

Mutation near the binding interfaces at AHSP is pathogenic

Supplementary Table 1. Interface energy and predicted hot spots interface residues of the template-target protein complex

Template	Target	Interface Energy	Interface Residues Contacts at Template <--> Target
AHSP	HBA1	-14.34	<p> pdb2_A_ASP_43 <--> pdb1_A_ASP_29 pdb2_A_VAL_26 <--> pdb1_A_TYR_51 pdb2_A_VAL_26 <--> pdb1_A_ASN_50 pdb2_A_GLN_24 <--> pdb1_A_TYR_51 pdb2_A_GLN_24 <--> pdb1_A_TYR_52 pdb2_A_ASP_29 <--> pdb1_A_PHE_47 pdb2_A_ASP_29 <--> pdb1_A_ASN_46 pdb2_A_ASP_29 <--> pdb1_A_ASP_43 pdb2_A_GLN_25 <--> pdb1_A_PHE_47 pdb2_A_GLN_25 <--> pdb1_A_TRP_44 pdb2_A_PHE_47 <--> pdb1_A_GLN_25 pdb2_A_PHE_47 <--> pdb1_A_GLN_24 pdb2_A_TYR_48 <--> pdb1_A_GLN_24 pdb2_A_PHE_47 <--> pdb1_A_VAL_26 pdb2_A_TYR_48 <--> pdb1_A_LEU_21 pdb2_A_VAL_20 <--> pdb1_A_GLU_17 pdb2_A_ASN_50 <--> pdb1_A_ASP_29 pdb2_A_GLN_24 <--> pdb1_A_PHE_47 pdb2_A_GLN_24 <--> pdb1_A_TYR_48 pdb2_A_VAL_26 <--> pdb1_A_PHE_47 pdb2_A_PHE_47 <--> pdb1_A_ASP_29 pdb2_A_TRP_44 <--> pdb1_A_TRP_44 pdb2_A_TYR_51 <--> pdb1_A_GLN_24 pdb2_A_ASN_46 <--> pdb1_A_ASP_29 pdb2_A_TYR_51 <--> pdb1_A_VAL_26 pdb2_A_ASN_50 <--> pdb1_A_VAL_26 pdb2_A_ASP_29 <--> pdb1_A_ASN_50 pdb2_A_LEU_21 <--> pdb1_A_LEU_21 pdb2_A_PHE_47 <--> pdb1_A_PRO_30 pdb2_A_GLU_17 <--> pdb1_A_GLN_24 pdb2_A_GLU_17 <--> pdb1_A_VAL_20 pdb2_A_TYR_52 <--> pdb1_A_GLN_24 pdb2_A_LEU_21 <--> pdb1_A_TRP_44 pdb2_A_GLN_24 <--> pdb1_A_GLU_17 </p>
AHSP	G60V of HBA1	-68.52	<p> pdb2_A_LEU_31 <--> pdb1_A_PHE_118 pdb2_A_LEU_31 <--> pdb1_A_ALA_111 pdb2_A_LEU_31 <--> pdb1_A_LEU_110 pdb2_A_GLN_24 <--> pdb1_A_SER_36 pdb2_A_GLN_24 <--> pdb1_A_LEU_35 pdb2_A_VAL_26 <--> pdb1_A_ARG_32 pdb2_A_PHE_47 <--> pdb1_A_THR_39 pdb2_A_SER_91 <--> pdb1_A_PRO_120 pdb2_A_ASP_43 <--> pdb1_A_VAL_97 pdb2_A_LEU_21 <--> pdb1_A_SER_36 pdb2_A_LEU_21 <--> pdb1_A_PHE_37 </p>

Mutation near the binding interfaces at AHSP is pathogenic

pdb2_A_LYS_90 <--> pdb1_A_PRO_120
pdb2_A_PHE_88 <--> pdb1_A_HIS_123
pdb2_A_LEU_21 <--> pdb1_A_PRO_38
pdb2_A_LEU_31 <--> pdb1_A_LEU_107
pdb2_A_ASP_29 <--> pdb1_A_ALA_112
pdb2_A_PRO_30 <--> pdb1_A_ALA_111
pdb2_A_ASP_29 <--> pdb1_A_ALA_111
pdb2_A_LEU_31 <--> pdb1_A_ASP_127
pdb2_A_LEU_31 <--> pdb1_A_HIS_123
pdb2_A_VAL_32 <--> pdb1_A_HIS_123
pdb2_A_VAL_32 <--> pdb1_A_HIS_104
pdb2_A_VAL_32 <--> pdb1_A_LEU_107
pdb2_A_VAL_32 <--> pdb1_A_ASP_127
pdb2_A_GLN_25 <--> pdb1_A_VAL_108
pdb2_A_GLN_25 <--> pdb1_A_HIS_104
pdb2_A_PHE_47 <--> pdb1_A_PHE_37
pdb2_A_LEU_89 <--> pdb1_A_PRO_120
pdb2_A_SER_33 <--> pdb1_A_HIS_123
pdb2_A_SER_33 <--> pdb1_A_ALA_124
pdb2_A_SER_33 <--> pdb1_A_ASP_127
pdb2_A_ASP_29 <--> pdb1_A_VAL_108
pdb2_A_PRO_30 <--> pdb1_A_HIS_123
pdb2_A_TYR_85 <--> pdb1_A_HIS_123
pdb2_A_PRO_30 <--> pdb1_A_VAL_108
pdb2_A_PRO_30 <--> pdb1_A_LEU_107
pdb2_A_PRO_30 <--> pdb1_A_HIS_104
pdb2_A_GLN_25 <--> pdb1_A_SER_36
AHSP L92F of HBA1 -53.37 pdb2_A_VAL_97 <--> pdb1_A_LEU_31
pdb2_A_VAL_97 <--> pdb1_A_VAL_32
pdb2_A_LYS_128 <--> pdb1_A_GLN_24
pdb2_A_SER_36 <--> pdb1_A_THR_39
pdb2_A_PRO_120 <--> pdb1_A_TYR_51
pdb2_A_ALA_124 <--> pdb1_A_LEU_21
pdb2_A_PRO_120 <--> pdb1_A_TYR_52
pdb2_A_ALA_124 <--> pdb1_A_GLN_24
pdb2_A_PHE_37 <--> pdb1_A_THR_39
pdb2_A_PHE_37 <--> pdb1_A_ASP_36
pdb2_A_PRO_96 <--> pdb1_A_LEU_31
pdb2_A_THR_135 <--> pdb1_A_ASP_29
pdb2_A_ASP_127 <--> pdb1_A_GLN_25
pdb2_A_ALA_121 <--> pdb1_A_GLU_17
pdb2_A_PRO_120 <--> pdb1_A_GLU_17
pdb2_A_PHE_118 <--> pdb1_A_TYR_51
pdb2_A_LEU_107 <--> pdb1_A_TRP_44
pdb2_A_LEU_101 <--> pdb1_A_ASP_36
pdb2_A_LEU_101 <--> pdb1_A_VAL_32
pdb2_A_THR_119 <--> pdb1_A_TYR_51
pdb2_A_PRO_115 <--> pdb1_A_TYR_51
pdb2_A_HIS_104 <--> pdb1_A_TRP_44

Mutation near the binding interfaces at AHSP is pathogenic

			pdb2_A_PRO_120 <--> pdb1_A_TYR_48
			pdb2_A_HIS_104 <--> pdb1_A_VAL_40
			pdb2_A_LYS_100 <--> pdb1_A_PRO_30
			pdb2_A_ASP_127 <--> pdb1_A_LEU_21
			pdb2_A_HIS_104 <--> pdb1_A_ASP_43
			pdb2_A_ALA_111 <--> pdb1_A_PHE_47
			pdb2_A_VAL_108 <--> pdb1_A_ASP_43
			pdb2_A_ASP_127 <--> pdb1_A_TRP_44
			pdb2_A_HIS_123 <--> pdb1_A_TYR_48
			pdb2_A_HIS_123 <--> pdb1_A_LEU_21
			pdb2_A_PHE_118 <--> pdb1_A_PHE_47
			pdb2_A_HIS_123 <--> pdb1_A_TRP_44
AHSP	K17M of HBA1	-47.51	pdb2_A_HIS_123 <--> pdb1_A_PHE_47
			pdb2_A_LEU_31 <--> pdb1_A_PHE_118
			pdb2_A_ASN_50 <--> pdb1_A_THR_39
			pdb2_A_LEU_31 <--> pdb1_A_ALA_111
			pdb2_A_PHE_27 <--> pdb1_A_LEU_3
			pdb2_A_ASN_46 <--> pdb1_A_THR_39
			pdb2_A_ASN_46 <--> pdb1_A_PRO_38
			pdb2_A_ASP_87 <--> pdb1_A_LEU_3
			pdb2_A_LEU_31 <--> pdb1_A_HIS_104
			pdb2_A_ASN_28 <--> pdb1_A_LYS_8
			pdb2_A_ASP_29 <--> pdb1_A_PHE_118
			pdb2_A_LEU_31 <--> pdb1_A_LEU_107
			pdb2_A_ASP_29 <--> pdb1_A_ALA_112
			pdb2_A_PRO_30 <--> pdb1_A_ALA_111
			pdb2_A_ASP_29 <--> pdb1_A_ALA_111
			pdb2_A_LEU_31 <--> pdb1_A_VAL_108
			pdb2_A_ASN_28 <--> pdb1_A_SER_4
			pdb2_A_ASN_28 <--> pdb1_A_ASP_7
			pdb2_A_ASP_29 <--> pdb1_A_PRO_115
			pdb2_A_ASP_29 <--> pdb1_A_VAL_11
			pdb2_A_ASN_28 <--> pdb1_A_VAL_11
			pdb2_A_ASP_43 <--> pdb1_A_PRO_38
			pdb2_A_ASP_43 <--> pdb1_A_SER_36
			pdb2_A_ASP_43 <--> pdb1_A_PHE_37
			pdb2_A_LEU_31 <--> pdb1_A_HIS_123
			pdb2_A_VAL_32 <--> pdb1_A_HIS_123
			pdb2_A_VAL_32 <--> pdb1_A_HIS_104
			pdb2_A_PHE_47 <--> pdb1_A_LEU_35
			pdb2_A_ASN_28 <--> pdb1_A_PRO_120
			pdb2_A_PHE_47 <--> pdb1_A_PRO_38
			pdb2_A_LEU_31 <--> pdb1_A_VAL_11
			pdb2_A_SER_33 <--> pdb1_A_ASP_127
			pdb2_A_PRO_30 <--> pdb1_A_VAL_108
			pdb2_A_ASP_43 <--> pdb1_A_LEU_101
			pdb2_A_PRO_30 <--> pdb1_A_HIS_104
AHSP	W15R of HBA1	-50.98	pdb2_A_ASN_28 <--> pdb1_A_PHE_118
			pdb2_A_VAL_97 <--> pdb1_A_LEU_31

Mutation near the binding interfaces at AHSP is pathogenic

pdb2_A_VAL_97 <--> pdb1_A_VAL_32
pdb2_A_LYS_128 <--> pdb1_A_GLN_24
pdb2_A_SER_36 <--> pdb1_A_THR_39
pdb2_A_PRO_120 <--> pdb1_A_TYR_51
pdb2_A_ALA_124 <--> pdb1_A_LEU_21
pdb2_A_PRO_120 <--> pdb1_A_TYR_52
pdb2_A_ALA_124 <--> pdb1_A_GLN_24
pdb2_A_PHE_37 <--> pdb1_A_THR_39
pdb2_A_LYS_100 <--> pdb1_A_ASP_29
pdb2_A_PRO_96 <--> pdb1_A_LEU_31
pdb2_A_ASP_127 <--> pdb1_A_GLN_25
pdb2_A_ALA_121 <--> pdb1_A_GLU_17
pdb2_A_PRO_120 <--> pdb1_A_GLY_14
pdb2_A_PRO_120 <--> pdb1_A_GLU_17
pdb2_A_PHE_37 <--> pdb1_A_ASP_36
pdb2_A_LEU_3 <--> pdb1_A_VAL_20
pdb2_A_PHE_118 <--> pdb1_A_TYR_51
pdb2_A_LEU_107 <--> pdb1_A_TRP_44
pdb2_A_LEU_101 <--> pdb1_A_VAL_32
pdb2_A_THR_119 <--> pdb1_A_TYR_51
pdb2_A_PHE_37 <--> pdb1_A_VAL_40
pdb2_A_PRO_115 <--> pdb1_A_TYR_51
pdb2_A_HIS_104 <--> pdb1_A_TRP_44
pdb2_A_PRO_120 <--> pdb1_A_TYR_48
pdb2_A_ASP_127 <--> pdb1_A_GLN_24
pdb2_A_HIS_104 <--> pdb1_A_VAL_40
pdb2_A_LYS_100 <--> pdb1_A_PRO_30
pdb2_A_ASP_127 <--> pdb1_A_LEU_21
pdb2_A_HIS_104 <--> pdb1_A_ASP_43
pdb2_A_ALA_111 <--> pdb1_A_PHE_47
pdb2_A_VAL_108 <--> pdb1_A_ASP_43
pdb2_A_ASP_127 <--> pdb1_A_TRP_44
pdb2_A_HIS_123 <--> pdb1_A_TYR_48
pdb2_A_HIS_123 <--> pdb1_A_LEU_21
pdb2_A_SER_4 <--> pdb1_A_GLU_17
pdb2_A_PHE_118 <--> pdb1_A_PHE_47
pdb2_A_ALA_116 <--> pdb1_A_TYR_51
pdb2_A_HIS_123 <--> pdb1_A_TRP_44
pdb2_A_HIS_123 <--> pdb1_A_PHE_47
HBA1 Y85C of AHSP -62.56 pdb1_A_VAL_97 <--> pdb2_A_LEU_31
pdb1_A_VAL_97 <--> pdb2_A_VAL_32
pdb1_A_LYS_128 <--> pdb2_A_GLN_24
pdb1_A_SER_36 <--> pdb2_A_THR_39
pdb1_A_PRO_120 <--> pdb2_A_TYR_51
pdb1_A_ALA_124 <--> pdb2_A_LEU_21
pdb1_A_PRO_120 <--> pdb2_A_TYR_52
pdb1_A_ALA_124 <--> pdb2_A_GLN_24
pdb1_A_PHE_37 <--> pdb2_A_THR_39
pdb1_A_LYS_100 <--> pdb2_A_ASP_29

Mutation near the binding interfaces at AHSP is pathogenic

			pdb1_A_PRO_96 <--> pdb2_A_LEU_31
			pdb1_A ASP_127 <--> pdb2_A_GLN_25
			pdb1_A_ALA_121 <--> pdb2_A_GLU_17
			pdb1_A_PRO_120 <--> pdb2_A_GLU_17
			pdb1_A_PHE_37 <--> pdb2_A ASP_36
			pdb1_A_PHE_118 <--> pdb2_A TYR_51
			pdb1_A_LEU_107 <--> pdb2_A TRP_44
			pdb1_A_LEU_101 <--> pdb2_A ASP_36
			pdb1_A_LEU_101 <--> pdb2_A_VAL_32
			pdb1_A_THR_119 <--> pdb2_A TYR_51
			pdb1_A_PHE_37 <--> pdb2_A_VAL_40
			pdb1_A_PRO_115 <--> pdb2_A TYR_51
			pdb1_A_HIS_104 <--> pdb2_A TRP_44
			pdb1_A_PRO_120 <--> pdb2_A TYR_48
			pdb1_A_HIS_104 <--> pdb2_A_VAL_40
			pdb1_A_LYS_100 <--> pdb2_A_PRO_30
			pdb1_A ASP_127 <--> pdb2_A_LEU_21
			pdb1_A_HIS_104 <--> pdb2_A ASP_43
			pdb1_A_ALA_111 <--> pdb2_A_PHE_47
			pdb1_A_VAL_108 <--> pdb2_A ASP_43
			pdb1_A ASP_127 <--> pdb2_A TRP_44
			pdb1_A_HIS_123 <--> pdb2_A TYR_48
			pdb1_A_HIS_123 <--> pdb2_A_LEU_21
			pdb1_A_PHE_118 <--> pdb2_A_PHE_47
			pdb1_A_HIS_123 <--> pdb2_A TRP_44
			pdb1_A_HIS_123 <--> pdb2_A_PHE_47
HBA1	L21P of AHSP	-60.0	pdb2_A_LEU_31 <--> pdb1_A_PHE_118
			pdb2_A ASP_43 <--> pdb1_A_LEU_101
			pdb2_A_LEU_31 <--> pdb1_A_ALA_111
			pdb2_A_LEU_31 <--> pdb1_A_LEU_110
			pdb2_A_SER_91 <--> pdb1_A_PRO_120
			pdb2_A_TRP_44 <--> pdb1_A_SER_36
			pdb2_A_LYS_90 <--> pdb1_A_PRO_120
			pdb2_A_PRO_21 <--> pdb1_A_SER_36
			pdb2_A_PRO_21 <--> pdb1_A_LEU_35
			pdb2_A_PRO_21 <--> pdb1_A_PRO_38
			pdb2_A_LEU_31 <--> pdb1_A_LEU_107
			pdb2_A ASP_29 <--> pdb1_A_ALA_112
			pdb2_A_PRO_30 <--> pdb1_A_ALA_111
			pdb2_A ASP_29 <--> pdb1_A_ALA_111
			pdb2_A ASP_36 <--> pdb1_A ASP_127
			pdb2_A_LEU_31 <--> pdb1_A ASP_127
			pdb2_A_LEU_31 <--> pdb1_A_HIS_123
			pdb2_A_VAL_32 <--> pdb1_A_HIS_123
			pdb2_A_VAL_32 <--> pdb1_A_HIS_104
			pdb2_A_VAL_32 <--> pdb1_A_LEU_107
			pdb2_A_VAL_32 <--> pdb1_A ASP_127
			pdb2_A_GLN_25 <--> pdb1_A_VAL_108
			pdb2_A_GLN_25 <--> pdb1_A_HIS_104

Mutation near the binding interfaces at AHSP is pathogenic

			pdb2_A_PHE_47 <--> pdb1_A_THR_39
			pdb2_A_PHE_47 <--> pdb1_A_PRO_38
			pdb2_A_SER_33 <--> pdb1_A_HIS_123
			pdb2_A_SER_33 <--> pdb1_A_ALA_124
			pdb2_A_SER_33 <--> pdb1_A_ASP_127
			pdb2_A_ASP_29 <--> pdb1_A_VAL_108
			pdb2_A_PRO_30 <--> pdb1_A_HIS_123
			pdb2_A_TYR_85 <--> pdb1_A_HIS_123
			pdb2_A_PRO_30 <--> pdb1_A_VAL_108
			pdb2_A_PRO_30 <--> pdb1_A_LEU_107
			pdb2_A_GLN_25 <--> pdb1_A_SER_36
			pdb2_A_LEU_89 <--> pdb1_A_HIS_123
HBA1	V56G of AHSP	-58.47	pdb1_A_VAL_97 <--> pdb2_A_LEU_31
			pdb1_A_VAL_97 <--> pdb2_A_VAL_32
			pdb1_A_LYS_128 <--> pdb2_A_GLN_24
			pdb1_A_SER_36 <--> pdb2_A_THR_39
			pdb1_A_PRO_120 <--> pdb2_A_TYR_51
			pdb1_A_ALA_124 <--> pdb2_A_LEU_21
			pdb1_A_PRO_120 <--> pdb2_A_TYR_52
			pdb1_A_ALA_124 <--> pdb2_A_GLN_24
			pdb1_A_PHE_37 <--> pdb2_A_THR_39
			pdb1_A_PHE_37 <--> pdb2_A_ASP_36
			pdb1_A_PRO_96 <--> pdb2_A_LEU_31
			pdb1_A_THR_135 <--> pdb2_A_ASP_29
			pdb1_A_ASP_127 <--> pdb2_A_GLN_25
			pdb1_A_ALA_121 <--> pdb2_A_GLU_17
			pdb1_A_PRO_120 <--> pdb2_A_GLU_17
			pdb1_A_PHE_118 <--> pdb2_A_TYR_51
			pdb1_A_LEU_107 <--> pdb2_A_TRP_44
			pdb1_A_LEU_101 <--> pdb2_A_ASP_36
			pdb1_A_LEU_101 <--> pdb2_A_VAL_32
			pdb1_A_THR_119 <--> pdb2_A_TYR_51
			pdb1_A_PRO_115 <--> pdb2_A_TYR_51
			pdb1_A_HIS_104 <--> pdb2_A_TRP_44
			pdb1_A_PRO_120 <--> pdb2_A_TYR_48
			pdb1_A_HIS_104 <--> pdb2_A_VAL_40
			pdb1_A_LYS_100 <--> pdb2_A_PRO_30
			pdb1_A_ASP_127 <--> pdb2_A_LEU_21
			pdb1_A_HIS_104 <--> pdb2_A_ASP_43
			pdb1_A_ALA_111 <--> pdb2_A_PHE_47
			pdb1_A_VAL_108 <--> pdb2_A_ASP_43
			pdb1_A_ASP_127 <--> pdb2_A_TRP_44
			pdb1_A_HIS_123 <--> pdb2_A_LEU_21
			pdb1_A_PHE_118 <--> pdb2_A_PHE_47
			pdb1_A_HIS_123 <--> pdb2_A_TRP_44
			pdb1_A_HIS_123 <--> pdb2_A_PHE_47
AHSP	HBA2	-7.05	pdb1_A_HIS_112 <--> pdb2_B_THR_8
			pdb1_A_PRO_114 <--> pdb2_B_LYS_11
			pdb1_A_GLU_116 <--> pdb2_B_LYS_7

Mutation near the binding interfaces at AHSP is pathogenic

			<p> pdb1_B_LYS_120 <--> pdb2_B_THR_8 pdb1_A_HIS_20 <--> pdb2_B_PRO_4 pdb1_B_HIS_116 <--> pdb2_B_ALA_71 pdb1_B_GLU_121 <--> pdb2_B_GLY_15 pdb1_B_LYS_120 <--> pdb2_B_LYS_11 pdb1_A_HIS_112 <--> pdb2_B_LYS_7 pdb1_B_GLY_119 <--> pdb2_B_LYS_11 pdb1_A_TYR_24 <--> pdb2_B_PRO_4 pdb1_A_PRO_114 <--> pdb2_B_HIS_72 pdb1_A_PRO_114 <--> pdb2_B_VAL_73 pdb1_A_PRO_114 <--> pdb2_B_ALA_71 pdb1_B_HIS_117 <--> pdb2_B_ALA_71 pdb1_B_GLU_121 <--> pdb2_B_LYS_11 pdb1_A_ALA_115 <--> pdb2_B_ASP_75 pdb1_B_LYS_120 <--> pdb2_B_ALA_12 pdb1_A_ALA_115 <--> pdb2_B_VAL_73 pdb1_B_PHE_118 <--> pdb2_B_LYS_11 pdb1_A_PRO_5 <--> pdb2_A_GLN_68 pdb1_B_PRO_52 <--> pdb2_A_ASN_50 pdb1_A_ALA_121 <--> pdb2_A_ASN_50 pdb1_A_ASN_10 <--> pdb2_A_ASN_46 pdb1_A_THR_9 <--> pdb2_A_ARG_71 pdb1_B_THR_51 <--> pdb2_A_TYR_51 pdb1_A_LYS_17 <--> pdb2_A_GLU_35 pdb1_C_SER_344 <--> pdb2_A_PRO_60 pdb1_A_SER_4 <--> pdb2_A_ARG_53 pdb1_A_PRO_5 <--> pdb2_A_ASP_64 pdb1_A_THR_119 <--> pdb2_A_ASP_43 pdb1_A_ALA_121 <--> pdb2_A_ASN_46 pdb1_B_SER_50 <--> pdb2_A_GLN_54 pdb1_B_ASP_53 <--> pdb2_A_PHE_47 pdb1_A_ALA_6 <--> pdb2_A_ARG_53 pdb1_B_THR_51 <--> pdb2_A_ASN_50 pdb1_A_ALA_6 <--> pdb2_A_ILE_49 pdb1_A_GLU_117 <--> pdb2_A_THR_39 pdb1_A_ALA_116 <--> pdb2_A_THR_39 pdb1_B_THR_51 <--> pdb2_A_TYR_51 pdb1_B_THR_51 <--> pdb2_A_ASN_50 pdb1_A_ALA_13 <--> pdb2_A_GLU_42 pdb1_A_SER_4 <--> pdb2_A_ARG_53 pdb1_A_THR_119 <--> pdb2_A_ASP_43 pdb1_B_SER_50 <--> pdb2_A_GLN_54 pdb1_B_PRO_52 <--> pdb2_A_ASN_50 pdb1_A_THR_9 <--> pdb2_A_ARG_71 pdb1_A_LYS_17 <--> pdb2_A_GLU_35 pdb1_A_ALA_6 <--> pdb2_A_ARG_53 pdb1_C_SER_344 <--> pdb2_A_PRO_60 pdb1_A_ALA_116 <--> pdb2_A_ASP_43 pdb1_A_ALA_121 <--> pdb2_A_ASN_50 </p>
HBA2	Y85C of AHSP	-1.77	
HBA2	L21P of AHSP	-3.74	

Mutation near the binding interfaces at AHSP is pathogenic

				<p> pdb1_A_ALA_116 <--> pdb2_A_THR_39 pdb1_A_PRO_5 <--> pdb2_A_GLN_68 pdb1_A_PRO_5 <--> pdb2_A_ASP_64 pdb1_B_ASP_53 <--> pdb2_A_PHE_47 pdb1_A_ASN_10 <--> pdb2_A_ASN_46 pdb1_A_VAL_122 <--> pdb2_A_ASN_46 pdb1_A_ALA_121 <--> pdb2_A_ASN_46 pdb1_A_ALA_6 <--> pdb2_A_ILE_49 pdb1_A_GLU_117 <--> pdb2_A_THR_39 </p>
HBA2	V56G of AHSP	‡		
AHSP	HBD	-13.21		<p> pdb2_B_VAL_60 <--> pdb1_A_ASN_46 pdb2_B_VAL_57 <--> pdb1_A_ASP_43 pdb2_A_GLN_76 <--> pdb1_A_GLN_54 pdb2_B_GLY_56 <--> pdb1_A_ASP_43 pdb2_B_GLU_53 <--> pdb1_A_TRP_44 pdb2_A_ILE_74 <--> pdb1_A_GLN_54 pdb2_B_SER_47 <--> pdb1_A_ASP_29 pdb2_B_LEU_49 <--> pdb1_A_GLN_25 pdb2_B_GLY_48 <--> pdb1_A_ASP_29 pdb2_A_MET_120 <--> pdb1_A_LEU_31 pdb2_A_MET_120 <--> pdb1_A_PRO_30 pdb2_B_LEU_49 <--> pdb1_A_ASP_29 pdb2_B_VAL_60 <--> pdb1_A_ASP_43 pdb2_A_LYS_122 <--> pdb1_A_ASP_36 pdb2_A_LYS_122 <--> pdb1_A_LEU_31 pdb2_A_LYS_122 <--> pdb1_A_SER_33 pdb2_A_LYS_122 <--> pdb1_A_VAL_32 pdb2_A_PRO_121 <--> pdb1_A_VAL_32 pdb2_A_ASP_77 <--> pdb1_A_GLN_54 pdb2_A_PRO_121 <--> pdb1_A_PRO_30 pdb2_A_ASP_77 <--> pdb1_A_ASN_50 pdb2_A_ASP_77 <--> pdb1_A_ARG_53 pdb2_B_LEU_49 <--> pdb1_A_PRO_30 pdb2_B_LYS_59 <--> pdb1_A_PHE_47 pdb2_C_ASP_68 <--> pdb1_A_ASP_29 pdb2_A_GLU_73 <--> pdb1_A_TYR_51 pdb2_A_GLU_73 <--> pdb1_A_GLN_54 pdb2_A_MET_120 <--> pdb1_A_ASP_29 pdb2_A_GLN_125 <--> pdb1_A_ASP_36 pdb2_B_GLU_63 <--> pdb1_A_ASN_50 pdb2_B_GLU_52 <--> pdb1_A_TRP_44 pdb2_B_GLU_52 <--> pdb1_A_LEU_21 pdb2_B_GLU_52 <--> pdb1_A_GLN_25 pdb2_A_GLN_125 <--> pdb1_A_THR_39 pdb2_A_PRO_121 <--> pdb1_A_VAL_40 pdb2_A_ASP_77 <--> pdb1_A_ARG_63 pdb2_A_ARG_116 <--> pdb1_A_LEU_31 </p>
HBD	Y85C of AHSP	-8.09		<p> pdb1_B_VAL_60 <--> pdb2_A_ASN_46 pdb1_A_GLN_125 <--> pdb2_A_VAL_40 </p>

Mutation near the binding interfaces at AHSP is pathogenic

			<p> pdb1_A_GLN_125 <--> pdb2_A_THR_39 pdb1_B_LYS_59 <--> pdb2_A_PHE_47 pdb1_B_LEU_49 <--> pdb2_A_VAL_26 pdb1_B_LEU_49 <--> pdb2_A ASP_29 pdb1_A_ARG_134 <--> pdb2_A ASP_43 pdb1_B_VAL_60 <--> pdb2_A ASP_43 pdb1_A_LYS_122 <--> pdb2_A ASP_36 pdb1_A_LYS_122 <--> pdb2_A LEU_31 pdb1_A_LYS_122 <--> pdb2_A PRO_30 pdb1_A_LYS_122 <--> pdb2_A SER_33 pdb1_A_LYS_122 <--> pdb2_A VAL_32 pdb1_A ASP_77 <--> pdb2_A_GLN_54 pdb1_A ASP_77 <--> pdb2_A ASN_50 pdb1_A ASP_77 <--> pdb2_A ARG_53 pdb1_A_ARG_129 <--> pdb2_A ASP_36 pdb1_A_ARG_129 <--> pdb2_A_GLU_35 pdb1_A_GLU_73 <--> pdb2_A_GLN_54 pdb1_A_ARG_128 <--> pdb2_A ASP_43 pdb1_A_MET_120 <--> pdb2_A ASP_29 pdb1_A_GLN_125 <--> pdb2_A ASP_36 pdb1_B_GLU_63 <--> pdb2_A ASN_50 pdb1_B_GLU_52 <--> pdb2_A LEU_21 pdb1_B_GLU_52 <--> pdb2_A_GLN_24 pdb1_A_ARG_116 <--> pdb2_A LEU_31 pdb1_A_GLN_125 <--> pdb2_A ASP_36 pdb1_B_LYS_59 <--> pdb2_A ASN_50 pdb1_A_ARG_129 <--> pdb2_A ASP_36 pdb1_B_GLU_63 <--> pdb2_A ARG_53 pdb1_B_LEU_49 <--> pdb2_A_GLN_25 pdb1_A_ARG_129 <--> pdb2_A_GLU_35 pdb1_B_GLU_52 <--> pdb2_A_PHE_47 pdb1_B_LEU_49 <--> pdb2_A_GLN_24 pdb1_B_GLN_27 <--> pdb2_A_GLN_54 pdb1_A_GLN_125 <--> pdb2_A_THR_39 pdb1_A_GLU_73 <--> pdb2_A ARG_53 pdb1_A_LYS_122 <--> pdb2_A ASP_36 pdb1_B_VAL_60 <--> pdb2_A ASN_46 pdb1_A_GLU_73 <--> pdb2_A_GLN_54 pdb1_A_GLN_125 <--> pdb2_A_VAL_40 pdb1_A_GLN_76 <--> pdb2_A ARG_63 pdb1_B_GLU_53 <--> pdb2_A ASP_43 pdb1_D_LYS_115 <--> pdb2_A LEU_31 pdb1_B_GLY_56 <--> pdb2_A ASP_43 pdb1_A ASP_77 <--> pdb2_A ARG_53 pdb2_A LEU_67 <--> pdb1_D ASP_77 pdb2_A ASP_43 <--> pdb1_D ARG_69 pdb2_A_GLN_54 <--> pdb1_D_GLN_76 pdb2_A_GLN_54 <--> pdb1_D ASP_77 pdb2_A_GLU_42 <--> pdb1_E_GLY_28 </p>
HBD	L21P of AHSP	-12.05	
HBD	V56G of AHSP	-4.66	

Mutation near the binding interfaces at AHSP is pathogenic

			pdb2_A_ARG_71 <--> pdb1_D_LEU_70
			pdb2_A_GLN_72 <--> pdb1_E_GLN_27
			pdb2_A_ASN_50 <--> pdb1_D_GLU_73
			pdb2_A_GLU_42 <--> pdb1_E_GLN_27
			pdb2_A_ASN_50 <--> pdb1_D_GLN_76
			pdb2_A_ARG_53 <--> pdb1_D_ASP_77
			pdb2_A_ARG_53 <--> pdb1_D_GLN_76
			pdb2_A_ASN_46 <--> pdb1_D_GLU_73
			pdb2_A_ARG_53 <--> pdb1_D_GLU_73
			pdb2_A_PRO_60 <--> pdb1_E_ARG_67
			pdb2_A_ASN_46 <--> pdb1_E_ILE_26
			pdb2_A_ARG_71 <--> pdb1_E_ILE_26
			pdb2_A_ARG_71 <--> pdb1_E_GLN_27
			pdb2_A_GLN_54 <--> pdb1_D_THR_80
			pdb2_A_ASP_64 <--> pdb1_E_GLU_63
			pdb2_A_ASP_64 <--> pdb1_E_ARG_67
			pdb2_A_ARG_63 <--> pdb1_D_PHE_78
			pdb2_A_ASN_75 <--> pdb1_E_GLN_27
			pdb2_A_THR_39 <--> pdb1_F_LEU_87
AHSP	KLF1	-6.79	pdb2_A_ARG_63 <--> pdb1_D_ASP_77
			pdb2_A_GLN_61 <--> pdb1_A_SER_23
			pdb2_A_ARG_71 <--> pdb1_A_HIS_38
			pdb2_A_ASN_46 <--> pdb1_A_VAL_37
			pdb2_A_GLU_34 <--> pdb1_A_GLU_10
			pdb2_A_GLN_68 <--> pdb1_A_SER_43
			pdb2_A_ASN_46 <--> pdb1_A_THR_39
			pdb2_A_GLN_72 <--> pdb1_A_THR_44
			pdb2_A_GLN_72 <--> pdb1_A_LYS_65
			pdb2_A_GLU_35 <--> pdb1_A_LYS_11
			pdb2_A_GLU_35 <--> pdb1_A_GLU_10
			pdb2_A_GLU_42 <--> pdb1_A_PHE_9
			pdb2_A_ASN_79 <--> pdb1_A_PRO_84
			pdb2_A_ASN_79 <--> pdb1_A_GLN_85
			pdb2_A_ASN_79 <--> pdb1_A_ARG_86
			pdb2_A_VAL_38 <--> pdb1_A_GLU_10
			pdb2_A_GLN_68 <--> pdb1_A_PRO_24
			pdb2_A_THR_39 <--> pdb1_A_VAL_12
			pdb2_A_THR_39 <--> pdb1_A_GLU_10
			pdb2_A_ASP_43 <--> pdb1_A_LYS_36
			pdb2_A_THR_39 <--> pdb1_A_LYS_36
			pdb2_A_GLU_42 <--> pdb1_A_HIS_38
			pdb2_A_VAL_38 <--> pdb1_A_PHE_9
			pdb2_A_GLN_68 <--> pdb1_A_VAL_41
			pdb2_A_GLN_68 <--> pdb1_A_THR_44
			pdb2_A_ASP_64 <--> pdb1_A_PRO_24
			pdb2_A_ASP_64 <--> pdb1_A_SER_23
			pdb2_A_ASN_75 <--> pdb1_A_GLN_85
			pdb2_A_ASN_75 <--> pdb1_A_HIS_87
			pdb2_A_THR_76 <--> pdb1_A_GLN_85

Mutation near the binding interfaces at AHSP is pathogenic

KLF1	Y85C of AHSP	-13.77	pdb2_A_ARG_71 <--> pdb1_A_HIS_87
			pdb1_A_PRO_24 <--> pdb2_A_LEU_77
			pdb1_A_THR_39 <--> pdb2_A_ASN_23
			pdb1_A_GLU_20 <--> pdb2_A_PHE_81
			pdb1_A_ASN_19 <--> pdb2_A_LEU_22
			pdb1_A_ASN_19 <--> pdb2_A_GLN_25
			pdb1_A_ASN_19 <--> pdb2_A_VAL_26
			pdb1_A_ASN_19 <--> pdb2_A_PHE_27
			pdb1_A_ASN_19 <--> pdb2_A_ASN_28
			pdb1_A_THR_28 <--> pdb2_A_VAL_26
			pdb1_A_GLU_20 <--> pdb2_A_MET_37
			pdb1_A_VAL_41 <--> pdb2_A_ASN_23
			pdb1_A_VAL_41 <--> pdb2_A_LEU_22
			pdb1_A_VAL_22 <--> pdb2_A_LEU_22
			pdb1_A_VAL_22 <--> pdb2_A_LEU_21
			pdb1_A_SER_23 <--> pdb2_A_PHE_81
			pdb1_A_VAL_22 <--> pdb2_A_TRP_44
			pdb1_A_GLU_26 <--> pdb2_A_LEU_22
			pdb1_A_GLU_26 <--> pdb2_A_ASN_23
			pdb1_A_ALA_25 <--> pdb2_A_PHE_81
			pdb1_A_VAL_22 <--> pdb2_A_PHE_81
			pdb1_A_PRO_24 <--> pdb2_A_LEU_22
			pdb1_A_ILE_107 <--> pdb2_A_LYS_84
			pdb1_A_GLN_106 <--> pdb2_A_LYS_84
			pdb1_A_ARG_110 <--> pdb2_A_LYS_84
			pdb1_A_SER_23 <--> pdb2_A_PHE_18
			pdb1_A_ASP_21 <--> pdb2_A_PHE_27
			pdb1_A_ASP_21 <--> pdb2_A_ASN_28
			pdb1_A_VAL_22 <--> pdb2_A_PHE_18
			pdb1_A_ASP_21 <--> pdb2_A_TRP_44
			pdb1_A_SER_23 <--> pdb2_A_ALA_78
			pdb1_A_ASP_21 <--> pdb2_A_VAL_41
			pdb1_A_ASP_21 <--> pdb2_A_VAL_40
pdb1_A_PRO_24 <--> pdb2_A_PHE_18			
pdb1_A_SER_23 <--> pdb2_A_LEU_77			
pdb1_A_GLU_20 <--> pdb2_A_ASN_28			
KLF1	L21P of AHSP	-23.27	pdb2_A_ASP_43 <--> pdb1_A_ASP_29
			pdb2_A_VAL_26 <--> pdb1_A_TYR_51
			pdb2_A_VAL_26 <--> pdb1_A_ASN_50
			pdb2_A_GLN_24 <--> pdb1_A_TYR_51
			pdb2_A_GLN_24 <--> pdb1_A_TYR_52
			pdb2_A_ASP_29 <--> pdb1_A_PHE_47
			pdb2_A_ASP_29 <--> pdb1_A_ASN_46
			pdb2_A_ASP_29 <--> pdb1_A_ASP_43
			pdb2_A_GLN_25 <--> pdb1_A_PHE_47
			pdb2_A_GLN_25 <--> pdb1_A_TRP_44
pdb2_A_PHE_47 <--> pdb1_A_GLN_25			
pdb2_A_PHE_47 <--> pdb1_A_GLN_24			
pdb2_A_TYR_48 <--> pdb1_A_GLN_24			

Mutation near the binding interfaces at AHSP is pathogenic

			<p> pdb2_A_PHE_47 <--> pdb1_A_VAL_26 pdb2_A_TYR_48 <--> pdb1_A_LEU_21 pdb2_A_VAL_20 <--> pdb1_A_GLU_17 pdb2_A_ASN_50 <--> pdb1_A_ASP_29 pdb2_A_GLN_24 <--> pdb1_A_PHE_47 pdb2_A_GLN_24 <--> pdb1_A_TYR_48 pdb2_A_VAL_26 <--> pdb1_A_PHE_47 pdb2_A_PHE_47 <--> pdb1_A_ASP_29 pdb2_A_TRP_44 <--> pdb1_A_TRP_44 pdb2_A_TYR_51 <--> pdb1_A_GLN_24 pdb2_A_ASN_46 <--> pdb1_A_ASP_29 pdb2_A_TYR_51 <--> pdb1_A_VAL_26 pdb2_A_ASN_50 <--> pdb1_A_VAL_26 pdb2_A_ASP_29 <--> pdb1_A_ASN_50 pdb2_A_LEU_21 <--> pdb1_A_LEU_21 pdb2_A_PHE_47 <--> pdb1_A_PRO_30 pdb2_A_GLU_17 <--> pdb1_A_GLN_24 pdb2_A_GLU_17 <--> pdb1_A_VAL_20 pdb2_A_TYR_52 <--> pdb1_A_GLN_24 pdb2_A_LEU_21 <--> pdb1_A_TRP_44 pdb2_A_GLN_24 <--> pdb1_A_GLU_17 </p>
KLF1	V56G of AHSP	‡	
AHSP	HBQ1	-26.08	<p> pdb1_A_PRO_80 <--> pdb2_A_ALA_36 pdb1_A_PRO_80 <--> pdb2_A_THR_33 pdb1_A_PRO_80 <--> pdb2_A_ARG_32 pdb1_A_THR_76 <--> pdb2_A_ARG_112 pdb1_A_PHE_81 <--> pdb2_A_ALA_36 pdb1_A_ASN_79 <--> pdb2_A_VAL_108 pdb1_A_PRO_80 <--> pdb2_A_CYS_105 pdb1_A_PRO_80 <--> pdb2_A_LEU_101 pdb1_A_THR_76 <--> pdb2_A_ARG_32 pdb1_A_ASP_87 <--> pdb2_A_GLN_100 pdb1_A_SER_19 <--> pdb2_A_LYS_41 pdb1_A_LYS_84 <--> pdb2_A_ALA_97 pdb1_A_SER_12 <--> pdb2_A_PRO_51 pdb1_A_LYS_16 <--> pdb2_A_SER_50 pdb1_A_LYS_16 <--> pdb2_A_PRO_51 pdb1_A_LEU_77 <--> pdb2_A_ALA_36 pdb1_A_LEU_77 <--> pdb2_A_LEU_35 pdb1_A_ALA_83 <--> pdb2_A_HIS_104 pdb1_A_LYS_84 <--> pdb2_A_PHE_37 pdb1_A_SER_19 <--> pdb2_A_LEU_35 pdb1_A_LEU_15 <--> pdb2_A_PRO_51 pdb1_A_LEU_22 <--> pdb2_A_PRO_38 pdb1_A_ASN_23 <--> pdb2_A_PRO_38 pdb1_A_LYS_84 <--> pdb2_A_LEU_101 pdb1_A_LEU_22 <--> pdb2_A_LEU_35 pdb1_A_LEU_22 <--> pdb2_A_ALA_36 pdb1_A_LEU_15 <--> pdb2_A_LEU_35 </p>

Mutation near the binding interfaces at AHSP is pathogenic

HBQ1	Y85C of AHSP	-28.89	<p> pdb2_A_GLN_54 <--> pdb1_A_ARG_112 pdb2_A_GLN_54 <--> pdb1_A_ALA_111 pdb2_A_GLU_59 <--> pdb1_A_LEU_101 pdb2_A_GLN_54 <--> pdb1_A_ARG_32 pdb2_A_ARG_53 <--> pdb1_A_VAL_108 pdb2_A_ASN_46 <--> pdb1_A_PRO_120 pdb2_A_ASN_50 <--> pdb1_A_PHE_118 pdb2_A_THR_57 <--> pdb1_A_HIS_104 pdb2_A_ARG_53 <--> pdb1_A_PHE_118 pdb2_A_ARG_53 <--> pdb1_A_ALA_111 pdb2_A_GLY_58 <--> pdb1_A_HIS_104 pdb2_A_THR_57 <--> pdb1_A_ALA_36 pdb2_A_PRO_60 <--> pdb1_A_GLN_100 pdb2_A_GLN_54 <--> pdb1_A_VAL_108 pdb2_A_ASN_50 <--> pdb1_A_ALA_111 pdb2_A_GLN_55 <--> pdb1_A_VAL_108 pdb2_A_GLU_59 <--> pdb1_A_PHE_37 pdb2_A_ARG_53 <--> pdb1_A_GLN_123 pdb2_A_ARG_53 <--> pdb1_A_PRO_120 pdb2_A_ARG_63 <--> pdb1_A_HIS_104 pdb2_A_VAL_56 <--> pdb1_A_VAL_108 pdb2_A_VAL_56 <--> pdb1_A_HIS_104 pdb2_A_ARG_63 <--> pdb1_A_GLN_123 pdb2_A_ASN_50 <--> pdb1_A_PRO_115 </p>
HBQ1	L21P of AHSP	-25.45	<p> pdb1_A_HIS_104 <--> pdb2_A_LYS_16 pdb1_A_PRO_120 <--> pdb2_A_ALA_6 pdb1_A_PRO_120 <--> pdb2_A_GLN_55 pdb1_A_PRO_120 <--> pdb2_A_VAL_56 pdb1_A_PRO_120 <--> pdb2_A_LEU_10 pdb1_A_ALA_111 <--> pdb2_A_GLU_17 pdb1_A_VAL_108 <--> pdb2_A_GLU_17 pdb1_A_VAL_108 <--> pdb2_A_LYS_16 pdb1_A_GLN_123 <--> pdb2_A_LEU_10 pdb1_A_PHE_118 <--> pdb2_A_ALA_13 pdb1_A_PHE_118 <--> pdb2_A_GLN_55 pdb1_A_GLN_123 <--> pdb2_A_ALA_13 pdb1_A_CYS_105 <--> pdb2_A_VAL_20 pdb1_A_SER_119 <--> pdb2_A_GLN_55 pdb1_A_ALA_36 <--> pdb2_A_VAL_20 pdb1_A_ALA_36 <--> pdb2_A_ASN_23 pdb1_A_ALA_36 <--> pdb2_A_GLN_24 pdb1_A_PRO_115 <--> pdb2_A_TYR_51 pdb1_A_LEU_35 <--> pdb2_A_GLN_24 pdb1_A_PRO_115 <--> pdb2_A_GLN_55 pdb1_A_PHE_37 <--> pdb2_A_VAL_20 pdb1_A_PHE_37 <--> pdb2_A_ASN_23 pdb1_A_ARG_32 <--> pdb2_A_GLN_24 pdb1_A_VAL_108 <--> pdb2_A_VAL_20 pdb1_A_ALA_124 <--> pdb2_A_ASP_9 </p>

Mutation near the binding interfaces at AHSP is pathogenic

HBQ1	V56G of AHSP	-34.64	pdb1_A_PRO_120 <--> pdb2_A ASP_9 pdb1_A_PRO_120 <--> pdb2_A ASN_7 pdb1_A_PRO_120 <--> pdb2_A ALA_6 pdb1_A_PRO_120 <--> pdb2_A GLN_55 pdb1_A_GLN_123 <--> pdb2_A GLU_17 pdb1_A_PRO_120 <--> pdb2_A LEU_10 pdb1_A_ALA_111 <--> pdb2_A GLU_17 pdb1_A_SER_119 <--> pdb2_A LEU_10 pdb1_A_VAL_108 <--> pdb2_A GLU_17 pdb1_A_VAL_108 <--> pdb2_A LYS_16 pdb1_A_PHE_118 <--> pdb2_A LEU_10 pdb1_A_GLN_123 <--> pdb2_A ALA_13 pdb1_A_CYS_105 <--> pdb2_A VAL_20 pdb1_A_ALA_36 <--> pdb2_A ASN_23 pdb1_A_ALA_36 <--> pdb2_A GLN_24 pdb1_A_LEU_35 <--> pdb2_A VAL_26 pdb1_A_LEU_35 <--> pdb2_A GLN_24 pdb1_A_PRO_115 <--> pdb2_A GLN_55 pdb1_A_HIS_104 <--> pdb2_A VAL_20 pdb1_A_PHE_37 <--> pdb2_A ASN_23 pdb1_A_ARG_32 <--> pdb2_A GLN_24 pdb1_A_ARG_32 <--> pdb2_A VAL_20 pdb1_A_LEU_107 <--> pdb2_A GLU_17 pdb1_A_VAL_108 <--> pdb2_A VAL_20 pdb1_A_ALA_124 <--> pdb2_A ASP_9 pdb1_A ASP_127 <--> pdb2_A LYS_16
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‡No interaction was found.