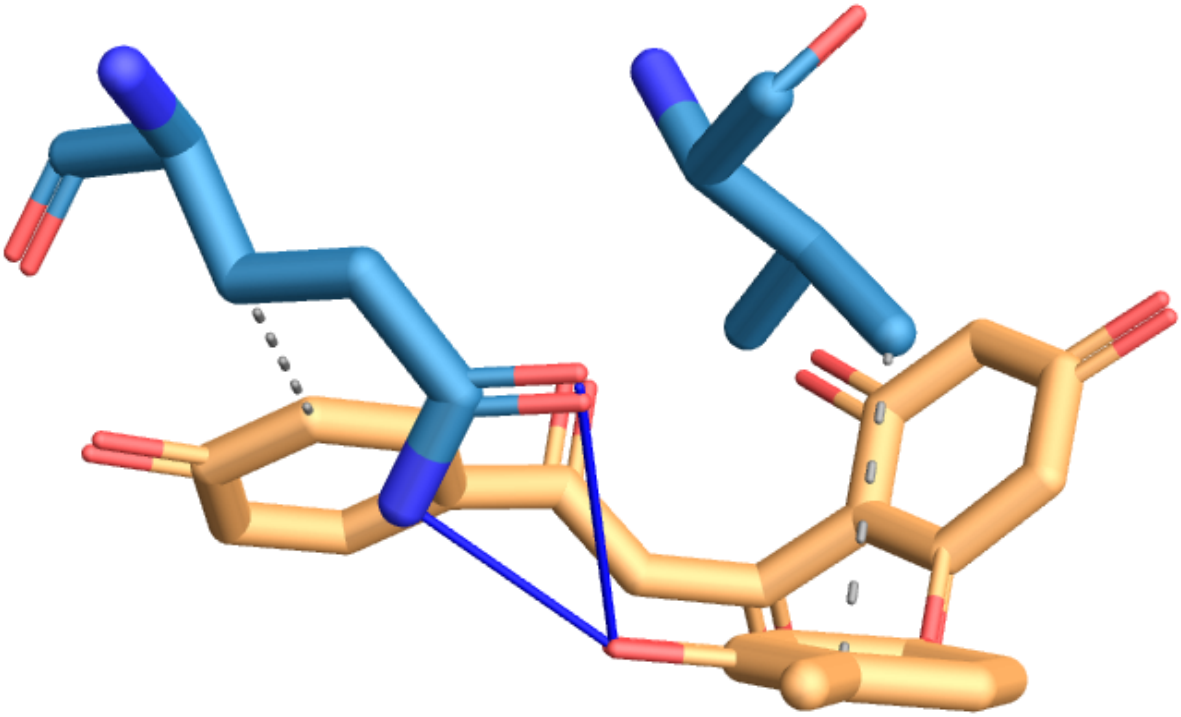
6lu7_pdb-Evolved-Amentoflavone

Docking Scores

No.	Affinity	rmsd l.b	rmsd u.b
1	-5.7	0	0
2	-5.3	3.745	6.984
3	-5.3	6.178	10.092
4	-5.2	4.729	7.459
5	-5.2	2.004	6.206
6	-5.1	2.116	6.308
7	-5.1	1.991	2.843
8	-5.1	3.013	8.477
9	-5	4.375	8.575

Visualisation



Natural Ligand 1

Hydrophobic Interactions

No.	Res.	AA	Dist	Ligand Atom	Proton Atom
1	25	THR	3.73	2416	178
2	26	THR	3.81	2416	185

Hydrogen Bonds

No.	Res.	AA	Dist H-A	Dist D-A	Don Angle	Protisdon?	Sidechain?	D. Atom	A. Atom
1	143	GLY	1.93	2.8	145.29	True	False	1105[Nam]	2412[O3]

Natural Ligand 2

Hydrophobic Interactions

No.	Res.	AA	Dist	Ligand Atom	Proton Atom
1	168	PRO	3.53	2372	1303

No Hydrogen Bonds Found

Natural Ligand 3

No Hydrophobic Interactions Found

Hydrogen Bonds

No.	Res.	AA	Dist H-A	Dist D-A	Don Angle	Protisdon?	Sidechain?	D. Atom	A. Atom
1	164	HIS	2.16	3.07	153.73	False	False	2398[N3]	1266[O2]
2	166	GLU	2.61	3.38	135.52	False	True	2399[Nam]	1289[O-]

Docked Ligand Interactions

Hydrophobic Interactions Found

Hydrophobic Interactions Found

Hydrogen Bonds Found

No Water Bridges Found

No Salt Bridges Found

No Pi Stacks Found

No Pi Cation Interactions Found

No Halogen Bonds Found

No Metal Complexes Found

Hydrophobic Interactions

No.	Res.	AA	Dist	Ligand Atom	Proton Atom
1	3	VAL	3.72	2435	2387
2	189	GLN	3.82	2430	1461

Hydrogen Bonds

No.	Res.	AA	Dist H-A	Dist D-A	Don Angle	Protisdon?	Sidechain?	D. Atom	A. Atom
1	189	GLN	1.93	2.81	146.83	True	True	1464[Nam]	2447[O3]
2	189	GLN	2.33	3.3	172.91	False	True	2447[O3]	1465[O2]

Figures

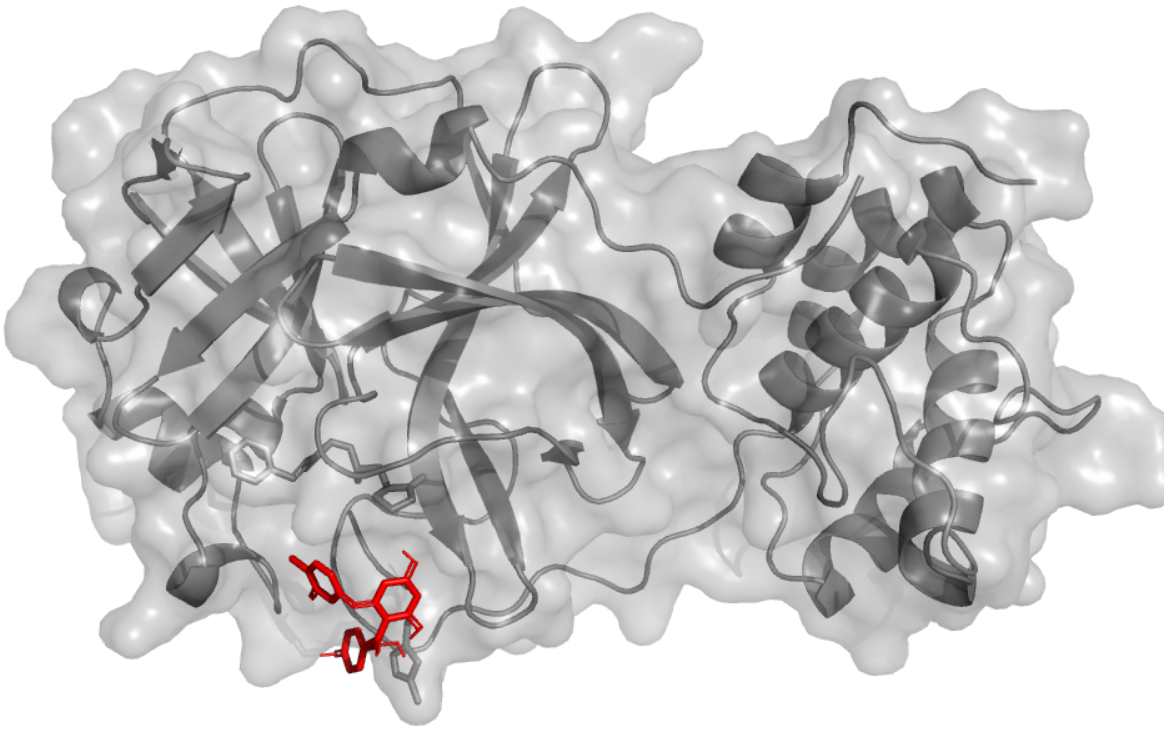


Figure 1: Back View

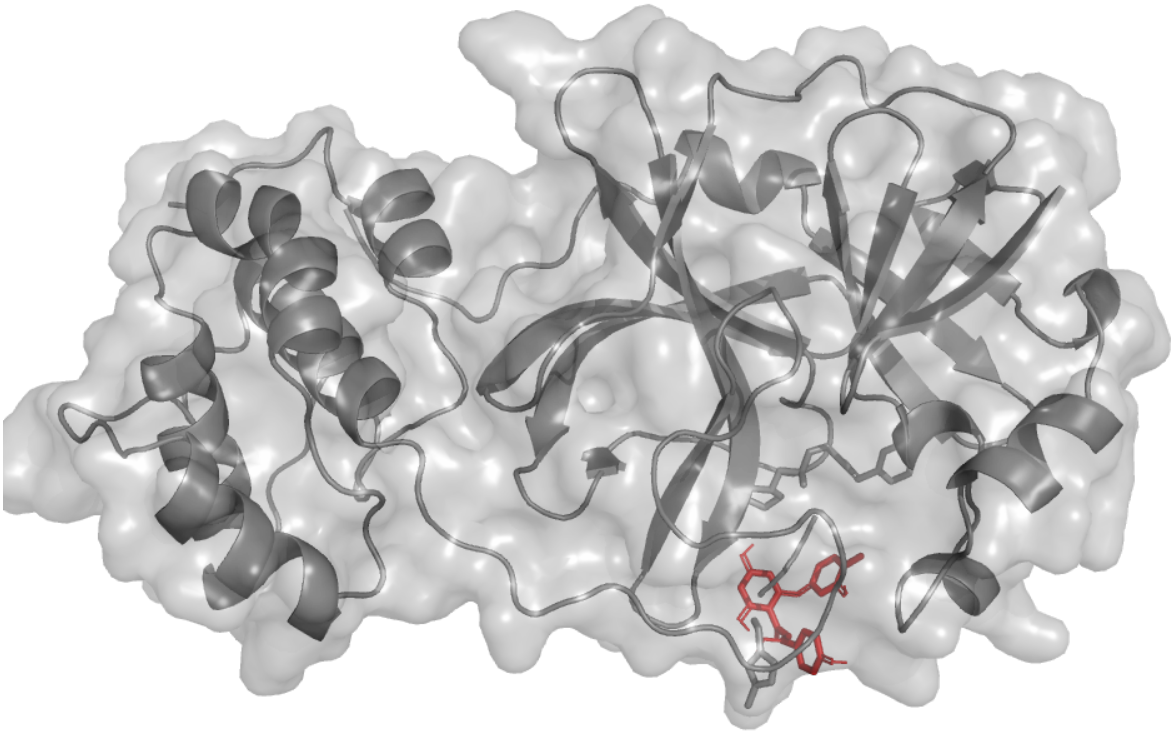


Figure 2: Front View

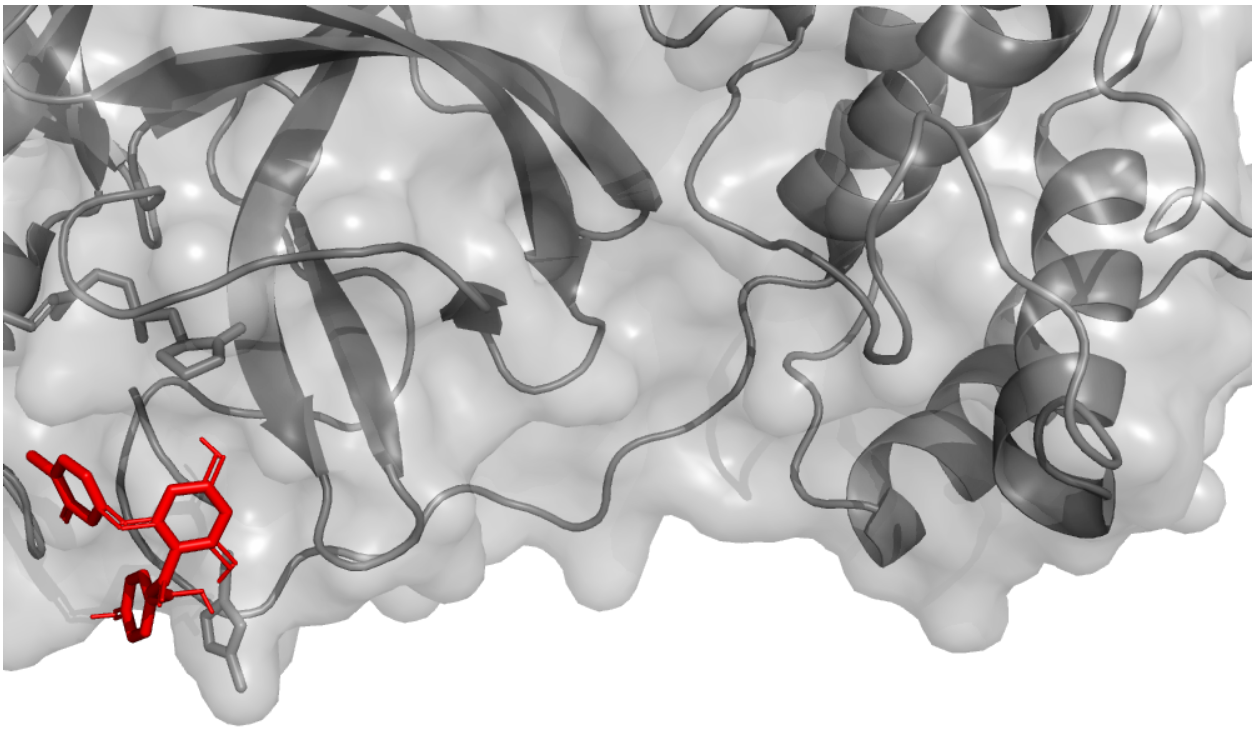


Figure 3: Close Up View of the Back

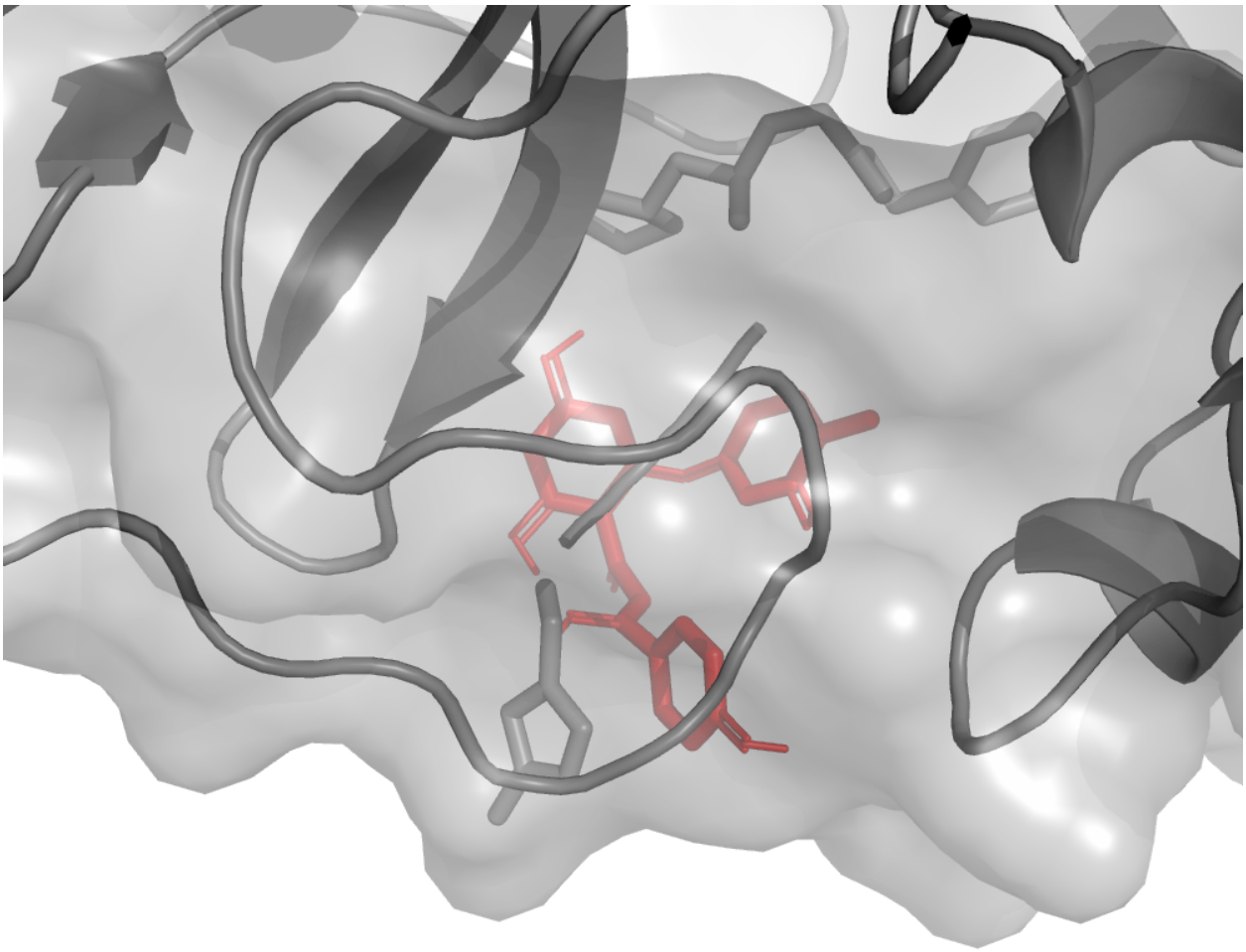


Figure 4: Close Up View of the Front