|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **PDB code or model** | 6BHV | 3HKV | 4X52 | 6TL1 | Model 1(Modeller)(3HKV based) | Model 2( I-Tasser) | Model 3(Robetta) |
| **Protein name** | **PARP1** | **PARP10** | **PARP13** | **TASOR** | **LRRC9** |
| **ADP-ribosylation activity:**  | P (poly-) | M (mono-) | inactive | inactive | not determined |
| NAD binding pocket hallmark residues (or counterparts of PARP H-Y-Y-E tetrad) *\*names of residues not included in the best pocket are italicized* | **H**-H862, G863,S864,**Y**- Y896,K903, **Y**-Y907, **E**-E988 | **H**-H887, G888,T889,**Y**-Y919,L926, **Y**-Y932, **E**-I987 | **H**-Y787, A788,T789,**Y**- Y819,Y826, **Y**-C831(N830), **E**-V876 | **H**-l184, M185,V186,**Y**- Y217,L224, **Y**-L225, **E**-Q299 | **H**-Y474, V475, F476,**Y**-E525, K532,**Y**-S538, **E**-K604 | ***H****-Y474, V475, F476*,**Y**-E525(I511?), *K532,****Y****-S538,* **E**-K604 | **H**-Y474, V475, F476,**Y**-E525 (I511?), *K532,****Y****-S538*,**E**-K604 |
| Parameters of the best pocket identified by DoGSiteScorer in the vicinity of the above hallmark residues |
| **simple score**  | 0.69 | 0.32 | 0.48 | 0.25 | 0.36 | 0.31 | 0.56 |
| **rank** | 1 | 1 | 1 | 1 | 2 | 1 | 1 |
| **Size and shape descriptors** |
| volume [Å³]  | 1090.88  | 478.14  | 708.93  | 474.94 | 586.05 | 515.2 | 821.82  |
| surface [Å²]  | 1192.78  | 613.62  | 1032.85  | 584.84 | 866.83 | 690.19 | 1075.79  |
| depth [Å]  | 19.69  | 13.28  | 21.08 | 12.82 | 18.44 | 17.73 | 17.85  |
| **Amino acid composition** |
| apolar amino acid ratio  | 0.32 | 0.39 | 0.34 | 0.46 | 0.40 | 0.36 | 0.37 |
| polar amino acid ratio  | 0.47 | 0.48 | 0.51 | 0.42  | 0.20 | 0.39 | 0.32 |
| positive amino acid ratio | 0.18 | 0.13 | 0.07 | 0.08  | 0.20 | 0.21 | 0.24 |
| negative amino acid ratio  | 0.03 | 0.00 | 0.07 | 0.04  | 0.20 | 0.04 | 0.08 |