

Protein Pharmacophore site	Site Details	Site Label	Number of acceptors for H-Bonds	Number of Donors for H-Bonds	Hydrophobic Interactions
Src__atom_1	/B/WAT`1/O	Donor	39	29	
Src__atom_2	/B/WAT`2/N	Acceptor	39	29	
Src__atom_3	/B/WAT`4/O	Donor	80	36	
Src__atom_4	/B/WAT`5/N	Acceptor	80	36	
Src__atom_5	/G/WAT`3/C	Grease			191
Src__atom_6	/G/WAT`6/C	Grease			87
Mcr__atom_1	/A/WAT`1/O	Acceptor	30	5	
Mcr__atom_2	/D/WAT`2/N	Donor	14	15	
Mcr__atom_3	/D/WAT`5/N	Donor	54	25	
Mcr__atom_4	/G/WAT`3/C	Grease			142
Mcr__atom_5	/G/WAT`4/C	Grease			93
Mcr__atom_6	/G/WAT`6/C	Grease			93
Mcr__atom_7	/G/WAT`7/C	Grease			130
Akt1_atom_1	/A/WAT`2/O	Acceptor	115	63	
Akt1_atom_2	/A/WAT`5/O	Acceptor	78	31	
Akt1_atom_3	/D/WAT`1/N	Donor	83	42	
Akt1_atom_4	/D/WAT`4/N	Donor	74	35	
Akt1_atom_5	/G/WAT`3/C	Grease			183
Ppara_atom_1	/B/WAT`2/O	Donor	120	2	
Ppara_atom_2	/B/WAT`3/N	Acceptor	120	5	
Ppara_atom_3	/G/WAT`1/C	Grease			159
Ppara_atom_4	/G/WAT`4/C	Grease			136
Ppara_atom_5	/G/WAT`5/C	Grease			164
Ppara_atom_6	/G/WAT`6/C	Grease			131
Ppara_atom_7	/G/WAT`7/C	Grease			206
Ppara_atom_8	/G/WAT`8/C	Grease			211
Ppara_atom_9	/G/WAT`9/C	Grease			152
Ppara_atom_10	/G/WAT`10/C	Grease			108
Urok_atom_1	/D/WAT`1/N	Donor	19	202	
Urok_atom_2	/G/WAT`2/C	Grease			224
Urok_atom_3	/G/WAT`3/C	Grease			265
Urok_atom_4	/G/WAT`4/C	Grease			179
Urok_atom_5	/G/WAT`5/C	Grease			179
Aldr_atom_1	/A/WAT`2/O	Acceptor	193	11	
Aldr_atom_2	/A/WAT`3/O	Acceptor	294	61	
Aldr_atom_3	/G/WAT`1/C	Grease			269
Aldr_atom_4	/G/WAT`4/C	Grease			284

Aldr_atom_5	/G/WAT`5/C	Grease			139
Aldr_atom_6	/G/WAT`6/C	Grease			268
Weel_atom_1	/B/WAT`2/O	Donor	31	9	
Weel_atom_2	/B/WAT`3/N	Acceptor	31	9	
Weel_atom_3	/D/WAT`1/N	Donor	20	19	
Weel_atom_4	/G/WAT`4/C	Grease			79
Weel_atom_5	/G/WAT`5/C	Grease			87
Weel_atom_6	/G/WAT`6/C	Grease			71
Weel_atom_7	/G/WAT`7/C	Grease			49
Weel_atom_8	/G/WAT`8/C	Grease			34
Weel_atom_9	/G/WAT`9/C	Grease			53
Met__atom_1	/A/WAT`3/O	Acceptor	81	32	
Met__atom_2	/A/WAT`9/O	Acceptor	27	25	
Met__atom_3	/B/WAT`7/O	Donor	86	40	
Met__atom_4	/B/WAT`8/N	Acceptor	86	40	
Met__atom_5	/G/WAT`1/C	Grease			28
Met__atom_6	/G/WAT`2/C	Grease			48
Met__atom_7	/G/WAT`4/C	Grease			251
Met__atom_8	/G/WAT`5/C	Grease			285
Met__atom_9	/G/WAT`6/C	Grease			146
Met__atom_10	/G/WAT`10/C	Grease			35
Met__atom_11	/G/WAT`11/C	Grease			37