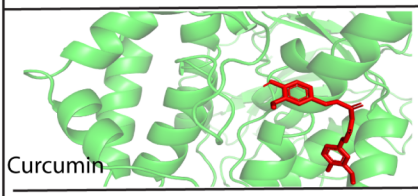
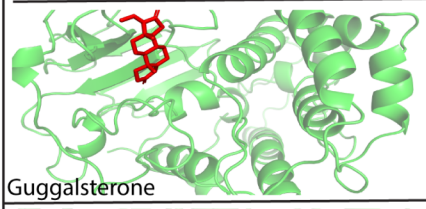
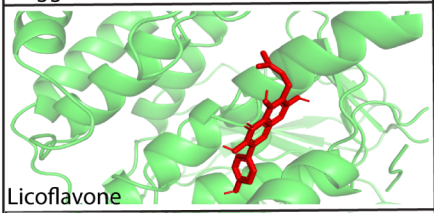
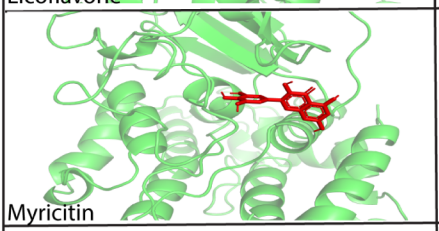
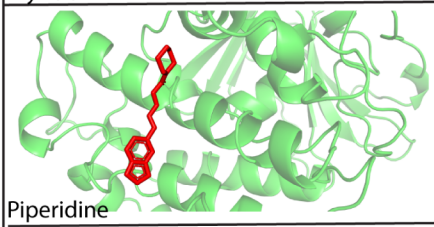
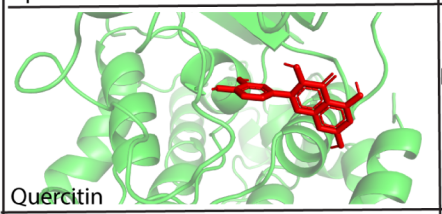
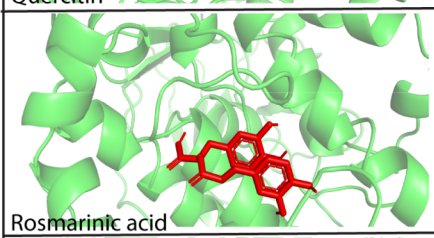
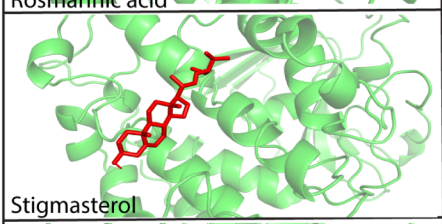
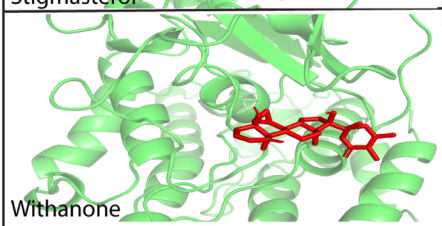
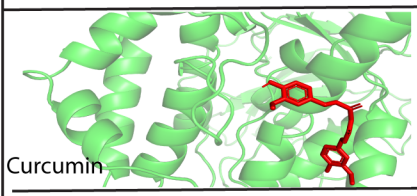
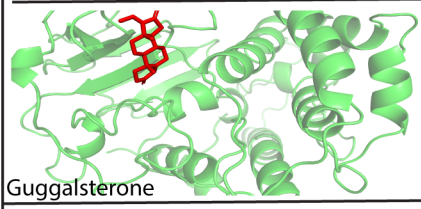
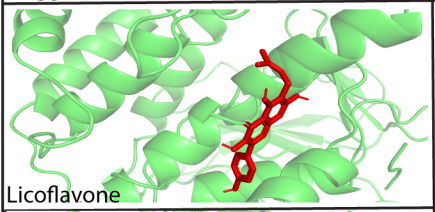
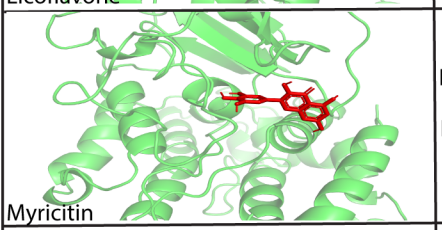
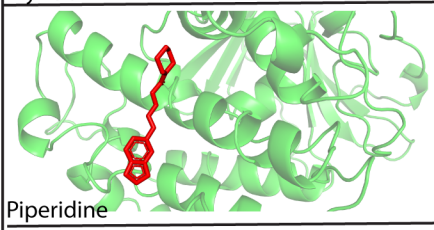
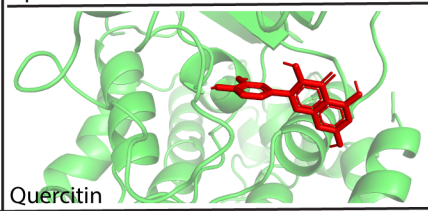
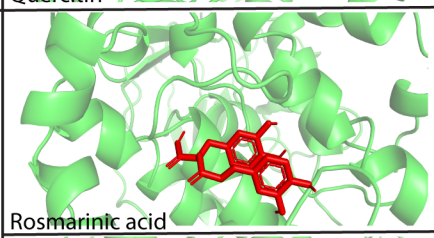
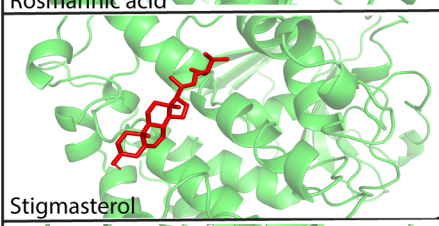
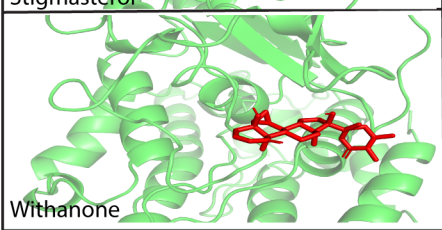
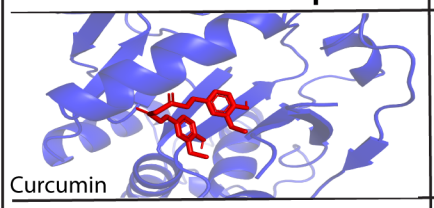
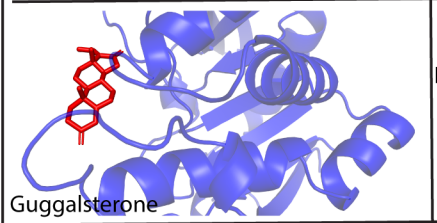
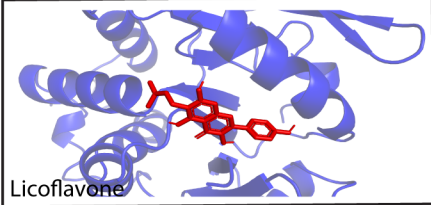
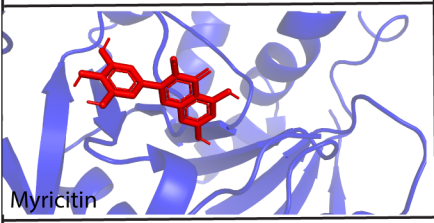
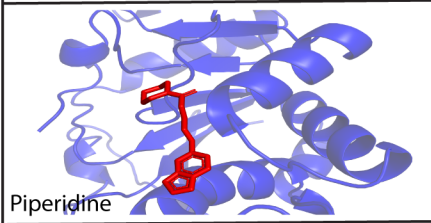
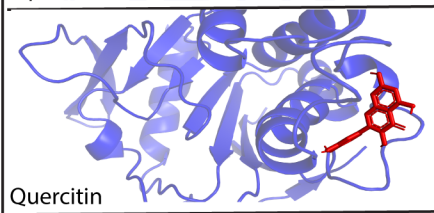
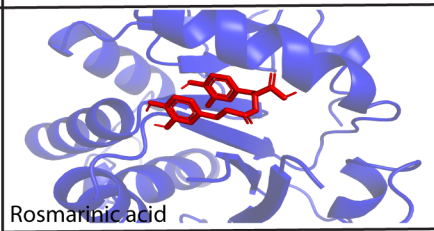
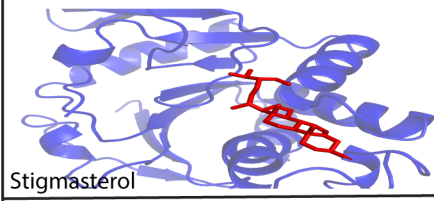
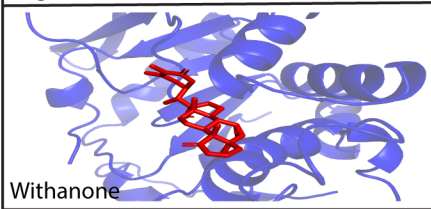
Supplementary Figure 1

Docked complex	Interactions
 Curcumin	Hydrophobic Bonds: Lys163,His167,Tyr160,Glu156,Asp136 Hydrogen Bonds: Thr138,Asn134,Pro139,Arg157
 Guggalsterone	Hydrophobic Bonds: Thr283,Lys311,Asn340,Asp310,Asn284,Asn285,Ile337 Hydrogen Bonds: Tyr289,Arg46
 Licoflavone	Hydrophobic Bonds: Thr160,Arg157,Arg205,Ile202,His167 Hydrogen Bonds: Glu156,Lys163,Asp201
 Myricitin	Hydrophobic Bonds: Ile337,Asn340,Thr283,Lys311 Hydrogen Bonds: Asp339,Tyr289,Arg46,Asp310
 Piperidine	Hydrophobic Bonds: His135,Tyr113,Asp136,Tyr160,Gln164,Ile202,Lys163,Asp201,Thr303 Hydrogen Bonds:
 Quercitin	Hydrophobic Bonds: Asn340,Ile337,Thr283,Lys311 Hydrogen Bonds: Tyr289,Asp339,Ile338,Arg46,Asp310
 Rosmarinic acid	Hydrophobic Bonds: Thr109,Asp136,Leu110,Asn111,Gly137,Tyr124,Phe107 Hydrogen Bonds: Lys108,His135,Lys133
 Stigmasterol	Hydrophobic Bonds: Ile202,His167,Lys163,Tyr160,Gln164,His135,Tyr113,Asp136 Hydrogen Bonds:
 Withanone	Hydrophobic Bonds: Glu341,Thr283,Asp339,Asp310,Lys311 Hydrogen Bonds: Asn287,Tyr289,Asn340

Supplementary Figure 2

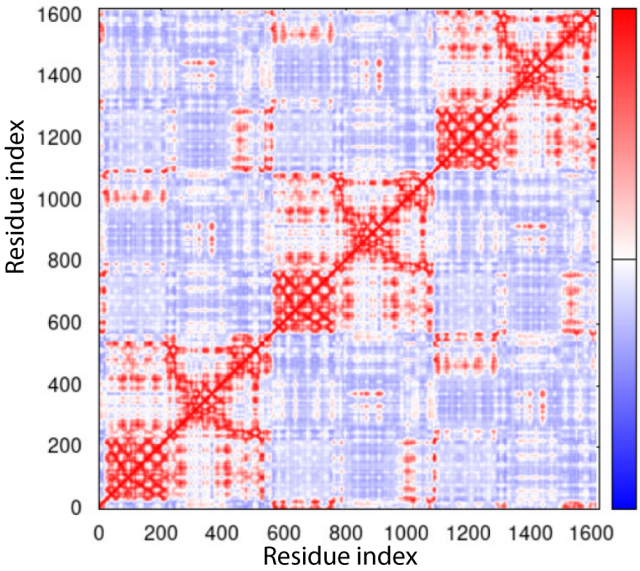
Docked complex	Interactions
 Curcumin	Hydrophobic Bonds: Lys163,His167,Tyr160,Glu156,Asp136 Hydrogen Bonds: Thr138,Asn134,Pro139,Arg157
 Guggalsterone	Hydrophobic Bonds: Thr283,Lys311,Asn340,Asp310,Asn284,Asn285,Ile337 Hydrogen Bonds: Tyr289,Arg46
 Licoflavone	Hydrophobic Bonds: Thr160,Arg157,Arg205,Ile202,His167 Hydrogen Bonds: Glu156,Lys163,Asp201
 Myricitin	Hydrophobic Bonds: Ile337,Asn340,Thr283,Lys311 Hydrogen Bonds: Asp339,Tyr289,Arg46,Asp310
 Piperidine	Hydrophobic Bonds: His135,Tyr113,Asp136,Tyr160,Gln164,Ile202,Lys163,Asp201,Thr303 Hydrogen Bonds:
 Quercitin	Hydrophobic Bonds: Asn340,Ile337,Thr283,Lys311 Hydrogen Bonds: Tyr289,Asp339,Ile338,Arg46,Asp310
 Rosmarinic acid	Hydrophobic Bonds: Thr109,Asp136,Leu110,Asn111,Gly137,Tyr124,Phe107 Hydrogen Bonds: Lys108,His135,Lys133
 Stigmasterol	Hydrophobic Bonds: Ile202,His167,Lys163,Tyr160,Gln164,His135,Tyr113,Asp136 Hydrogen Bonds:
 Withanone	Hydrophobic Bonds: Glu341,Thr283,Asp339,Asp310,Lys311 Hydrogen Bonds: Asn287,Tyr289,Asn340

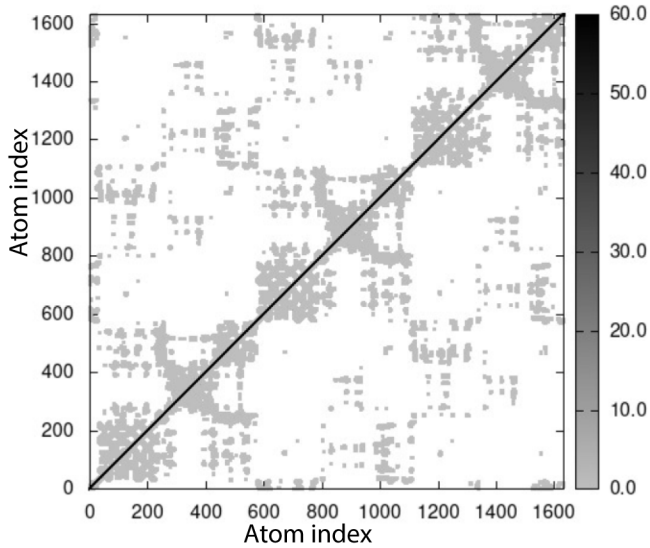
Supplementary Figure 3

Docked complex	Interactions
 Curcumin	Hydrophobic Bonds: Tyr62,Arg137,Lys141,His144,Leu140,Ala4,Glu119 Hydrogen Bonds: Thr6, Tyr120
 Guggalsterone	Hydrophobic Bonds: Phe212,Gly211,Tyr213,Phe214 Hydrogen Bonds: Thr91, Thr94
 Licoflavone	Hydrophobic Bonds: Asp61,Arg137,Lys5,Leu140,Val118,His144,Arg191 Hydrogen Bonds: Lys117,Glu119,Ala4,Thr6
 Myricitin	Hydrophobic Bonds: His293,Ala233,Ala234,Glu165,Thr158 Hydrogen Bonds: Val237,Arg154,Ile157,Lys161
 Piperidine	Hydrophobic Bonds: Val183,Tyr213,Phe212,Ser210,Gly211,Cys90,Thr91,Ser209 Hydrogen Bonds: Phe214
 Quercitin	Hydrophobic Bonds: Ala99,Ile72,Asp75,Arg96,Tyr78,Lys95,Ser83 Hydrogen Bonds: Glu92,Phe82
 Rosmarinic acid	Hydrophobic Bonds: Lys141,Tyr120,Ala4,His144,Leu140 Hydrogen Bonds: Thr6,Glu119,Asp61,Arg137
 Stigmasterol	Hydrophobic Bonds: Cys90,Thr94,Ser209,Ser210,Phe212,Gly211,Phe214,Tyr213 Hydrogen Bonds: Asn87,Met89
 Withanone	Hydrophobic Bonds: Cys99,Gly211,Phe212,Tyr213,Phe214 Hydrogen Bonds: Thr94,Thr91

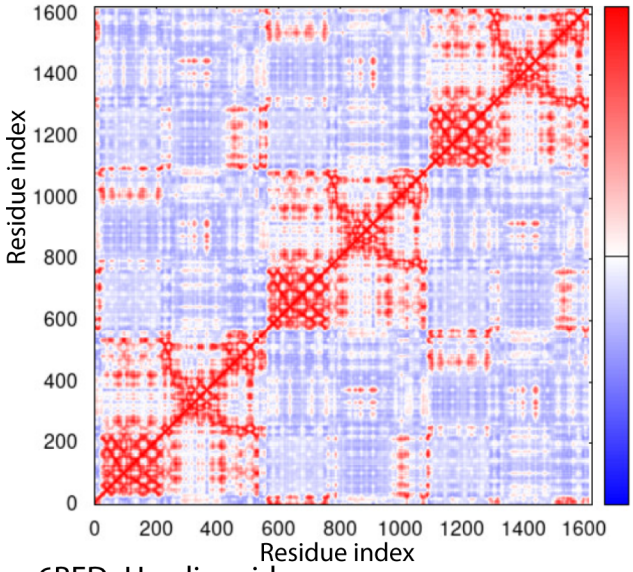
Supplementary Figure 4

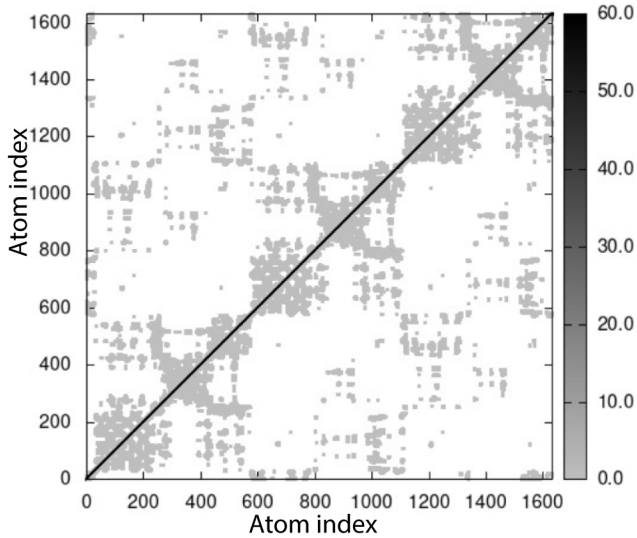
6BED_Silibinin





6BED_Oleanolic acid





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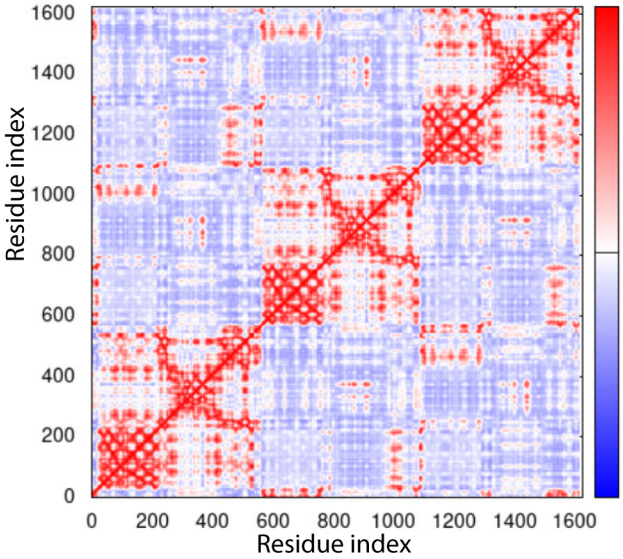
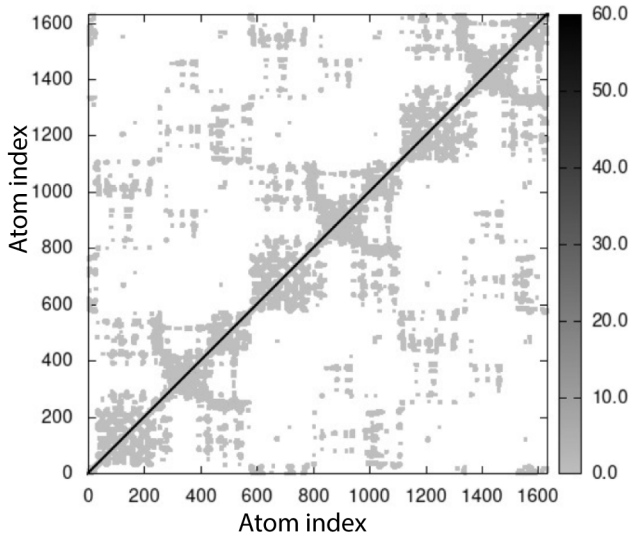
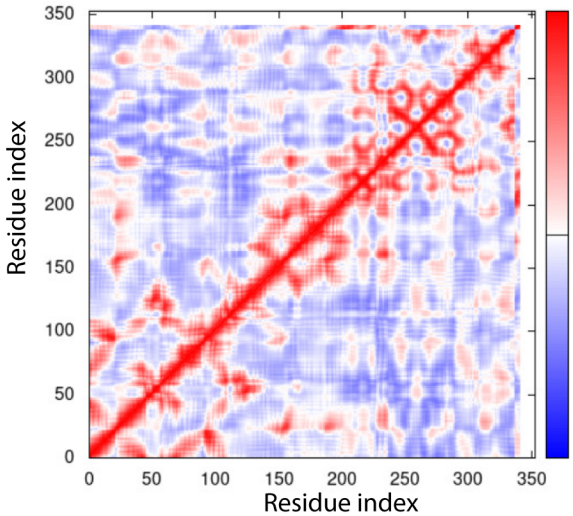
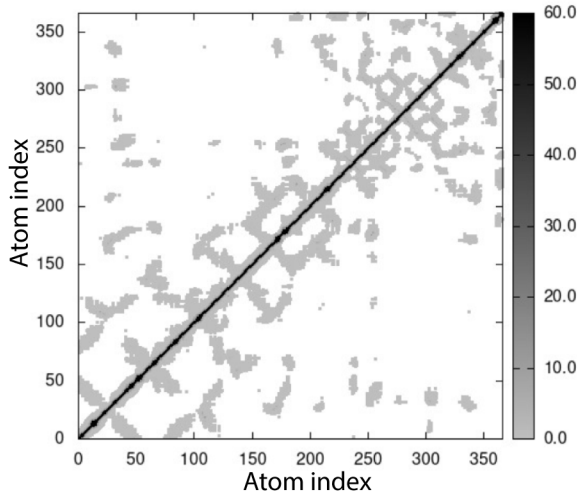




Supplementary Figure 5

6A9S_Silibinin





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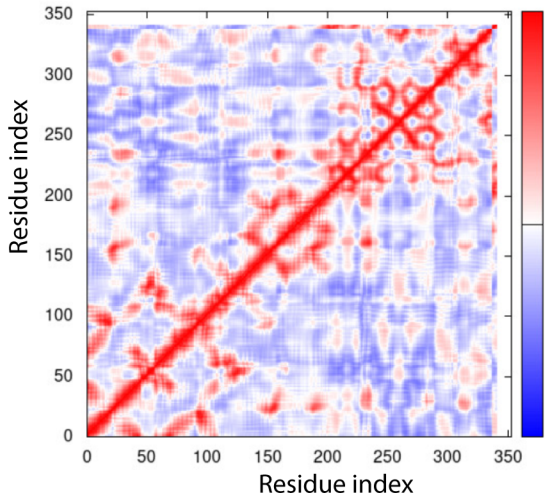

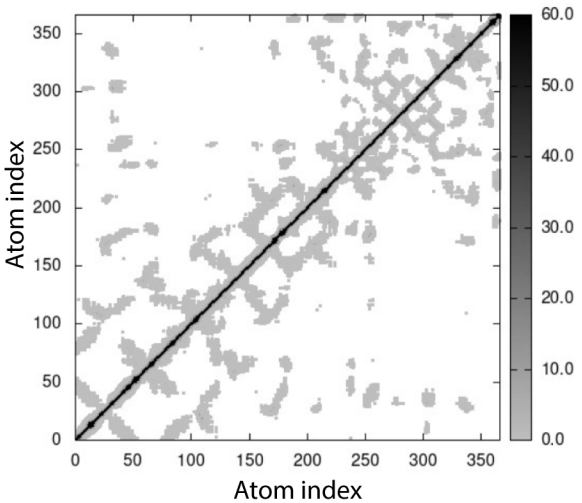

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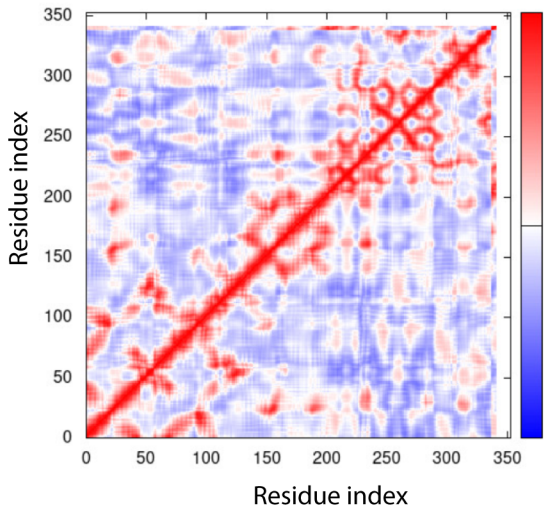

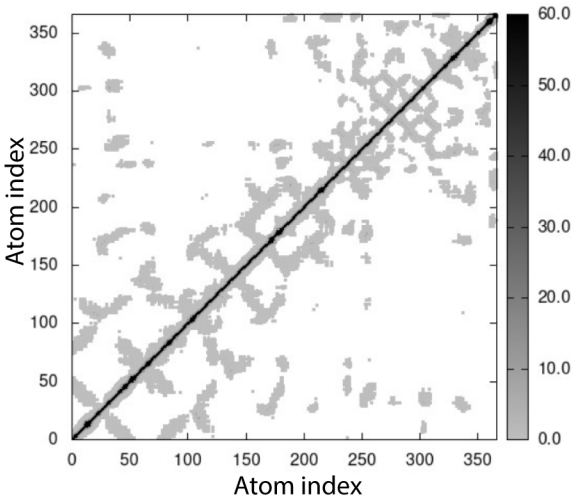

Supplementary Figure 6