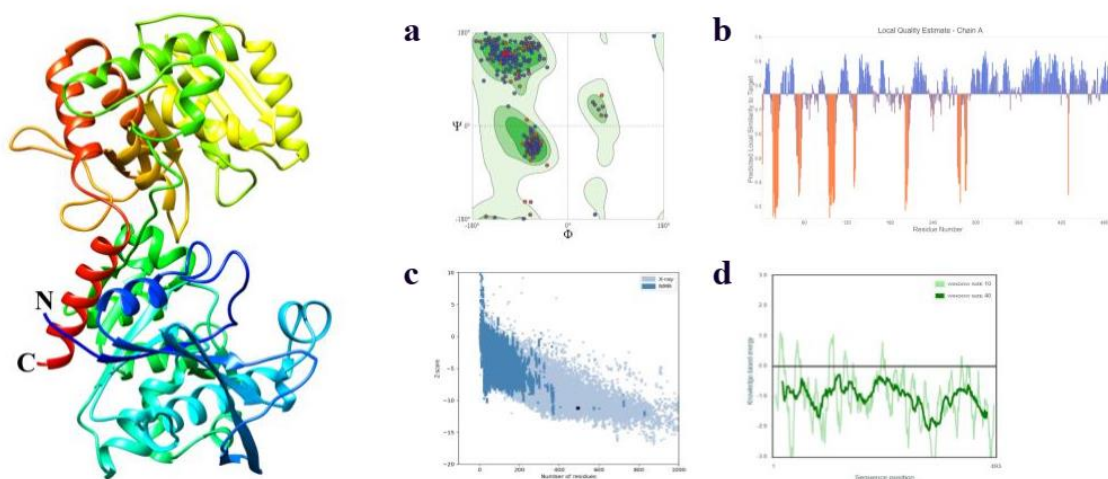
S1 Figure 5. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Prunus avium*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



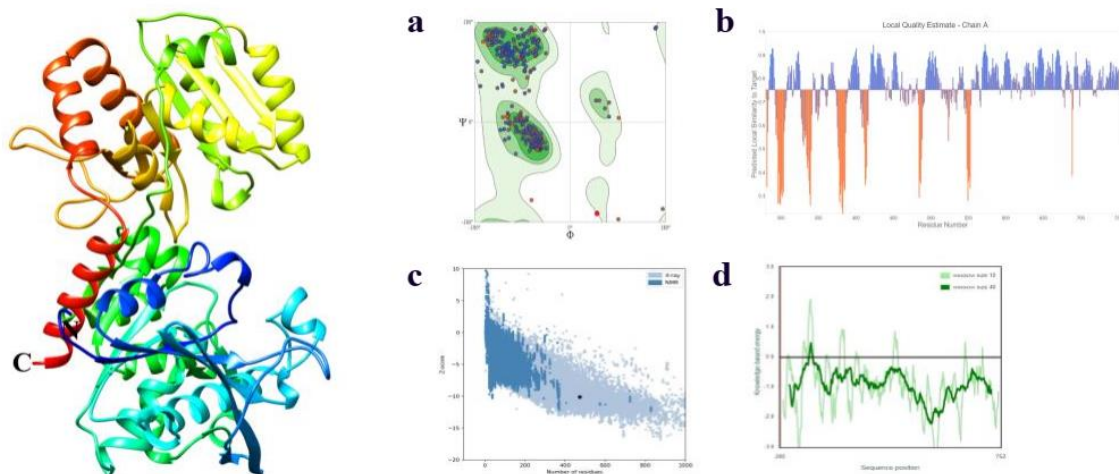
S1 Figure 6. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Solanum tuberosum*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



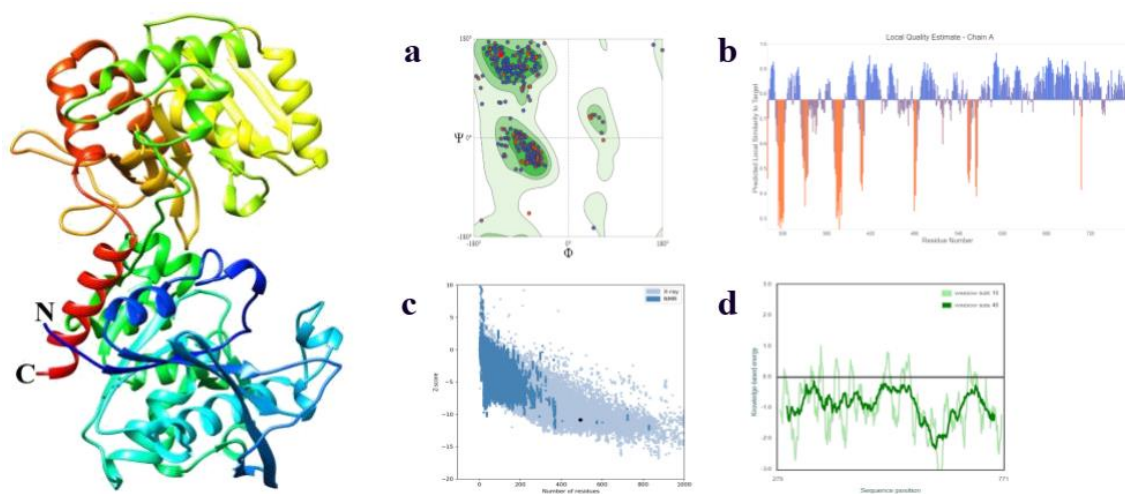
S1 Figure 7. Theoretical structure of the Granule-Bound Starch Synthase II enzyme from *Coffea eugenioides*. (a) Stereochemical analysis, (b) QNEMAN composite score analysis, (c) Zscore, (d) Energy graph.



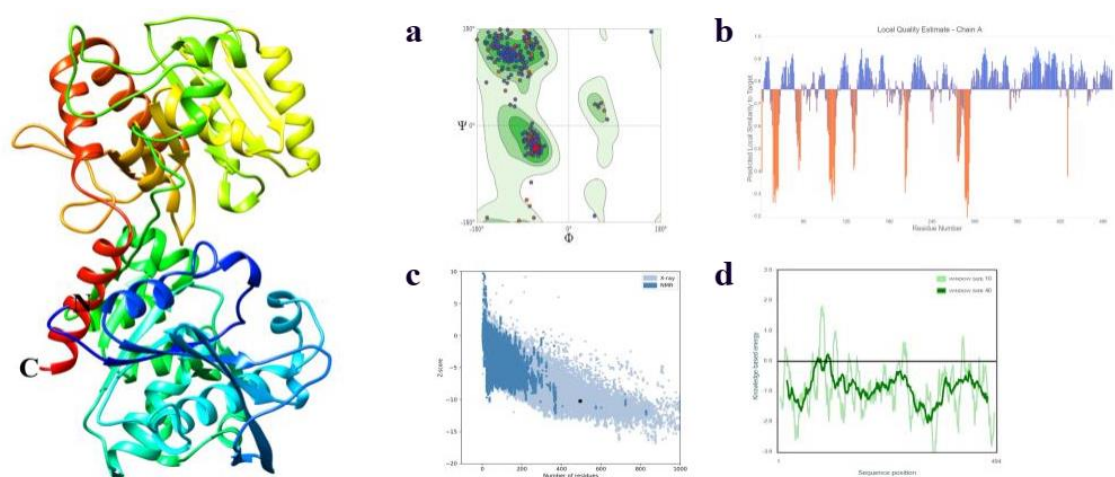
S1 Figure 8. Theoretical structure of the Granule-Bound Starch Synthase II enzyme from *Glycine soja*. (a) Stereochemical analysis, (b) QNEMAN composite score analysis, (c) Zscore, (d) Energy graph.



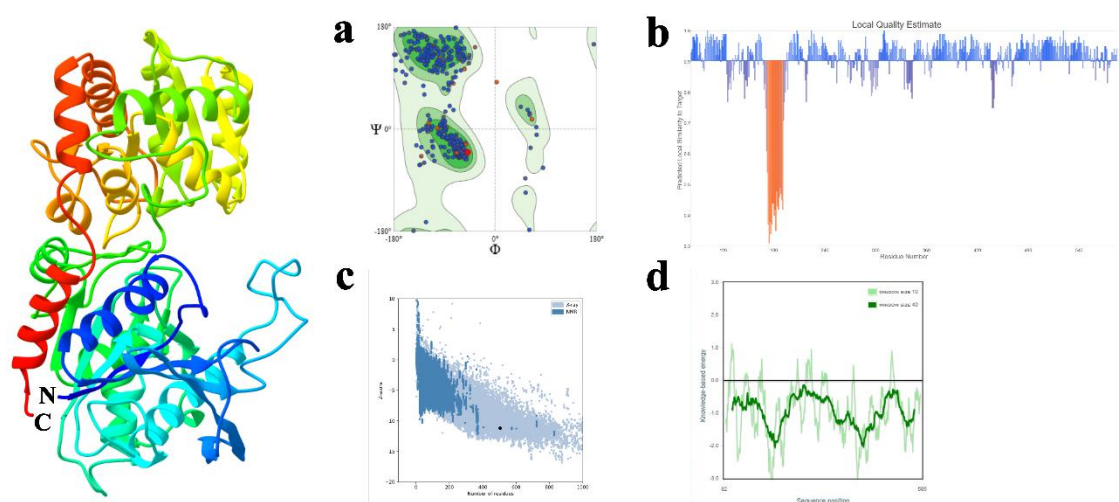
S1 Figure 9. Theoretical structure of the Granule-Bound Starch Synthase II enzyme from *Musa acuminata*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



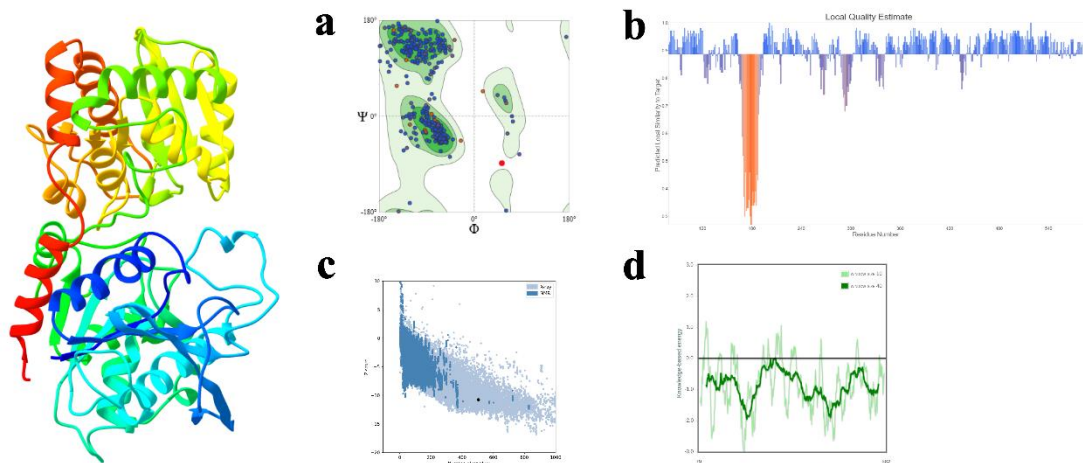
S1 Figure 10. Theoretical structure of the Granule-Bound Starch Synthase II enzyme from *Prunus avium*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



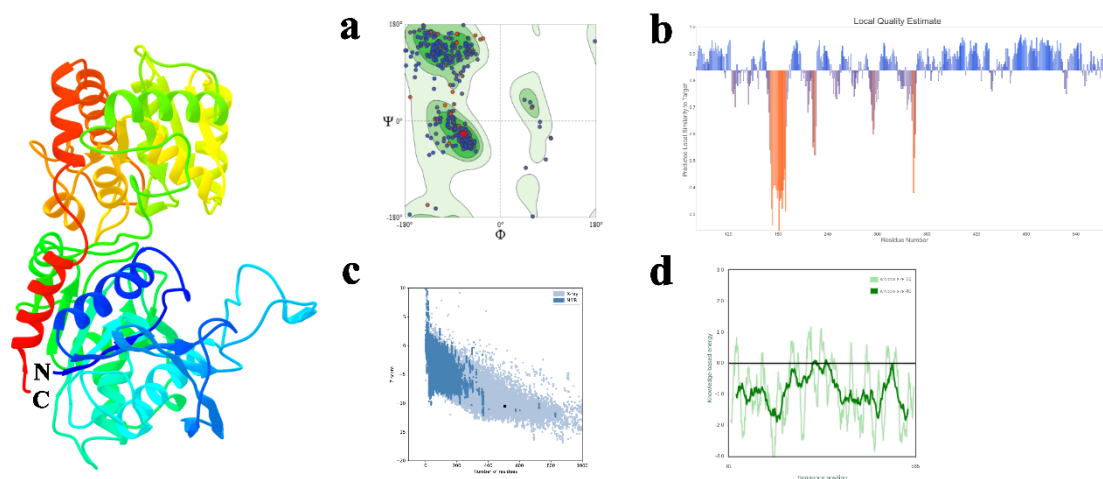
S1 Figure 11. Theoretical structure of the Granule-Bound Starch Synthase II enzyme from *Solanum tuberosum*. (a) Stereochemical analysis, (b) QNEMAN composite score analysis, (c) Zscore, (d) Energy graph.



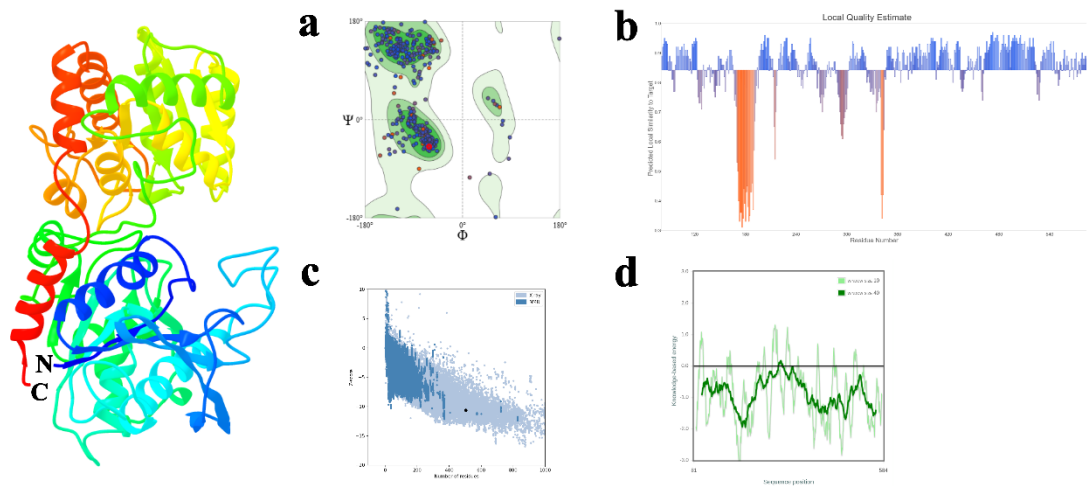
S1 Figure 12. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Oryza brachyantha*. (a) Stereochemical analysis, (b) QNEMAN composite score analysis, (c) Zscore, (d) Energy graph.



S1 Figure 13. Theoretical structure of the Granule-Bound Starch Synthase I enzyme from *Sorghum leiocladum*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



S1 Figure 14. Theoretical structure of the Granule-Bound Starch Synthase II enzyme from *Oryza brachyantha*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.



S1 Figure 15. Theoretical structure of the Granule-Bound Starch Synthase II enzyme from *Sorghum bicolor*. **(a)** Stereochemical analysis, **(b)** QNEMAN composite score analysis, **(c)** Zscore, **(d)** Energy graph.