S1 Text. Description of the GDT-HA and lDDT metrics for model quality evaluation.

**GDT-HA.** To evaluate the backbone quality of the 3D models we used the global distance test - high accuracy (GDT-HA) metric, one of the most frequently used in literature and in CASP experiments [1]. Once a 3D model is superposed to the target experimentally-determined structure, GDT-HA is computed as:

\[
GDT-HA = \frac{p_{0.5} + p_{1.0} + p_{2.0} + p_{4.0}}{4}
\]

where \(p_d\) is the fraction of C\(_\alpha\) atoms of the 3D model found at a distance of less than \(d\) Å of their equivalent atoms in the experimentally-determined structure. GDT-HA values range from 0 to 1 (with 1 corresponding to a maximum of accuracy). In order to compute GDT-HA scores, we used the TM-score program available at:

https://zhanglab.ccmb.med.umich.edu/TM-score.

**lDDT.** In order to evaluate the quality of local structures and side chains of the models we used the local distance difference test (lDDT) metric [2]. This metric is computed by considering all pairs of heavy atoms in the target experimentally-determined structure at a distance closer than 15.0 Å and not belonging to the same residue. These interatomic distances are compared with the equivalent ones in the 3D model. A distance in the model is presumed to be correctly modeled if the difference between its value and that of its equivalent distance in the target is below a specific cutoff. The lDDT score is computed as:

\[
lDDT = \frac{f_{0.5} + f_{1.0} + f_{2.0} + f_{4.0}}{4}
\]

where \(f_d\) is the fraction of distances being correctly modeled by considering a cutoff value of \(f\) Å. lDDT values range from 0 to 1 (with 1 corresponding to a maximum of accuracy). In order to compute this metric, we used the lDDT program available at:


**References**
