

Composition of training, validation, and test sets

	PDBBIND	DTC binding	DTC nonbinding	Docked Negatives
Training_1	1573	64551	19957	84508
Validation_1	142	275	46	321
Test_1	136	271	46	317
Training_2	1420	64602	19680	84282
Validation_2	140	273	45	318
Test_2	137	279	48	327
Training_3	1446	61026	19137	80163
Validation_3	144	274	48	322
Test_3	135	276	45	321
Training_4	1453	58995	20779	79774
Validation_4	141	275	46	321
Test_4	138	274	45	319
Training_5	1582	59024	20124	79148
Validation_5	135	275	50	325
Test_5	139	272	45	317