**Table S6: Validity of averaging fingerprints over bound structures solved by NMR. Pairwise correlation coefficients between the fingerprints for models 1-5 and the average fingerprint of the 5 ligand-bound MDM2 structures (PDB ID 2lzg).**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Model** | **Model 1** | **Model 2** | **Model 3** | **Model 4** | **Model 5** | **Average** |
| 1 |  | 0.794 | 0.91 | 0.84 | 0.963 | 0.954 |
| 2 |  |  | 0.874 | 0.897 | 0.804 | 0.922 |
| 3 |  |  |  | 0.857 | 0.876 | 0.953 |
| 4 |  |  |  |  | 0.86 | 0.943 |
| 5 |  |  |  |  |  | 0.954 |