I**. Mean score of EP-39 and BVM** for each observed location. Mean score is computed over the 10 best scores, including all locations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Cup | | Barrel | | Barrel bottom |
|  | BVM | EP-39 | BVM | EP-39 | BVM |
| mean score | 22.4 | 25.1 | 22.9 | 25.4 | 22.5 |
| mean HB term | 2.6 | 2.8 | 0.9 | 1.77 | 0 |
| mean lipo term | 185 | 197 | 213 | 233 | 287 |

**II. Contacts and potential hydrogen bonds**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Cup** | | **Barrel** | | **Barrel bottom** |
|  | **BVM** | **EP-39** | **BVM** | **EP-39** | **BVM** |
| **G156** | L | H |  |  |  |
| **P157** | L |  |  |  |  |
| **K158** | G L  N(L).CO(3) | H I J NZ(I)-NH2(28)  NZ(I)-CO(28) | J K  NZ(J)-CO(28) | I J K  NZ(I)-CO(28)  NZ(J)-NH2(28) |  |
| **E159** | L | H |  |  |  |
| **P160** | G | I |  |  |  |
| **R162** | G  NH12(G)-CO2H(3) | I NH12(I)-CO2H(3) |  |  |  |
| **G222** | H | J  CO(J)-NH2(28) | K | K  CO(K)-NH2(28) |  |
| **G223** |  |  |  | K |  |
| **P224** |  | J K | L | K |  |
| **K227** | G | I J | J K | J K  NZ(J)-NH2(28) | G H L |
| **L231** |  |  | H I J K | G H I J K | G H I J K L |
| **M4** |  |  | I | H J K L | G H I J K L |

Color code:

MHR, purple;

GVGG β-turn, yellow;

CA C-terminal, coral;

CA-L231, red;

SP1, deep pink.

Green color represents contacts between the ligand (BVM or EP-39) and the monomer(s) of the hexameric structure of CACter-SP1

Blue color represents the Hbonds between the ligand (BVM or EP-39) and the monomer(s) of the hexameric structure of CACter-SP1

*[NB : NH12 = NH1 et/ou NH2 de ARG (notation Sybyl) → jusqu'à 2 liaisons H possibles avec le CO2H du ligand]*