

Supplementary Materials

Effect of T68A/N126Y mutations on conformational and ligand binding landscape of Coxsackievirus B3 3C protease

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Name and structure of the ligand/inhibitor: O-tert-butyl-N-[(9H-fluoren-9-yl methoxy) carbonyl]-L-threonyl-N-[(2R)-5-ethoxy-5-oxo-1-[(3S)-2-oxopyrrolidin-3-yl]pentan-2-yl]-L-phenylalaninamide (Codename: 3CPI)

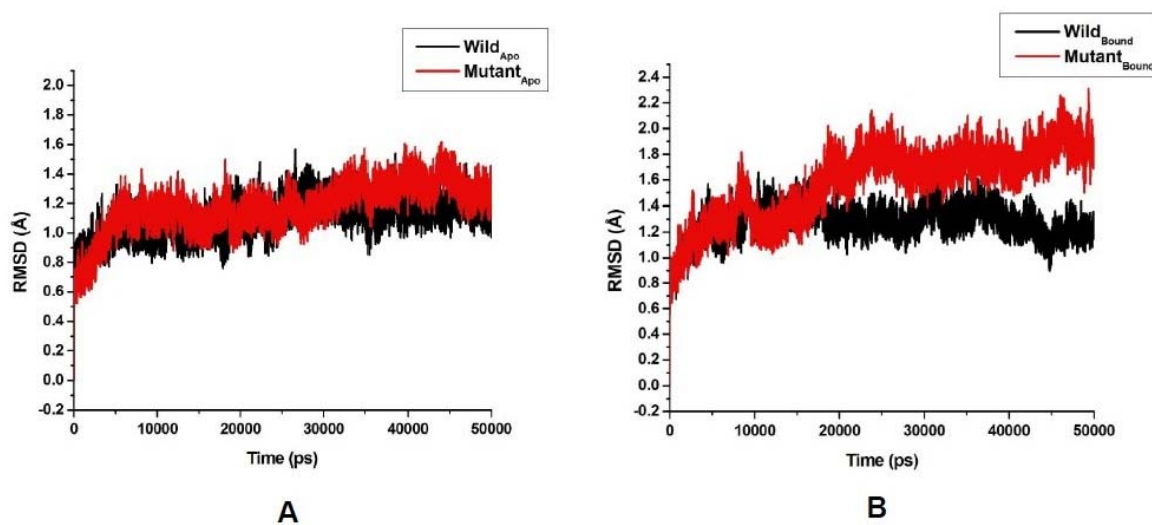
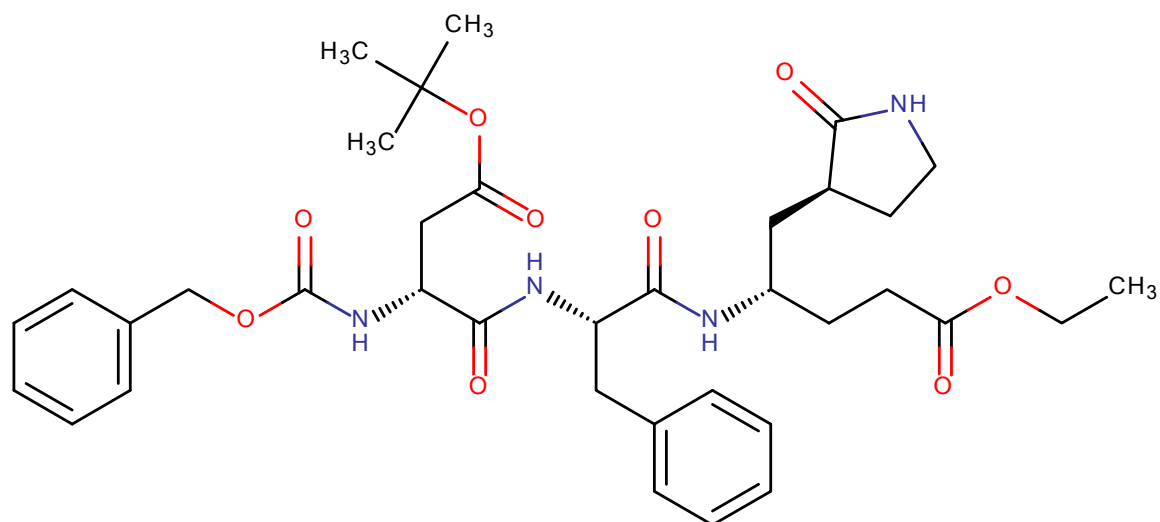


Figure S1. The C- α fluctuation against time for apo and bound conformations of CVB3 3C protease.

H-bond occupancy Wild_{Bound}

#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
G83_182@O35	GLY_164@H	GLY_164@N	50440	0.5044	2.8850	156.5692
G83_182@O66	HIS_161@HE2	HIS_161@NE2	13261	0.1326	2.8823	149.8232
VAL_162@O	G83_182@H49	G83_182@N49	12882	0.1288	2.9179	160.0781
GLY_164@O	G83_182@H21	G83_182@N21	9468	0.0947	2.9123	156.0555
ARG_143@O	G83_182@H69	G83_182@N69	8262	0.0826	2.9024	148.7288
G83_182@O66	THR_142@HG1	THR_142@OG1	1022	0.0102	2.8481	156.0733
THR_142@O	G83_182@H69	G83_182@N69	984	0.0098	2.9158	155.8300
THR_142@OG1	G83_182@H69	G83_182@N69	770	0.0077	2.9317	154.1160

G83_182@O86	GLY_145@H	GLY_145@N	505	0.0050	2.9176	155.1281
G83_182@O19	GLY_128@H	GLY_128@N	178	0.0018	2.9041	155.3498
G83_182@O86	HIS_40@HE2	HIS_40@NE2	66	0.0007	2.8868	147.6999
G83_182@O88	GLY_145@H	GLY_145@N	26	0.0003	2.8903	156.1542
G83_182@O88	HIS_40@HE2	HIS_40@NE2	24	0.0002	2.8778	145.3545
G83_182@O66	CYS_147@H	CYS_147@N	20	0.0002	2.9475	144.7418
G83_182@O88	CYS_147@H	CYS_147@N	15	0.0001	2.8791	157.1797
ARG_143@N	G83_182@H69	G83_182@N69	11	0.0001	2.9492	147.9790
G83_182@O1	GLY_128@H	GLY_128@N	7	0.0001	2.9224	153.2327
G83_182@O15	ASN_165@HD22	ASN_165@ND2	5	0.0001	2.9178	157.3201
GLN_146@O15	G83_182@H69	G83_182@N69	5	0.0001	2.9488	156.0656
G83_182@N69	THR_142@HG1	THR_142@OG1	5	0.0001	2.9562	153.1496
G83_182@O66	GLN_146@H	GLN_146@N	4	0.0000	2.9369	142.2436
G83_182@N69	HIS_161@HE2	HIS_161@NE2	4	0.0000	2.9469	140.4831
G83_182@O15	ASN_165@HD21	ASN_165@ND2	3	0.0000	2.8900	151.2552
G83_182@O66	GLY_164@H	GLY_164@N	1	0.0000	2.7959	136.8724
G83_182@N69	GLY_166@H	GLY_166@N	1	0.0000	2.9543	137.5968
G83_182@O66	GLY_166@H	GLY_166@N	1	0.0000	2.9571	135.6166
GLY_166@N	G83_182@H69	G83_182@N69	1	0.0000	2.9793	136.6475
G83_182@O86	CYS_147@H	CYS_147@N	1	0.0000	2.9899	168.6648

H-bond occupancy Mutant_{Bound}

#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
G83_181@O35	GLY_164@H	GLY_164@N	34051	0.3840	2.8956	157.6263
G83_181@O66	HIE_161@HE2	HIE_161@NE2	23389	0.2637	2.8937	158.5958
G83_181@O15	ASN_165@HD22	ASN_165@ND2	5135	0.0579	2.8985	156.1966
VAL_162@O	G83_181@H49	G83_181@N49	4520	0.0510	2.9303	162.0290
GLY_164@O	G83_181@H21	G83_181@N21	1371	0.0155	2.9244	156.4146
THR_142@OG1	G83_181@H69	G83_181@N69	1189	0.0134	2.9329	153.8576
G83_181@O19	GLY_128@H	GLY_128@N	591	0.0067	2.9030	158.2981
G83_181@O15	ASN_165@HD21	ASN_165@ND2	436	0.0049	2.8735	162.0789
G83_181@O66	THR_142@HG1	THR_142@OG1	374	0.0042	2.8438	152.0207
ARG_143@O	G83_181@H69	G83_181@N69	313	0.0035	2.8999	145.9651
G83_181@O66	CYS_147@H	CYS_147@N	246	0.0028	2.9061	146.1727
G83_181@O86	TYR_22@HH	TYR_22@OH	177	0.0020	2.8100	158.0970
G83_181@O66	GLN_146@H	GLN_146@N	125	0.0014	2.9174	144.8618
G83_181@O66	GLN_146@HE22	GLN_146@NE2	102	0.0012	2.8931	155.2064
G83_181@O1	ASN_165@HD22	ASN_165@ND2	77	0.0009	2.8776	152.5278
G83_181@O66	GLY_145@H	GLY_145@N	68	0.0008	2.9020	144.4633
ASN_165@OD1	G83_181@H21	G83_181@N21	64	0.0007	2.9054	157.5828
THR_142@O	G83_181@H69	G83_181@N69	47	0.0005	2.9094	154.2204
G83_181@O2	ASN_165@HD22	ASN_165@ND2	41	0.0005	2.8989	160.1364
G83_181@N69	THR_142@HG1	THR_142@OG1	12	0.0001	2.9283	144.7846
G83_181@O88	HIE_40@HE2	HIE_40@NE2	11	0.0001	2.8606	144.2498
G83_181@N69	HIE_161@HE2	HIE_161@NE2	11	0.0001	2.9571	150.4724
G83_181@O86	GLY_145@H	GLY_145@N	9	0.0001	2.9399	152.3438
ASN_165@ND2	G83_181@H21	G83_181@N21	4	0.0000	2.9566	142.2089
HIE_161@NE2	G83_181@H69	G83_181@N69	2	0.0000	2.9185	140.9090
G83_181@O2	ASN_165@HD21	ASN_165@ND2	1	0.0000	2.8308	135.1057
G83_181@O88	TYR_22@HH	TYR_22@OH	1	0.0000	2.9450	167.6373
G83_181@O88	GLY_145@H	GLY_145@N	1	0.0000	2.9709	145.0692
G83_181@O15	GLY_128@H	GLY_128@N	1	0.0000	2.9912	164.9176