

Mutation	Mutant_PDB_ID	Wildtype_Protein_PDB_ID	Ligand_ID_in_PDB	Multiple_Binding_Sites	Impact_of_Mutation_on_Binding_Affinity	Fold_Change
G48H	1A9M	1GNO	U0E	No	Decreased Affinity	-5.95
V82F	1BWA	1BV9	XV6	No	Decreased Affinity	-22.7272727
L22Y	1DLS	1U72	MTX	No	Decreased Affinity	-3205.88235
Y101F	1E2L	1E2K	TMC	No	Decreased Affinity	-4.51754386
V82D	1GNM	1GNO	U0E	No	Decreased Affinity	-28
V82N	1GNN	1GNO	U0E	No	Decreased Affinity	-105
R218H	1HK2	1HK1	T44	Yes	Increased Affinity	13.52941176
R218P	1HK3	1HK1	T44	Yes	Increased Affinity	8.846153846
R218H	1HK5	1HK4	T44	No	Decreased Affinity	-1.16734694
C59R/ S108N	1J3J	3QGT	CP6	No	Decreased Affinity	-49
N51I/ C59R/ S108N/ I164L	1J3K	1J3I	WRA	No	Decreased Affinity	-3.36363636
K213E	1JQV	2DOR	ORO	No	Decreased Affinity	-4.03448276
R57A	1JQX	2DOR	ORO	No	Decreased Affinity	-3.27586207
P56A	1JRB	2DOR	ORO	No	Decreased Affinity	-50
N67A	1JRC	2DOR	ORO	No	Decreased Affinity	-1.51724138
F93A	1MGO	1HLD	PFB	No	Decreased Affinity	-17
V292T	1N8K	1N92	NAJ	No	Decreased Affinity	-30
N229C	1NJA	1NJE	DCM	No	Increased Affinity	600
N229D	1NJC	1NJE	DCM	No	Increased Affinity	20
W57L	1OBO	1FLV	FMN	No	Decreased Affinity	-25.8461539
Y94F	1OBV	1FLV	FMN	No	Decreased Affinity	-4
K136E	1OVD	2DOR	ORO	No	Increased Affinity	3.815789474
L90M	1SDU	1SDT	MK1	No	Increased Affinity	6.279069767
V82A	1SDV	1SDT	MK1	No	Decreased Affinity	-3.35185185
Y187F	1SYI	1SYH	CPW	No	Decreased Affinity	-8.47328244
S96P	1TPW	1TPH	PGH	No	Decreased Affinity	-14.2
L22R	1U70	1U72	MTX	No	Decreased Affinity	-1344.11765
W92A	1W6Y	1OH0	EQU	No	Decreased Affinity	-2.2
S292Q	1X7W	1U5B	TDP	No	Decreased Affinity	-38.0625
S292E	1X7X	1U5B	TDP	No	Decreased Affinity	-32.875
S292N	1X7Y	1U5B	TDP	No	Decreased Affinity	-34
S292D	1X7Z	1U5B	TDP	No	Decreased Affinity	-25.1875
I219A	1YDK	1K3L	GTX	No	Decreased Affinity	-18.5714286
Y408C	1YKL	3PCA	DHB	No	Decreased Affinity	-22.8
Y408H	1YKP	3PCA	DHB	No	Decreased Affinity	-15.6
Y120F	1YP6	1QY1	PRZ	No	Decreased Affinity	-6.63333333
A328V	1ZOA	1JPZ	140	No	Increased Affinity	7.111111111
D597N	1ZZQ	1P6J	DP9	No	Decreased Affinity	-200
D597N/ M336V	1ZZR	1P6J	DP9	No	Decreased Affinity	-420
N368D	1ZZS	1P6N	DP9	No	Increased Affinity	21.56862745
N368D/ V106M	1ZZT	1P6N	DP9	No	Increased Affinity	100
D597N/ M336V	1ZZU	1P6H	DP1	No	Decreased Affinity	-211
R21L	2CAQ	2CA8	GSH	No	Decreased Affinity	-12.9545455
Y10F	2F8F	2CA8	GSH	No	Increased Affinity	1.047619048
V82A	2IDW	2IEN	17	No	Decreased Affinity	-1.3
I84V	2IEO	2IEN	17	No	Decreased Affinity	-3.2
C298A/ W219Y	2IPW	2IS7	2CL	No	Increased Affinity	4.4

C298A/ W219Y	2ISF	2INE	PAC	No	Decreased Affinity	-3.75
N199A	2OGY	2E7F	C2F	No	Decreased Affinity	-2.65
K57A	2ONZ	2ONY	TMJ	No	Increased Affinity	161.5384615
V47I	2PD9	1PWM	FID	No	Decreased Affinity	-1.27503839
F121P	2PDC	2PZN	393	No	Decreased Affinity	-6.44186556
L300P	2PDH	2PDG	47D	No	Decreased Affinity	-6.44186556
L300A	2PDJ	2PZN	393	No	Decreased Affinity	-2.15852453
L301M	2PDL	2FZD	TOL	No	Decreased Affinity	-2.75220163
S302R	2PDN	2PDG	47D	No	Decreased Affinity	-109.6772
S302R	2PDP	2PZN	393	No	Decreased Affinity	-70.2517332
C303D	2PDQ	2PDG	47D	No	Decreased Affinity	-57.3747748
C303D	2PDU	2PZN	393	No	Decreased Affinity	-64.7862173
C303D	2PDW	1PWM	FID	No	Decreased Affinity	-5.70492615
S302R/ C303D	2PDY	1PWM	FID	No	Decreased Affinity	-24.5126117
N88D	2PYM	2Q64	1UN	No	Decreased Affinity	-12.8571429
A71V	2PYN	2Q64	1UN	No	Decreased Affinity	-5
L90M	2Q63	2Q64	1UN	No	Decreased Affinity	-7.07142857
D30N	2QCI	2Z4O	65	No	Decreased Affinity	-17.037037
I50V	2QD6	2Z4O	65	No	Decreased Affinity	-7.77777778
V82A	2QD7	2Z4O	65	No	Decreased Affinity	-2.96296296
I84V	2QD8	2Z4O	65	No	Decreased Affinity	-3.14814815
E88G/ N92L	2YGE	1A4H	GDM	No	Decreased Affinity	-8.41328413
L89V/ L93I/ V136M	2YGF	1A4H	GDM	No	Decreased Affinity	-1.70848709
M372A/ K316A	3AM5	3AM3	TCL	No	Decreased Affinity	-1.35714286
G48V	3CYW	3TKW	17	No	Decreased Affinity	-29.3103448
I54M	3D1Z	3TKW	17	No	Decreased Affinity	-2.75862069
I54V	3D20	3TKW	17	No	Decreased Affinity	-8.62068966
Y43F	3DGO	3DGL	ATP	No	Increased Affinity	1.388888889
Q35K	3F8Y	3FS6	DH1	No	Increased Affinity	27.71084337
Q35S/ N64S	3F8Z	3FS6	DH1	No	Increased Affinity	3.484848485
Q35K/ N64F	3F91	3FS6	DH1	No	Increased Affinity	17.69230769
F98Y	3FRA	3FRF	XCF	No	Decreased Affinity	-20
F98Y	3FRB	3FRE	TOP	No	Decreased Affinity	-16.6666667
F98Y	3FY8	3FYW	XCF	No	Decreased Affinity	-3.91304348
F98Y	3FY9	3FYV	XCF	No	Decreased Affinity	-15.9090909
D816H	3G0F	3G0E	B49	No	Decreased Affinity	-1.1
L308V	3GUG	3C3U	C2U	No	Decreased Affinity	-13.220339
T113C	3LBO	1US0	LDT	No	Increased Affinity	13.07769009
T113S	3LD5	1US0	LDT	No	Decreased Affinity	-5.36181466
T113C	3LEP	2IKI	388	No	Decreased Affinity	-1.27020982
T113A	3LQG	2IKI	388	No	Decreased Affinity	-3.71532999
T113A	3LQL	1US0	LDT	No	Decreased Affinity	-7.55911261
T113V	3LZ5	1US0	LDT	No	Decreased Affinity	-3.6434088
N88S	3LZU	3LZS	17	No	Decreased Affinity	-7.98165138
T113V	3M4H	2IKI	388	No	Decreased Affinity	-13.4692591
A467G	3MOE	3DT7	SPV	No	Decreased Affinity	-1.92307692
V32I	3NU4	3NU3	478	No	Decreased Affinity	-10
I50V	3NU5	3NU3	478	No	Decreased Affinity	-30
I54M	3NU6	3NU3	478	No	Decreased Affinity	-3.33333333
I84V	3NU9	3NU3	478	No	Decreased Affinity	-6

I54V	3NUJ	3NU3	478	No	Decreased Affinity	-2.73333333
L90M	3NUO	3NU3	478	No	Decreased Affinity	-1.06666667
T90S/ W108V/ L110T/ F29L/ S52G/ R53S	3RDO	3RY2	BTN	No	Decreased Affinity	-215.384615
S35K	3S3V	3NOH	TOP	Yes	Increased Affinity	1.056506849
A16V/ S108T	3UM6	3UM8	1CY	No	Decreased Affinity	-948.75