Benchmark

β-Lactamases:

(Bös and Pleiss, 2008)

Query protein: 1AXB_A

User defined list:
1AXB_A,1BT5_A,1BTL_A,1ERM_A,1ERO_A,1ERQ_A,1ESU_A,1FQG_A,1JVJ_A,1JWP_A,1JWV_A,1JWZ_A,1LHY_A,1LI0_A,1LI9_A,1M40_A,1NXY_A,1NY0_A,1NYM_A,1NYY_A,1TEM_A,1XPB_A,1YT4_A,1ZG4_A,1ZG6_A,1N9B_A,1ONG_A,1Q2P_A,1RCJ_A,1SHV_A,1TDG_A,1TDL_A,1VM1_A,2A3U_A,2A49_A,1YLJ_A,1YLP_A,1YLT_A,1YLW_A,1YLY_A,1YLY_B,1YLZ_A,1YLZ_B,1YM1_A,1YM1_B,1YMS_A,1YMS_B,1YMX_A,1YMX_B

Degree of conservation cutoff: 0.9

The output files are in **1axb_a_0.9** directory.

Degree of conservation cutoff: 0.8

The output files are in **1axb_a_0.8** directory.

	By PyWATER	In reference paper
No of water molecules	15713	-
No. of clusters	2049	-
No. of clusters with >= 80% conservation	18	-
No. of clusters with >= 90% conservation	12	13

PyWATER identified 12 water molecules out of 13 described, which have a degree of conservation of at least 0.9 (present in 90% of all structures). The 13th water molecule was not identified because more than one position was defined in one crystal structure. PyWATER discarded this water molecule from the cluster and thus its degree of conservation fell to 0.89 in this case. Thus, it was not found with the criteria of 90% conservation.

MHC class – I

(Ogata and Wodak, 2002)

Query protein: 1I4F_A

User defined list:
1I4F_A,1TMC_A,1AGD_A,1HSA_A,1A1N_A,1E27_A,1A1M_A,1QLF_A,1QO3_A,1KBG_H,1ED3_A,1MHC_A

X-ray structure refinement assessing method : No refinement

Degree of conservation cutoff: 0.5

The output files are in **1i4f_a_0.5** directory.

	By PyWATER	In reference paper
No of water molecules	2033	-
No. of clusters	864	-
No. of clusters with >= 90% conservation	68	67

BPTI:

(Sanschagrin and Kuhn, 1998)

Query protein: 4PTI_A

User defined list: 4PTI_A,5PTI_A,6PTI_A,9PTI_A

X-ray structure refinement assessing method : Mobility

Degree of conservation cutoff: 0.5

The output files are in **4pti_a_0.5** directory.

	By PyWATER	In reference paper
No of water molecules	259 (+4 removed by Mobility filter)	263
No. of clusters	132	134
No. of clusters with >= 50% conservation	69	73
No. of clusters with >= 100% conservation	17	18

Trypsin:

(Sanschagrin and Kuhn, 1998)

1tpo_a_0.5

Query protein: 1TPO_A

User defined list: 1TPO_A,2PTN_A,3PTN_A

X-ray structure refinement assessing method : Mobility

Degree of conservation cutoff: 0.5

The output files are in **1tpo_a_0.5** directory.

	By PyWATER	In reference paper
No of water molecules	243 (+5 removed by Mobility filter)	248
No. of clusters	104	106
No. of clusters with >= 50% conservation	82	82
No. of clusters with >= 100% conservation	57	60

Thrombin:

(Sanschagrin and Kuhn, 1998)

Sanschagrin and Kuhn performed the study on whole structure together, while with PyWATER we performed study for heavy chain and light chain separately.

Chain H (heavy chain):

Query protein: 1HAI_H

User defined list:
1HAI_H,1ABJ_H,1PPB_H,1TMB_H,1HAH_H,1TMT_H,1ABI_H,1THR_H,1THS_H,1IHS_H

X-ray structure refinement assessing method : Mobility

Degree of conservation cutoff: 0.5

The output files are in **1hai_h_0.5** directory.

	By PyWATER	In reference paper
No of water molecules	1770	-
No. of clusters	662	-
No. of clusters with >= 50% conservation	115	-
No. of clusters with >= 100% conservation	26	-

Chain L (Light chain):

Query protein: 1HAI_L

User defined list:

1HAI_L,1ABJ_L,1PPB_L,1TMB_L,1HAH_L,1TMT_L,1ABI_L,1THR_L,1THS_L,1IHS_L

X-ray structure refinement assessing method : Mobility

Degree of conservation cutoff: 0.5

The output files are in **1hai_l_0.5** directory.

	By PyWATER	In reference paper
No of water molecules	220	-
No. of clusters	102	-
No. of clusters with >= 50% conservation	8	-
No. of clusters with >= 100% conservation	1	-

Though, it is not comparable directly. We show the total numbers for heavy chain and light chain study.

Total of heavy chain and Light chain:

	By PyWATER	In reference paper
No of water molecules	1990	2075
No. of clusters	764	708
No. of clusters with >= 50% conservation	123	131
No. of clusters with >= 100% conservation	27	28

Bromodomain containing protein 4

(Lucas *et al.*, 2013)

Query protein: 4LYW_A (with default parameters)

Sequence identity cutoff: 95

Resolution cutoff: 2.0

X-ray structure refinement assessing method : Mobility

Degree of conservation cutoff: 0.5

The output files are in **4lyw_a_0.7** directory.

	By PyWATER	In reference paper
No of water molecules		
No. of clusters		
No. of clusters with >= 70% conservation		

Bös,F. and Pleiss,J. (2008) Conserved water molecules stabilize the Omega-loop in class A beta-lactamases. *Antimicrob. Agents Chemother.*, **52**, 1072–9.

Lucas,X. *et al.* (2013) 4-Acyl Pyrroles: Mimicking Acetylated Lysines in Histone Code Reading. *Angew. Chem. Int. Ed. Engl.*, **52**, 14055–9.

Ogata,K. and Wodak,S.J. (2002) Conserved water molecules in MHC class-I molecules and their putative structural and functional roles. *Protein Eng.*, **15**, 697–705.

Sanschagrin,P.C. and Kuhn,L. a (1998) Cluster analysis of consensus water sites in thrombin and trypsin shows conservation between serine proteases and contributions to ligand specificity. *Protein Sci.*, **7**, 2054–64.