Structurally Conserved Binding Sites of Hemagglutinin as Targets for Influenza Drug and Vaccine Development

Supporting Information

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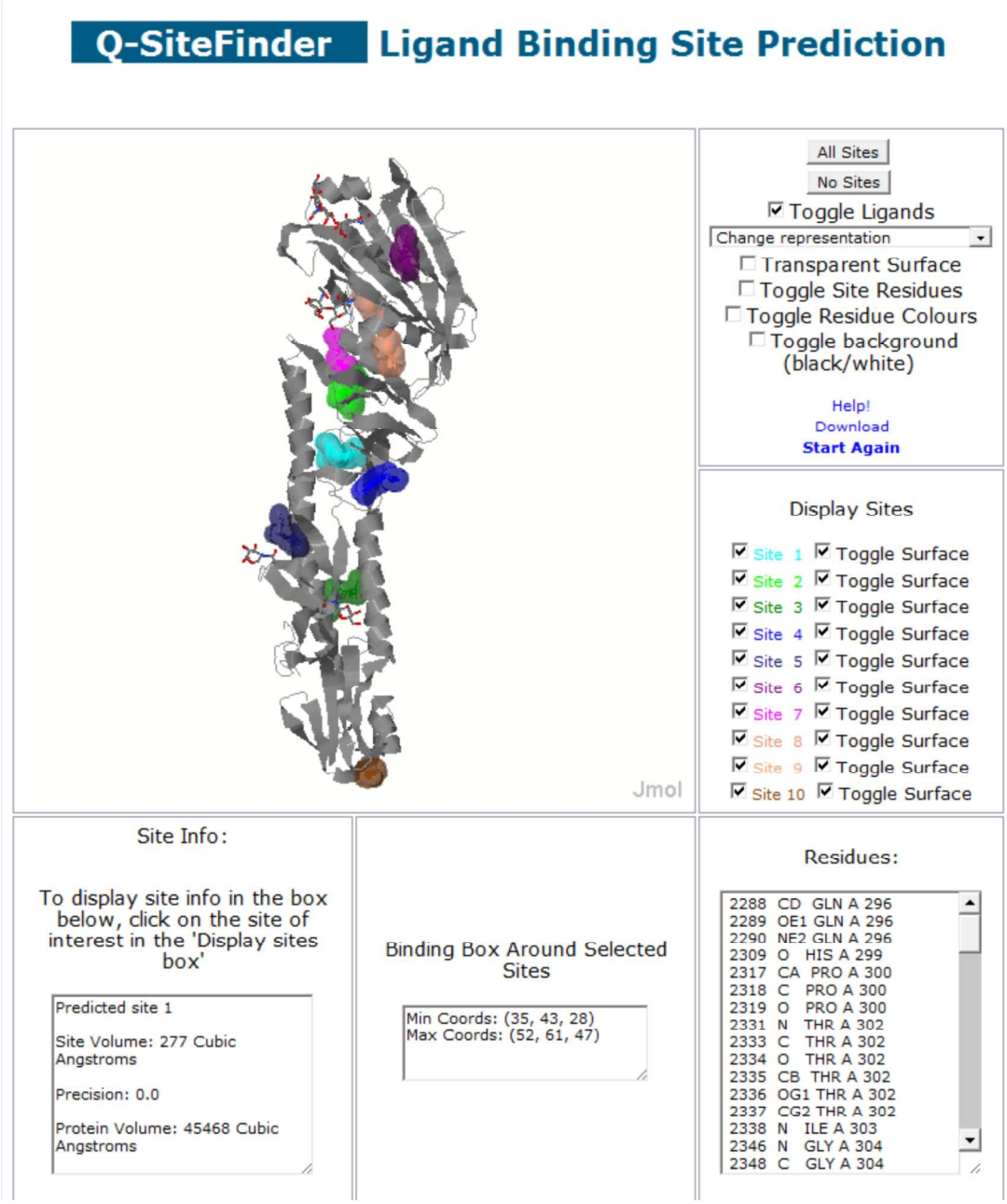

Figure S1. The output page of Q-Site Finder

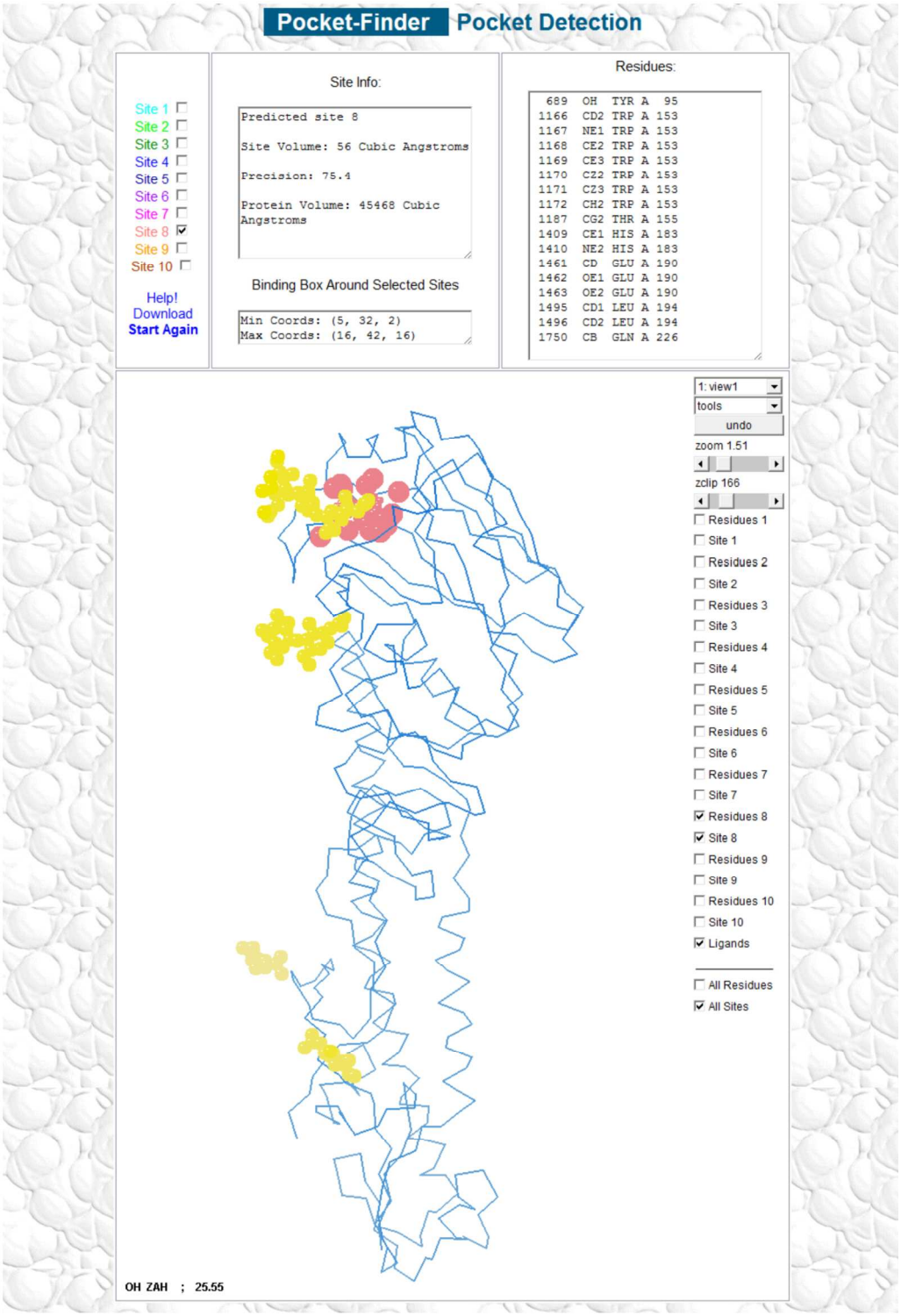

Figure S2. The output page of Pocket Finder

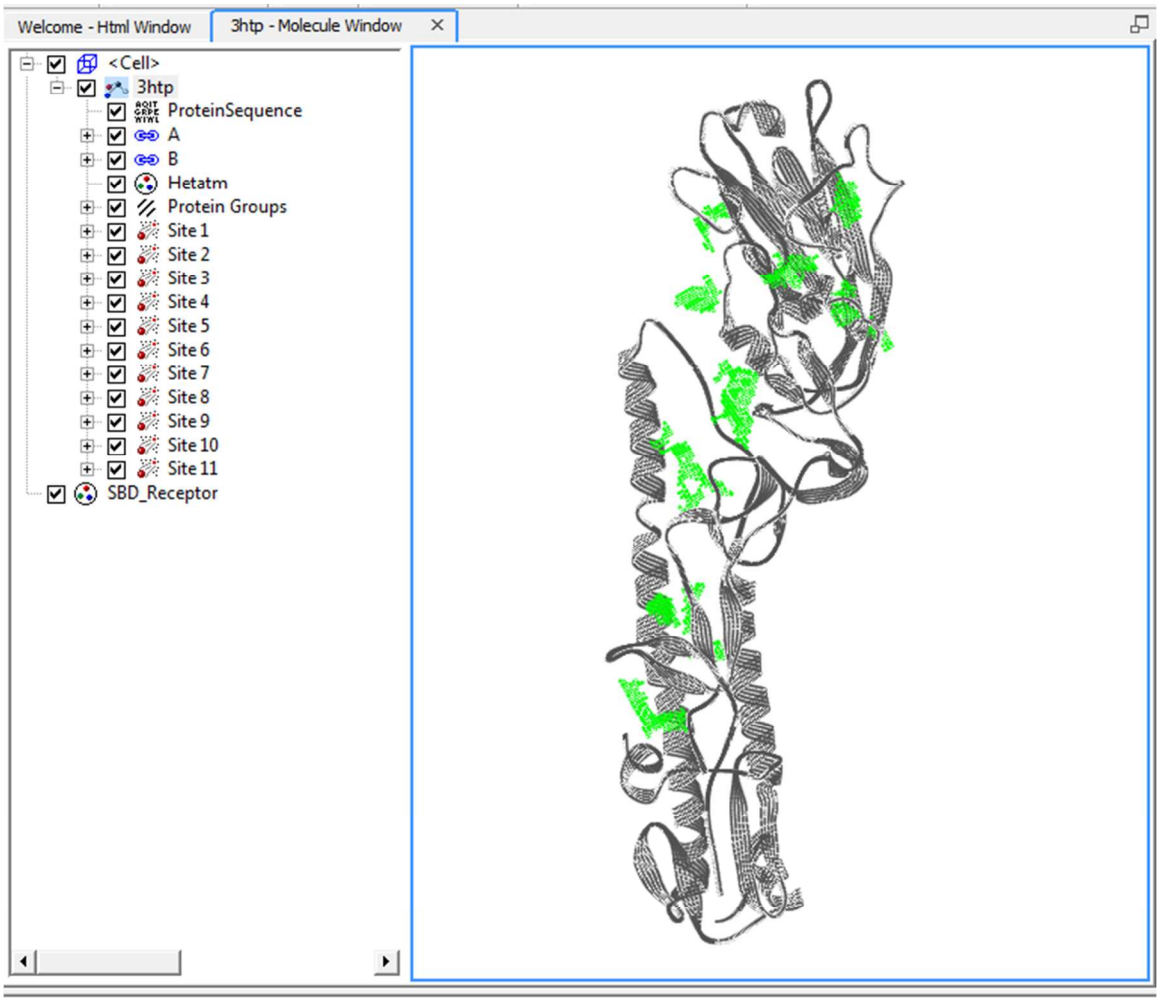

Figure S3. The output display of Binding Site Tools in Accelrys Discovery Studio

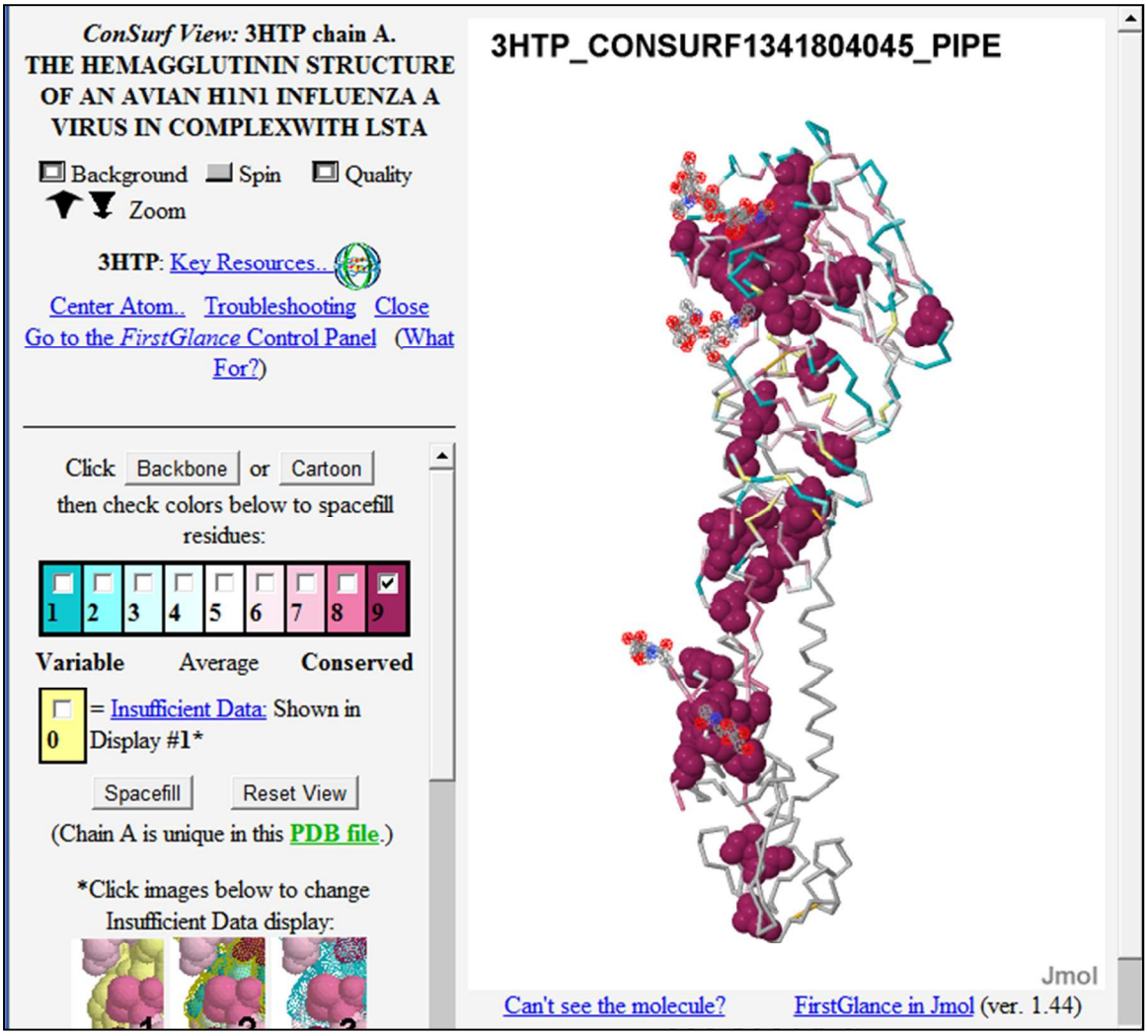

Figure S4. The output page of ConSurf

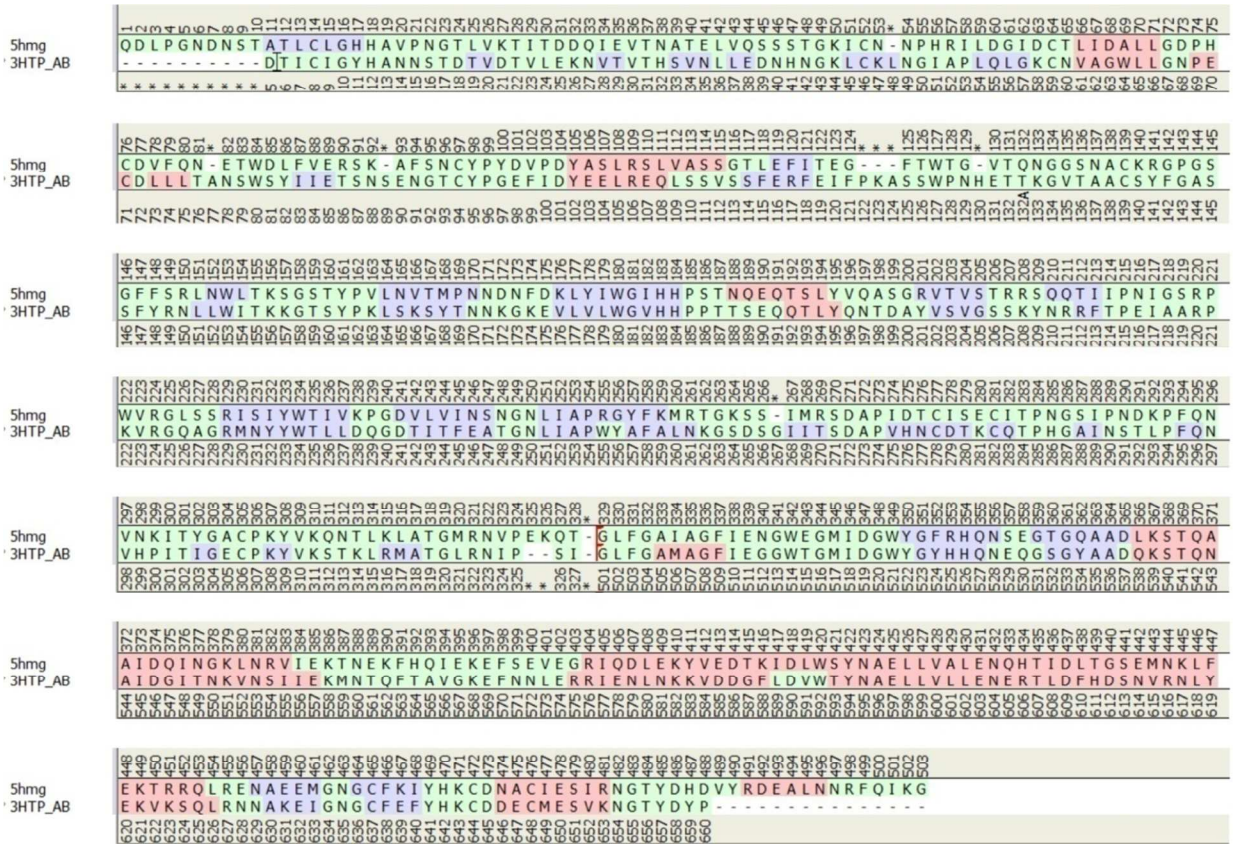

Figure S5. Numbering alignment between H3 ((A/Aichi/2/1968(H3N2), PDB ID 5HMG) and H1 (PDB ID 3HTP)
*red line indicates the separator between HA1 and HA2 (Chain A and B).

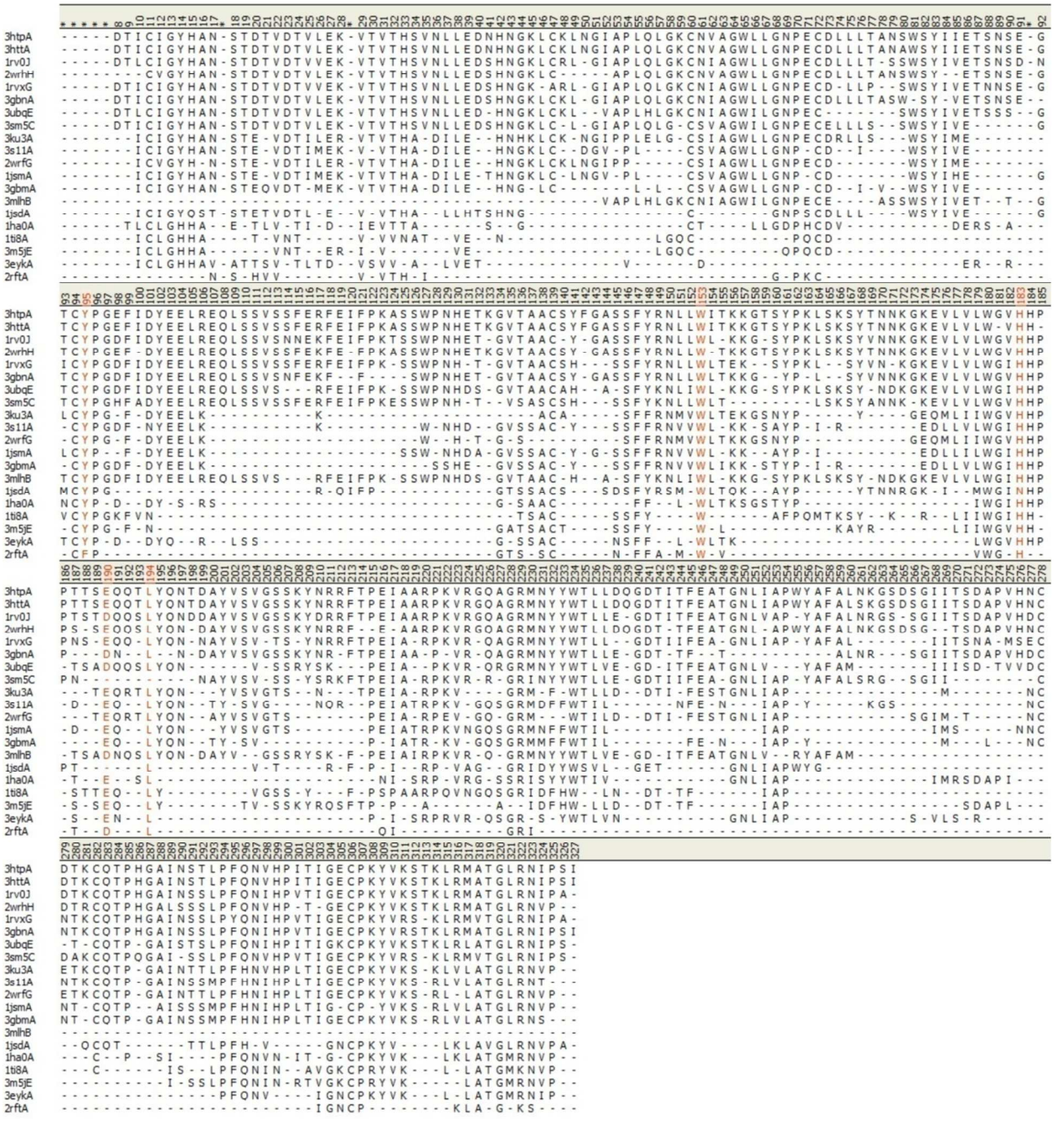

Figure S6. The structural alignment of 3HTP_A query resulted from ProBiS

Table S1. Prediction score of each conserved residue according to rank order of all predictors.

Rank Order	Predictors									
	ProBiS		Q-Site Finder		Pocket Finder		ADS		ConSurf	
1st Score	P69	R229	H299	T561	E103	I303	E103	I301	D5	G304
	C71	M230	P300	Q562	E104	A565	R106	T302	I7	C306
	C94	C306	T302	T564	R106	V566	E107	I303	C8	P307
	Y95	P307	I303	V566	E107	G567	S110	A565	H12	Y309
	P96	Q542	G304	V584	S110	K568	S266	V566	N14	L315
	G134	A544	E305	D585	D265	E569	G267	G567	S16	G320
	T136	I545	C306	F588	S266	F570	I268	K568	V20	R322
	A138	D546	P307	L589	G267	E578	I269	E569	T22	N323
	C139	I548	K308		I268	N581	Q283		V30	P325
	F147	T549	Y309		I269	K582			T31	G501
	Y148	V552			P300	D585			C46	A505
	L151	N553			I301	D586			G67	A507
	W153	L580			T302				P69	G508
	L179	K582							S81	E511
	W180	V584							E85	G513
	G181	D585							C94	G520
	H183	D590							Y95	G523
	L194	D609							P96	N528
									L105	G531
									G134	A536
									C139	D537
									F147	S540
									N170	T541
									W180	Q542
									H183	A544
									H184	N553
									Y195	N560
									P215	N604
									R220	T607
									R229	D612
									G249	L626
									P254	N629
									S266	A630
									S271	G636
									C282	C637
									G287	H642
									F295	T656
									N297	
2nd Score	C8	Q296	E103	I301	Q296	Y309	L36	V552	G10	I252
	I9	V298	R106	T302	H299	T561	P294	I555	Y11	A253
	G10	G304	E107	T303	P300	Q562	F295	I556	A13	C278
	Y11	Y309	S110	A565	T302	T564	L315	A596	T17	P294
	V20	V310	S266	V566	G304	V566	R316	L599	N27	Q296
	T22	M317	G267	G567	C306	D585	M317	V600	T29	H299
	V28	A318	I268	K568	P307	F588	A318	E603	S33	K308
	C59	T319	I269	E569	K308		T319	N604	N35	S312
	G67	G320	T270				I548	T607	L36	M317
	N68	L321					K551		L37	A318
	E70	R322							E38	T319
	E85	N323							L56	I327
	V135	K551							C59	G504
	S146	I577							G63	M506
	Y161	E578							N68	F509
	P162	N579							C71	I510
	V182	K583							I83	G512
	H184	D586							G97	G516
	E190	L589							E104	W521
	P215	V591							R106	Y522
	I217	T593							S110	H526
	V223	L602							W127	G533
	G228	E603							T136	A535
	Y233	E605							S146	I548
	W234	T607							W153	K551
	T235	L608							I154	M559

	L236	N614							Y161	E569
	L237	V615							L177	F570
	F295	L618							G181	L601
									P185	L608
									Q191	N614
									L194	L618
									V204	G634
									S206	F638
									Y233	C648
									W234	V652
									Q239	N654
									D241	Y657
									I243	Y659
									A247	P660
									N250	
3rd Score	I7	K308	L502	N550	G63	A77	Y11	M506	T6	A257
	H12	K311	F503	K551	W64	F115	H12	A507	I9	I268
	S16	I324	G547		L65	E116	A13	G513	D21	T280
	D18	P325	I548		G67	R117	T22	W521	E25	T284
	V30	N550			N68	R149	V28	Y522	V28	A288
	T31	I556			C71	F258	T31	N604	H32	I289
	L37	R576			D72	A259	G320	E605	N60	S291
	E38	N581			L74	L260	L321	L608	A62	I303
	D72	Y594			L75		R322	D609	D72	V310
	A137	N595			T76		N323	H611	W80	L321
	R149	L598					I324	D612	Y82	S326
	P185	V600					G501	V615	T86	F503
	Q191	N604					L502		S89	W514
	R220	R606							N91	I545
	P221	H611							G92	T549
	I252	D612							H130	S554
	P294	S613							R149	E574
	N297	N617							N150	R576
	E305	E620							P162	D586
									Y168	D590
									V202	T593
									S203	N595
									I217	A596
									P221	L599
									V223	V600
									R224	E603
									Q226	V615
									G228	V622
									M230	C644
									G240	D645
									E246	S651
									T248	G655
4th Score	A13	N231	E38	C282	K123	Y148	G63	L75	D18	L237
	V23	Y232	N40	A288	T132	L151	W64	A77	L45	F245
	E25	F245	H41	I289	T132A	L152	L65	F115	L48	L251
	S33	A253	N42	N290	K133	W153	G67	R117	G50	Y256
	L36	P254	D279	S291	G134	W255	N68	R149	Q55	I269
	G43	I269	T280	T292	V135		P69	N150	L66	Q283
	P53	H299	K281		F147		C71	F258	I84	N290
	N60	T302					D72		E103	L293
	L65	I303					L74		E107	T302
	L66	L315							S111	K311
	T93	R316							V112	K314
	G97	G523							S114	R316
	D101	N543							R117	L502
	Y102	S554							P122	Y524
	R106	I555							A138	Q530
	S145	R575							Y148	I556
	L152	W592							L151	K558
	I154	A596							S167	V566
	L177	E597							V176	E597
	V178	L599							V182	R606
	T187	L601							N210	D609

	Y195	F610							R212	E632
	S206	R616							Y232	N635
	E216	Y619							T235	
	A227	V622								
5th Score	T19	G249	T19	K314	S291	K308	L65	V178	N15	F258
	D21	I289	V20	L315	T292	I556	L66	L179	L24	A259
	L24	S291	D21	R316	L293	M559	F99	W180	V34	G267
	H32	L502	K26	M317	P294	N560	I100	Y232	H41	P300
	L54	F503	S312		E305	T561	R117	Y233	N42	I324
	S81	W521	T313		C306		F118	W234	L74	T515
	Y82	Y522			P307		I120	L237	F99	D519
	I84	Y524					F121	I243	D101	N550
	E98	A536					N150	F245	F115	Q562
	F99	D537					L151	P254	E116	T564
	E103	K539					K166	W255	I120	I577
	N150	S540					S167	Y256	L152	N579
	T155	T541					Y168	A257	E175	N581
	S160	E557					N170	F258	T187	Y594
	K174	E574					V176		A200	L598
	V176	K621					L177		Y201	E605
	V204	K623							S207	H611
	K222	L626							Y209	E639
	R224	C648							E216	F640
	Q226	S651							A218	
									G225	
8th Score					Y95	E190				
					W153	L194				
					T155	Q226				
					H183					