**Supplementary Data**

Diagram

Description automatically generated

Figure S1:Ramachandran plot for Alphafold2 predicted hNECD model shows around 87% of residues in most favored regions and 12% in additional allowed regions.

A picture containing graphical user interface

Description automatically generated

Figure S2: Errat plot for AlphaFold2 hNECD model showing 99% of protein residues falls below the 95% rejection limit.

Graphical user interface, chart

Description automatically generated

Figure S3: RMSD and distance between salt bridge forming atoms to check stability of hNECD-VS2’ complex.

Supplementary Table 1: List of interaction of hNECD interface residues with VS2’ interface residues in hNECD-VS2’ protein complex obtained through PPCheck protein-protein interaction prediction tool

|  |  |  |
| --- | --- | --- |
| hNECD residues | Type of Interaction | VS2’ interacting residues |
| B112LYS | E,E,V,V,V,V,V,V,V,V,V,V,V | A867ASP,A868GLU,A1056ALA,A1057PRO,A1058HIS,A1059GLY,A823PHE,A863PRO,A866THR,A867ASP,A868GLU,A869MET,A871ALA |
| B113CYS | V,V,V,V,V,V,V,V | A863PRO,A864LEU,A865LEU,A866THR,A867ASP,A868GLU,A869MET,A870ILE |
| B114SER | V,V,V,V,V,V,V,V | A864LEU,A866THR,A868GLU,A869MET,A870ILE,A871ALA,A872GLN,A873TYR |
| B115ASN | V,V,V,V,V,V | A864LEU,A865LEU,A866THR,A868GLU,A869MET,A872GLN |
| B116SER | V,V,V,V,V | A863PRO,A864LEU,A865LEU,A866THR,A869MET |
| B117GLY | H,V,V,V,V,V,V | A864LEU,A862PRO,A863PRO,A864LEU,A865LEU,A866THR,A869MET |
| B118ILE | V,V,V,V,V,V | A832GLY,A861LEU,A862PRO,A863PRO,A864LEU,A865LEU |
| B119GLU | E,V,V,V | A868GLU,A862PRO,A863PRO,A864LEU |
| B121ASP | V | A834ILE |
| B126CYS | V | A864LEU |
| B127ILE | V | A864LEU |
| B128ASN | V | A864LEU |
| B129PRO | V,V | A862PRO,A864LEU |
| B132TRP | V,V,V | A832GLY,A833PHE,A862PRO |
| B144ASP | V | A833PHE |
| B146ASN | V,V | A833PHE,A836GLN |
| B147ARG | E,V,V,V,V | A835LYS,A833PHE,A834ILE,A835LYS,A836GLN |
| B148CYS | V,V | A833PHE,A836GLN |
| B149VAL | V,V,V | A833PHE,A836GLN,A837TYR |
| B150ARG | E,V,V,V,V,V,V,V,V,V,V | A830ASP,A830ASP,A832GLY,A833PHE,A835LYS,A836GLN,A837TYR,A859THR,A860VAL,A861LEU,A862PRO |
| B151LEU | V,V,V,V,V,V,V,V | A833PHE,A836GLN,A837TYR,A838GLY,A839ASP,A854LYS,A857GLY,A859THR |
| B152TYR | V,V,V,V,V,V,V,V | A837TYR,A853GLN,A854LYS,A855PHE,A856ASN,A857GLY,A858LEU,A859THR |
| B153GLY | V,V,V,V,V,V,V,V,V | A837TYR,A841LEU,A853GLN,A854LYS,A855PHE,A856ASN,A857GLY,A858LEU,A859THR |
| B154PRO | V,V,V,V,V,V,V,V,V,V,V,V,V | A1000ARG,A841LEU,A842GLY,A854LYS,A855PHE,A856ASN,A857GLY,A966LEU,A967SER,A975SER,A976VAL,A977LEU,A978ASN |
| B155ASN | V,V,V,V,V,V,V,V,V | A1000ARG,A841LEU,A855PHE,A856ASN,A975SER,A976VAL,A977LEU,A978ASN,A979ASP |
| B156PHE | V,V,V,V,V,V,V,V,V,V | A837TYR,A838GLY,A839ASP,A840CYS,A841LEU,A854LYS,A855PHE,A856ASN,A857GLY,A978ASN |
| B159GLN | V,V | A837TYR,A859THR |
| B161TYR | V,V | A833PHE,A861LEU |
| B166LYS | V,V | A861LEU,A864LEU |
| B167SER | V | A861LEU |
| B168TRP | V,V,V,V,V,V | A833PHE,A836GLN,A859THR,A860VAL,A861LEU,A862PRO |
| B187ASP | V | A836GLN |
| B188MET | V,V,V | A833PHE,A836GLN,A837TYR |
| B189GLY | V | A836GLN |
| B190TYR | V,V,V,V,V,V | A835LYS,A836GLN,A837TYR,A838GLY,A839ASP,A840CYS |
| B198GLN | V | A978ASN |
| B199GLY | V,V | A978ASN,A981LEU |
| B200ILE | V,V,V,V,V,V | A976VAL,A977LEU,A978ASN,A979ASP,A981LEU,A993ILE |
| B201VAL | V,V,V,V,V,V,V,V | A977LEU,A978ASN,A981LEU,A986LYS,A989ALA,A990GLU,A993ILE,A997ILE |
| B202ASP | V,V,V,V | A1000ARG,A977LEU,A993ILE,A997ILE |
| B203ASP | E,V,V,V,V,V,V,V,V | A1000ARG,A1000ARG,A1001LEU,A1004LEU,A977LEU,A993ILE,A996LEU,A997ILE,A998THR |
| B204SER | V,V,V | A1000ARG,A1001LEU,A997ILE |
| B205GLY | V,V | A1001LEU,A997ILE |
| B234LYS | V,V | A986LYS,A990GLU |
| B238SER | V | A978ASN |
| B240ARG | V,V,V | A838GLY,A839ASP,A841LEU |
| B241CYS | V,V,V | A837TYR,A838GLY,A839ASP |
| B242ILE | V,V,V | A838GLY,A839ASP,A841LEU |
| B243ALA | V,V | A838GLY,A839ASP |

Supplementary Table 2: List of interface residues of hNECD and VS2’ in hNECD-VS2’ complex

|  |  |
| --- | --- |
| hNECD\_interface residues | VS2’ interface residues |
| B112LYS | A823PHE |
| B113CYS | A830ASP |
| B114SER | A832GLY |
| B115ASN | A833PHE |
| B116SER | A834ILE |
| B117GLY | A835LYS |
| B118ILE | A836GLN |
| B119GLU | A837TYR |
| B121ASP | A838GLY |
| B126CYS | A839ASP |
| B127ILE | A840CYS |
| B128ASN | A841LEU |
| B129PRO | A842GLY |
| B132TRP | A853GLN |
| B144ASP | A854LYS |
| B146ASN | A855PHE |
| B147ARG | A856ASN |
| B148CYS | A857GLY |
| B149VAL | A858LEU |
| B150ARG | A859THR |
| B151LEU | A860VAL |
| B152TYR | A861LEU |
| B153GLY | A862PRO |
| B154PRO | A863PRO |
| B155ASN | A864LEU |
| B156PHE | A865LEU |
| B159GLN | A866THR |
| B161TYR | A867ASP |
| B166LYS | A868GLU |
| B167SER | A869MET |
| B168TRP | A870ILE |
| B187ASP | A871ALA |
| B188MET | A872GLN |
| B189GLY | A873TYR |
| B190TYR | A966LEU |
| B198GLN | A967SER |
| B199GLY | A975SER |
| B200ILE | A976VAL |
| B201VAL | A977LEU |
| B202ASP | A978ASN |
| B203ASP | A979ASP |
| B204SER | A981LEU |
| B205GLY | A986LYS |
| B234LYS | A989ALA |
| B238SER | A990GLU |
| B240ARG | A993ILE |
| B241CYS | A996LEU |
| B242ILE | A997ILE |
| B243ALA | A998THR |
|  | A1000ARG |
|  | A1001LEU |
|  | A1004LEU |
|  | A1056ALA |
|  | A1057PRO |
|  | A1058HIS |
|  | A1059GLY |