Supplement materials

Identification of a binding pocket of Letermovir in the terminase subunit pUL56 of human Cytomegalovirus

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Figure S1. Model of the 3D structure of pUL56 with indicated regions for data processing.

Table S1. Amino acids for processing

| Amino acids for processing SwissDock conformations | | | | | | | | | | |
|--|------|------|------|------|------|------|------|------|------|--|
| polar | T244 | T245 | R246 | S333 | Y337 | | | | | |
| nonpolar | L240 | L243 | 1247 | L250 | C325 | L238 | M329 | 1332 | L336 | |

| pUL56 Variant | пвм | ΔG_{mean} in kcal/mol | p-value, pwc with wt | significance |
|---------------|-----|-------------------------------|----------------------|--------------|
| Wildtype | 318 | -9.09 ± 0.91 | - | - |
| V236M | 400 | -9.15 ± 0.86 | 0.72 | |
| C325W | 445 | -9.06 ± 0.75 | 0.95 | |
| C325F | 51 | -9.09 ± 0.91 | 0.72 | |
| C325Y | 48 | -8.40 ± 0.96 | <0.0001 | *** |

Table S2: Mean values of Gibb's free energy in kcal/mol for each pUL56 variant.

(p <0.05: *, p <0.01: **, p <0.001: ***). Correction of p-values was done using Holm's method.

 Δ G-values were directly obtained by SwissDock for each Letermovir binding mode. Δ G-values were averaged by the remaining conformation after processing. Number of binding modes remaining after processing are given as n_{BM}. The "p-value, pwc with wt" column notes the p-value resulting from a pairwise comparison (pwc) between mutant and wild-type (wt).