Supplementary file 2. Bonds involved in the multimerization of TDP-43 as deduced from the complex RRM1-2/(GU)12 MD model. Physical parameters of the established interactions between atoms of residues of RRM2 pocket around V220 and those located in RRM1 loop 3 from monomer 1 and 2, respectively, are shown. Values in brackets indicates the energy contribution (in kcal/mol) of amino acid residues to the protein-protein interface stability. Energies were averaged over 100 ns of MD simulation and values are reported in kcal/mol with variant of fluctuations being ± 0.1 kcal/mol. *1bb and vdW correspond to backbone and van der Waals, respectively.*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Monomer 1** | **Atom** | **Monomer 2** | **Atom** | **Distance (**Å**)** | **Interaction type** | **Energy contribution** |
|
| E204 | O2 | K140  (-6.21) | H3 | 1.83 | ionic | -8.27 |
| C | C | 3.7 | vdW*1* |
| C | T141  (-2.06) | C | 4.01 | vdW |
| C | C | 4.05 | vdW |
| D205 | C | K140  (-2.14) | C | 3.8 | vdW | -2.14 |
| R208 | HH12  (of NH1) | D138  (-0.72) | O (C=O) | 2.27 | H-bond | -4.9 |
| HH11  (of NH1) | L139  (-1.51) | O (C=O) | 2.42 | H-bond |
| HH12  (of NH1) | O (C=O) | 2.55 | H-bond |
| HH11  (of NH1) | K140  (-0.81) | O (C=O) | 2.29 | H-bond |
| HH11  (of NH1) | T141  (-1.47) | O (C=O) | 2.68 | H-bond |
| NH1 | G142 ( -0,4) | HN (bb*1*) | 3.43 | H-bond |
| M218 | O (C=O) | K137  (-2.85) | N | 3.24 | H-bond | -2.85 |
| D219 | O2 | K137  (-1.41) | N | 4.26 | ionic | -7.22 |
| C | T141  (-2.22) | C2 | 3.1 | vdW |
| C | G142  (-1.21) | C | 4.3 | vdW |
| C | H143  (-2.38) | C | 3.76 | vdW |
| C | C | 3.53 | vdW |
| V220 | HN (bb*1*) | T141  (-8.06) | O (C=O) | 1.82 | H-bond | -9.47 |
| O (C=O) | H  (of O) | 3.24 | H-bond |
| HN (bb) | H143  (-1.41) | N1 | 3.5 | H-bond |
| F221 | C | H143  (-0.67) | C1 | 3.08 | vdW | -0.67 |