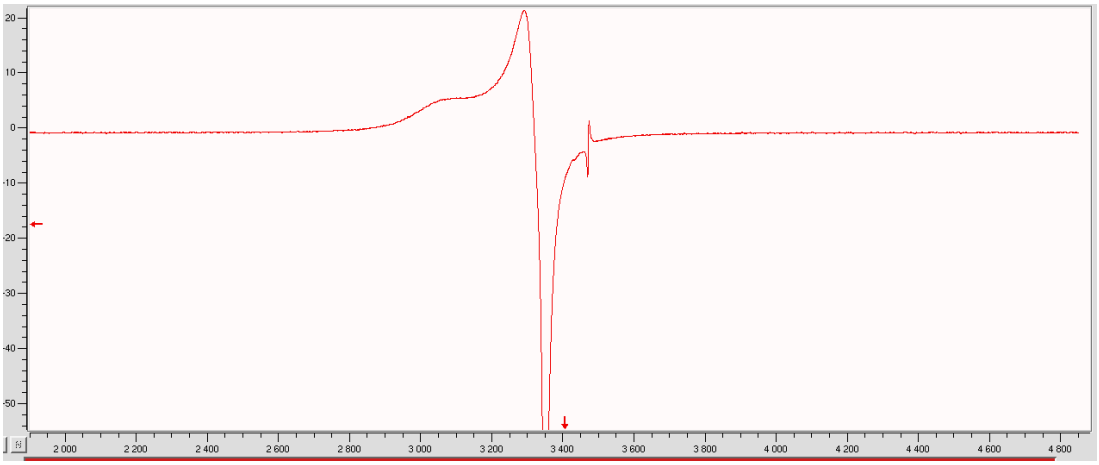
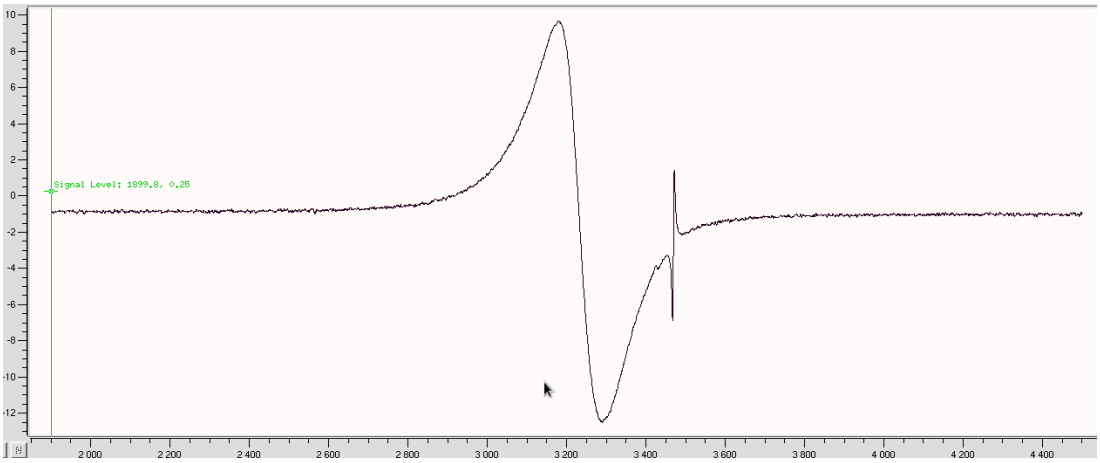
Supporting Information

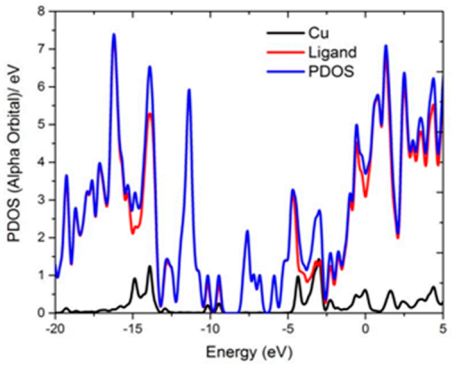


2

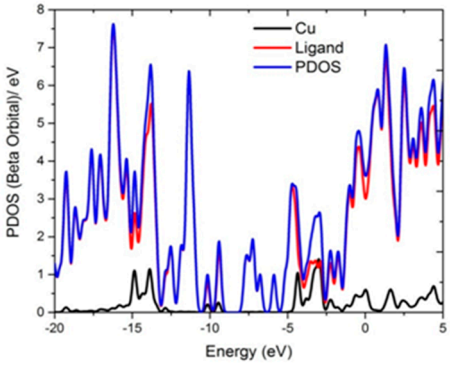


3

Figure S1. EPR spectra for powder samples of **2** and **3** at 300 K.

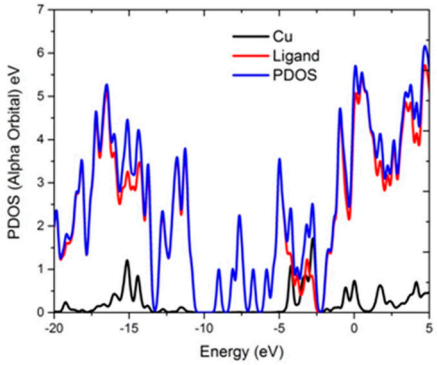


Alpha MOS	Cu	Ligand
L+5	1	99
L+4	0	100
L+3	0	100
L+2	1	99
L+1	1	99
LUMO	26	74
HOMO	21	79
H-1	1	99
H-2	1	99
H-3	0	100
H-4	0	100
H-5	0	100

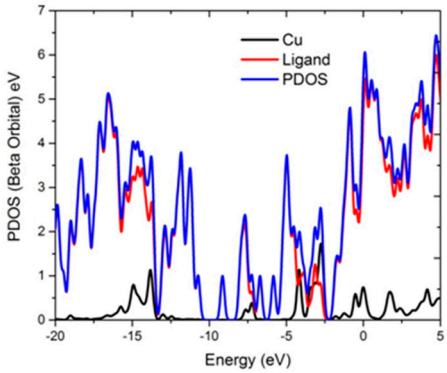


Beta MOS	Cu	Ligand
L+5	0	100
L+4	1	99
L+3	1	99
L+2	1	99
L+1	2	98
LUMO	25	75
HOMO	21	79
H-1	1	99
H-2	0	100
H-3	0	100
H-4	0	100
H-5	0	100

1



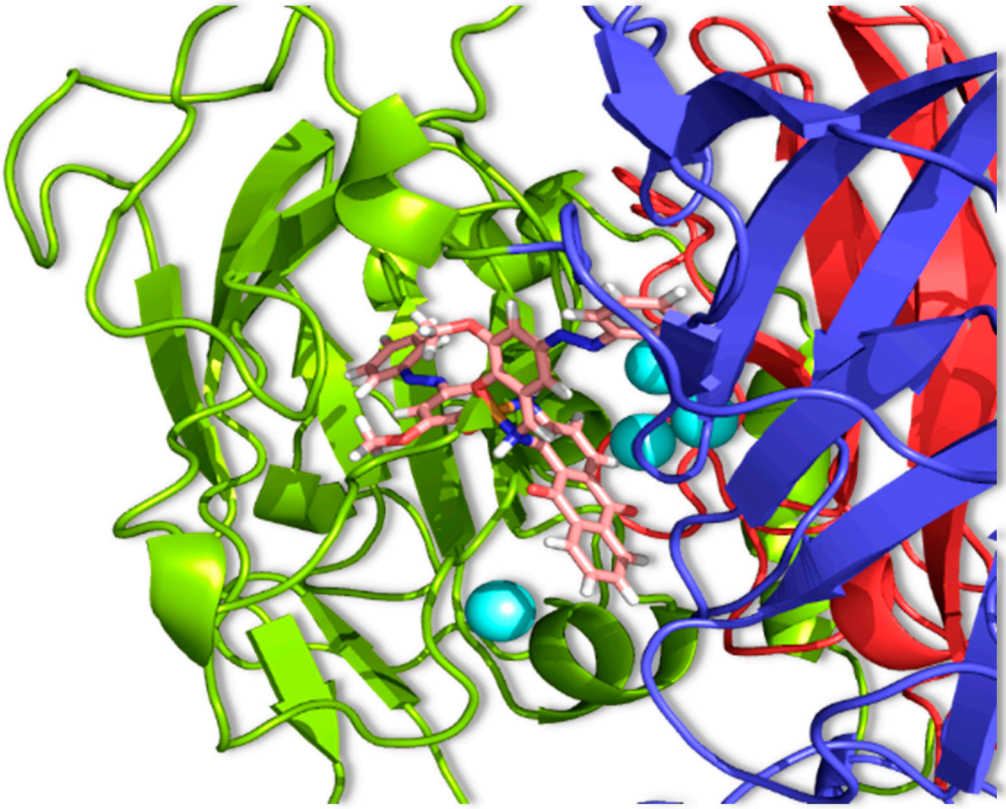
Alpha MOs	Cu	Ligand
L+5	1	99
L+4	0	100
L+3	0	100
L+2	1	99
L+1	0	100
LUMO	0	100
HOMO	1	99
H-1	1	99
H-2	0	100
H-3	1	99
H-4	1	99
H-5	7	93



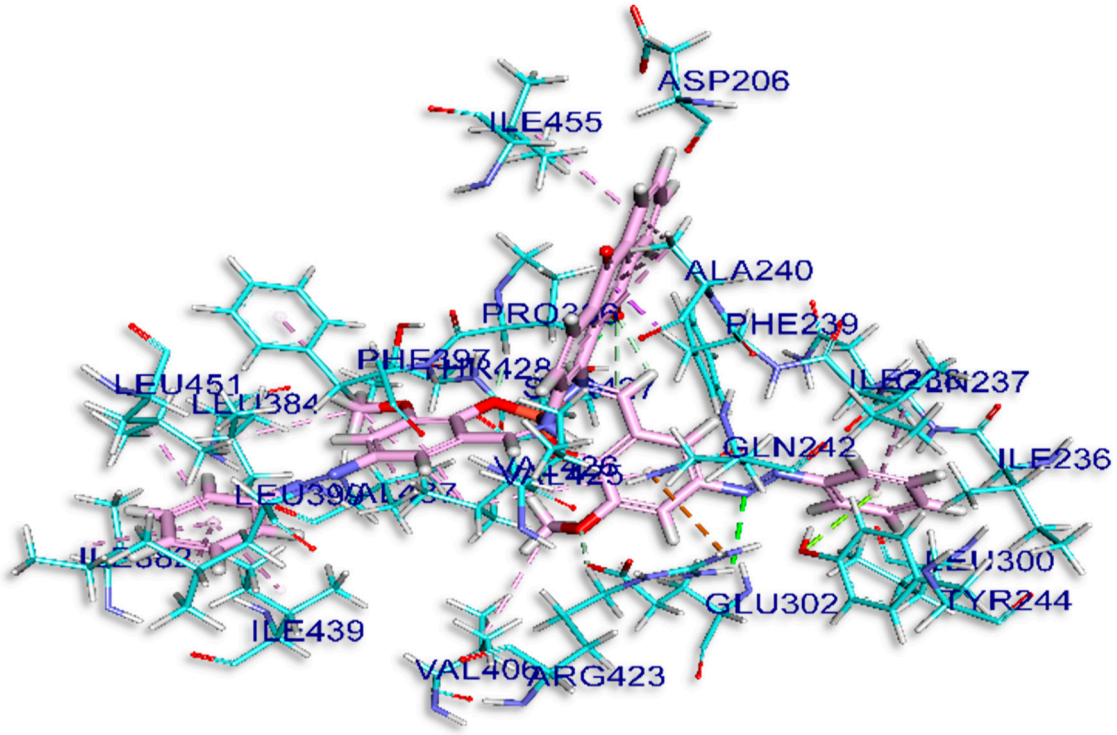
Beta MOs	Cu	Ligand
L+5	38	62
L+4	11	89
L+3	12	88
L+2	2	98
L+1	1	99
LUMO	1	99
HOMO	1	99
H-1	1	99
H-2	0	100
H-3	0	100
H-4	0	100
H-5	1	99

2

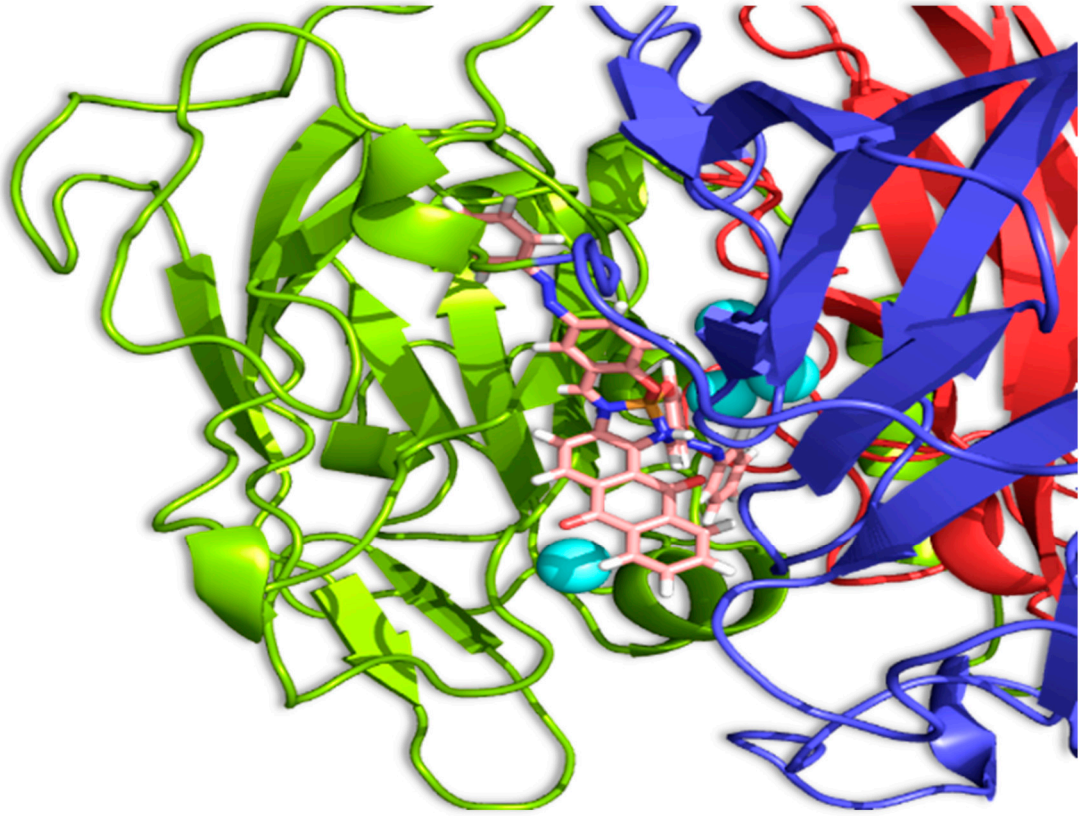
Figure S2. PDOS with orbital contribution for **1** and **2**.



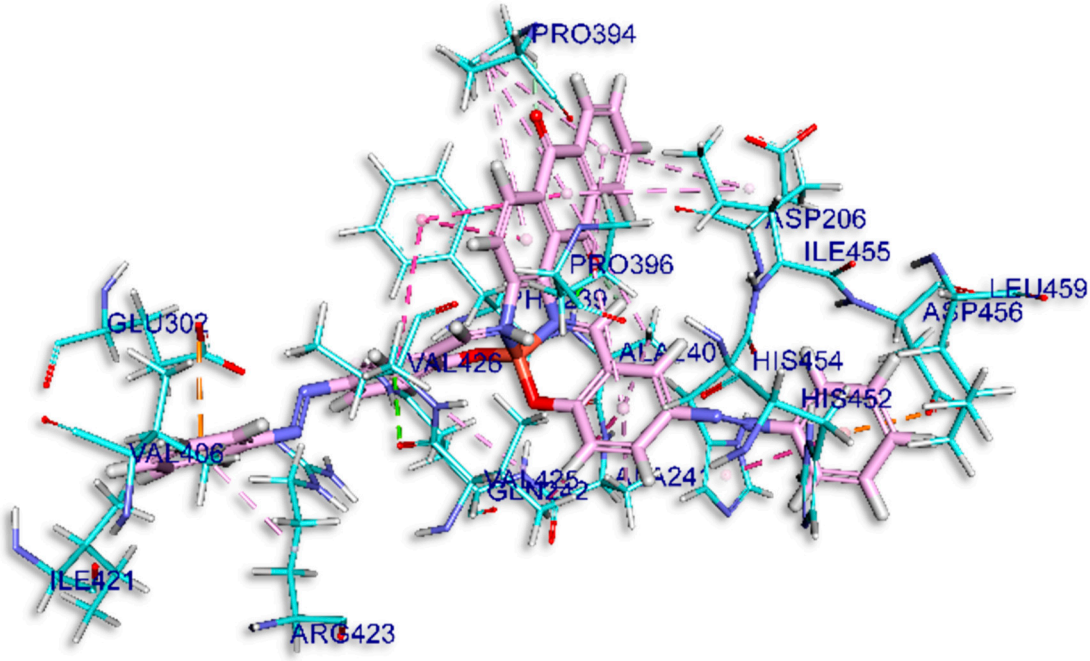
(a)


ASP206
ILE455
ALA240
PHE239
LEU451
GLN242
ILE236
GLU302
TYR244
ILE439
ARG423

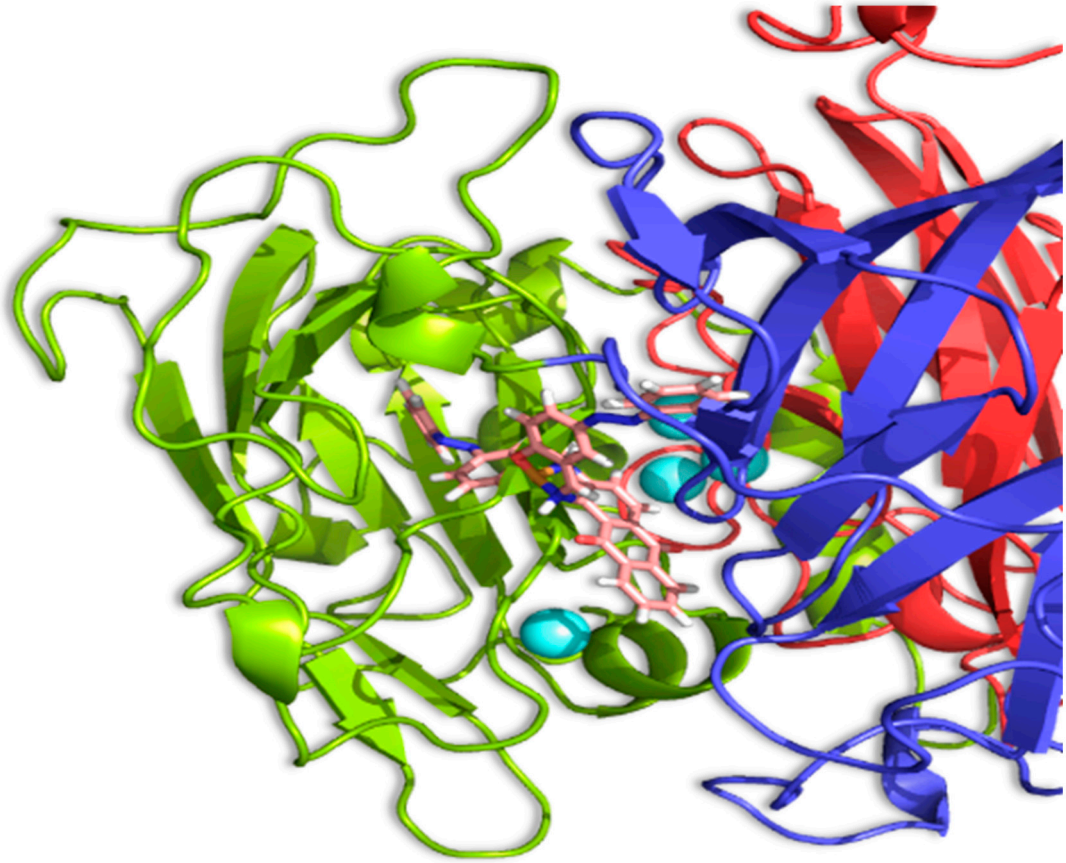
(b)



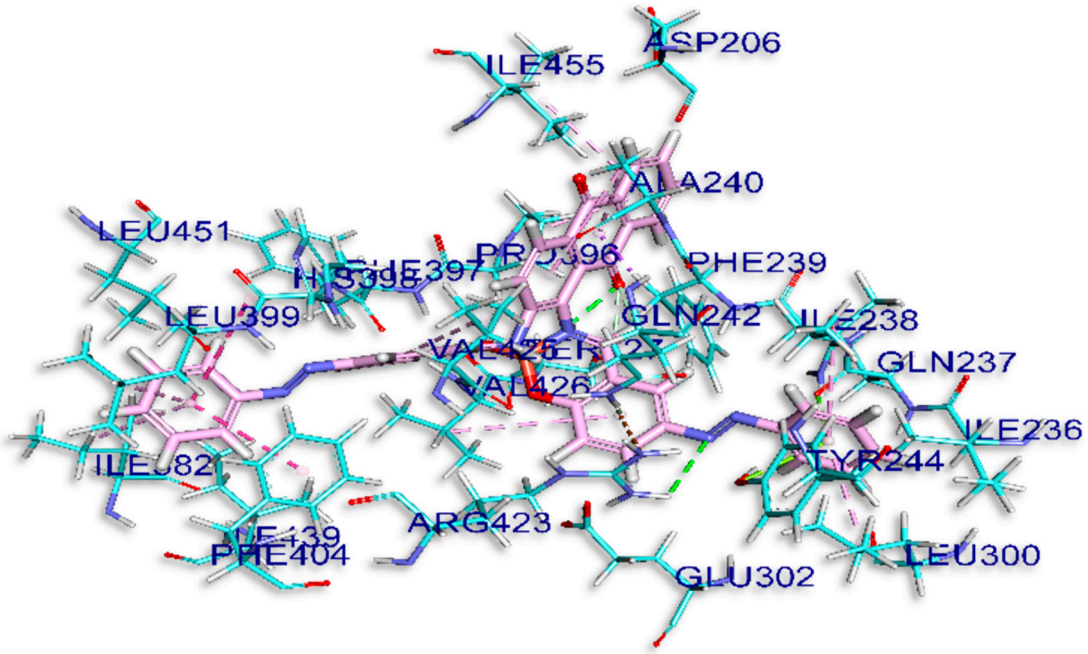
(c)


PRO394
ASP206
ILE455
LEU459
PRO396
GLU302
VAL426
HIS454
HIS452
VAL406
ILE421
ARG423

(d)



(e)



(f)

Figure S3. Comprehensive laccase receptor and copper complex interaction after docking. The copper complex is docked at the active site of the laccase receptor. The secondary structure of the laccase receptor is represented by the ribbon model, and the copper complex is represented by the stick model. Interactions of copper complex ligands (pink) with laccase receptor amino acids (sky blue)

omitting the laccase receptor, ligand surrounded amino acids are represented in a three letter code marked in dark blue. a, b represents ligand **1**, c, d represents ligand **2** and e, f represents ligand **3**.

Table S1. Summary of the results of DFT calculations for **1** and **2.**

	Wave-length (nm)	Oscillator Strength	Symmetry	Major Contribution	Minor Contribution
1	837.109	0.06	2.590-A	H-5(B)->LUMO(B)(12%) H-4(B)->L+1(B) (12%)	H-7(A)->LUMO(A) (5%) H-4(A)->LUMO(A) (4%) H-10(B)->L+1(B) (8%) H-9(B)->LUMO(B) (3%) H-9(B)->L+1(B) (7%) H-8(B)->LUMO(B) (8%) H-8(B)->L+1(B) (3%) H-6(B)->LUMO(B) (8%) H-4(B)->LUMO(B) (7%) H-3(B)->L+1(B) (9%) H-2(B)->L+1(B) (2%) H-13(A)->L+1(A) (2%) H-11(A)->LUMO(A)(2%) H-8(A)->LUMO(A) (2%) HOMO(A)->L+1(A) (4%) H-12(B)->L+1(B) (3%) H-9(B)->LUMO(B) (3%) H-5(B)->LUMO(B) (2%) HOMO(B)->L+1(B) (6%)
2	607.438	0.5	2.872-A	H-10(A)>LUMO(A)(20%) H-6(A)->LUMO(A)(17%) H-3(A)->LUMO(A)(10%) H-11(B)->LUMO(B)(14%)	

Table S2. Bond distances and type between laccase receptor and **Complex 2(L2) and Complex 3(L3).**

Complex 2(L2)			
P:L2:H16 - P:L2:O1	2.20	Hydrogen Bond	Conventional Hydrogen Bond
A:PRO394:HD1 - P:L2:O2	2.31	Hydrogen Bond	Carbon Hydrogen Bond
P:L2:H15 - P:L2:O1	2.36	Hydrogen Bond	Carbon Hydrogen Bond
A:VAL425:O - P:L2	2.74	Other	Pi-Lone Pair
A:ASP456:OD2 - P:L2	3.33	Electrostatic	Pi-Anion
A:GLU302:OE2 - P:L2	3.49	Electrostatic	Pi-Anion
P:L2 - A:ALA241	3.58	Hydrophobic	Pi-Alkyl
P:L2 - A:ARG423	3.68	Hydrophobic	Pi-Alkyl
A:HIS454 - P:L2	3.92	Hydrophobic	Pi-Pi T-shaped
A:PHE239 - P:L2	4.07	Hydrophobic	Pi-Pi T-shaped
P:L2 - A:PRO396	4.20	Hydrophobic	Pi-Alkyl
A:PHE239 - P:L2	4.49	Hydrophobic	Pi-Pi T-shaped
P:L2 - A:ALA240	4.66	Hydrophobic	Pi-Alkyl
P:L2 - A:PRO394	4.73	Hydrophobic	Pi-Alkyl
P:L2 - A:VAL425	4.73	Hydrophobic	Pi-Alkyl
A:PHE239 - P:L2	5.11	Hydrophobic	Pi-Pi T-shaped
P:L2 - A:ILE455	5.21	Hydrophobic	Pi-Alkyl
P:L2 - A:PRO394	5.22	Hydrophobic	Pi-Alkyl
P:L2 - A:VAL426	5.27	Hydrophobic	Pi-Alkyl
P:L2 - A:ALA240	5.31	Hydrophobic	Pi-Alkyl
P:L2 - A:PRO396	5.39	Hydrophobic	Pi-Alkyl
A:ALA241:C,O;GLN242:N - P:L2	5.40	Hydrophobic	Amide-Pi Stacked

P:L2 - A:ILE455	5.42	Hydrophobic	Pi-Alkyl
P:L2 - A:PRO394	5.44	Hydrophobic	Pi-Alkyl
Complex 3**(L3).**			
A:GLN242:HE22 - P:L3	1.06	Hydrogen Bond	Pi-Donor Hydrogen Bond
A:PRO396:HA - P:L3:O3	1.85	Hydrogen Bond	Carbon Hydrogen Bond
A:PHE239:HB1 - P:L3	2.05	Hydrophobic	Pi-Sigma
P:L3:H16 - P:L3:O1	2.20	Hydrogen Bond	Conventional Hydrogen Bond
P:L3:H15 - P:L3:O1	2.36	Hydrogen Bond	Carbon Hydrogen Bond
A:GLN237:O - P:L3	2.63	Other	Pi-Lone Pair
A:SER427:HB2 - P:L3:O1	2.90	Hydrogen Bond	Carbon Hydrogen Bond
A:ARG423:HH12 - P:L3:N3	2.94	Hydrogen Bond	Conventional Hydrogen Bond
A:TYR244:OH - P:L3	2.95	Other	Pi-Lone Pair
P:L3 - A:PRO396	3.74	Hydrophobic	Pi-Alkyl
P:L3 - A:LEU399	3.75	Hydrophobic	Pi-Alkyl
P:L3 - A:LEU300	3.90	Hydrophobic	Pi-Alkyl
P:L3 - A:ALA240	4.03	Hydrophobic	Pi-Alkyl
A:PHE404 - P:L3	4.49	Hydrophobic	Pi-Pi Stacked
A:ARG423:NH2 - P:L3	4.61	Electrostatic	Pi-Cation
P:L3 - A:ILE455	4.64	Hydrophobic	Pi-Alkyl
P:L3 - A:ALA240	4.65	Hydrophobic	Pi-Alkyl
P:L3 - A:ILE238	4.68	Hydrophobic	Pi-Alkyl
P:L3 - A:ALA240	4.82	Hydrophobic	Pi-Alkyl
A:HIS398:C,O;LEU399:N - P:L3	5.03	Hydrophobic	Amide-Pi Stacked
P:L3 - A:ILE382	5.13	Hydrophobic	Pi-Alkyl
P:L3 - A:VAL426	5.38	Hydrophobic	Pi-Alkyl
P:L3 - A:VAL425	5.45	Hydrophobic	Pi-Alkyl