**Supplementary Table S1.** Comparative analysis of the secondary structures and solvent accessibility of native and *truncated* AGBL3 protein predicted by SPPIDER.

| | Secondary structure | | | Solvent accessibility (SABLE) | |
|---|---|---|---|---|---|
| **Position** | **Helix** | **Coil** | **Beta strand** | ***Fully buried areas*** | ***Exposed areas*** |
| Native AGBL3 Protein | 84 | 219 | **106** | **37** | **5** |
| *Truncated* AGBL3 Protein | 0 | 57 | **38** | **21** | **5** |

**Supplementary Table S2.** Stabilising residues of native and *truncated* AGBL3 proteins analysed by SRide.

| **Protein** | **Stabilising residues** | |
|---|---|---|
| | **Present** | **Newly formed** |
| Native AGBL3 Protein | PHEA210, PHEA223, SERA279, LEUA280 | |
| *Truncated* AGBL3 Protein | | GLNA192, LEUA193 |

**Supplementary Table S3.** Flexpred predicted changes in flexible residue positions in native and *truncated* AGBL3 protein structures. The positions of the additional flexible residues are shown in bold.

| **Protein** | **Flexible residues** |
|---|---|
| Native AGBL3 Protein | 1, 2, 3, 4, 5, 40, 92, 93, 106, 107, 108, 109, 110, 111, 112, 114, 127, 128, 153, 154, 158, 185, 186, 187, 188, 189, 221, 222, 223, 224, 311, 312, 313, 314, 315, 316, 317, 337, 338, 352, 353, 354, 355, 356, 357, 383, 384, |
| *Truncated* AGBL3 Protein | 1, 2, 3, 4, 5, **15, 37, 38, 39**, 40, **41, 54, 55, 56,68, 71,74, 76, 79, 80, 81, 88, 91,** 92, 93, **94** |

**Supplementary Table IV.** Intermolecular hydrogen bond frequency estimates in HBAT and native and *truncated* AGBL3 proteins.

| **Protein** | **N-H..O** | **O-H..O** | **N-H..N** | **O-H..N** | **C-H..O** | **C-H..N** | **N-H..S** | **O-H..S** | **C-H..S** |
|---|---|---|---|---|---|---|---|---|---|
| Native AGBL3 Protein | 434 | 30 | 220 | 10 | 73 | 22 | 2 | 1 | 6 |
| *Truncated* AGBL3 Protein | 62 | 1 | 44 | 1 | 15 | 8 | 0 | 0 | 1 |