

Supporting information

Table S1. MODEL-1 (GPO_AuNS) Conventional Hydrogen Bonds

Donor Residue	Donor Residue No	Donor Atom	Acceptor Residue	Acceptor Residue No	Acceptor Atom	Occupancy%
GLY	7	N	PRO	5	O	89.60
GLY	7	N	PRO	8	O	70.58
GLY	10	N	PRO	8	O	86.68
GLY	10	N	PRO	8	O	85.27
GLY	10	N	PRO	11	O	80.60
GLY	13	N	PRO	11	O	81.33
GLY	16	N	PRO	14	O	87.30
GLY	16	N	PRO	17	O	79.17
GLY	16	N	PRO	14	O	77.56
GLY	19	N	PRO	20	O	73.64
GLY	19	N	PRO	17	O	62.94
GLY	22	N	PRO	20	O	75.99
GLY	22	N	PRO	23	O	72.58
GLY	25	N	PRO	23	O	53.32
GLY	25	N	PRO	23	O	51.04

Table S2. MODEL-2 (GPP_AuNS) Conventional Hydrogen Bonds

Donor Residue	Donor Residue NO	Donor Atom	Acceptor Residue	Acceptor Residue NO	Acceptor Atom	Occupancy%
GLY	4	N	PRO	2	O	31.81
GLY	4	N	PRO	2	O	62.48
GLY	4	N	PRO	5	O	71.61
GLY	7	N	PRO	5	O	93.15
GLY	7	N	PRO	5	O	94.58
GLY	7	N	PRO	8	O	70.32
GLY	10	N	PRO	8	O	78.82
GLY	10	N	PRO	8	O	92.89
GLY	10	N	PRO	11	O	95.37
GLY	13	N	PRO	11	O	78.17
GLY	13	N	PRO	11	O	88.61
GLY	13	N	PRO	14	O	94.39
GLY	16	N	PRO	14	O	91.45
GLY	16	N	PRO	14	O	92.95
GLY	16	N	PRO	17	O	92.73
GLY	19	N	PRO	17	O	89.57
GLY	19	N	PRO	17	O	90.49
GLY	19	N	PRO	20	O	90.93
GLY	22	N	PRO	20	O	92.18
GLY	22	N	PRO	20	O	92.50
GLY	22	N	PRO	23	O	92.28
GLY	25	N	PRO	23	O	92.11
GLY	25	N	PRO	23	O	92.78

Table S3. MODEL-3 (TYPEIII_AuNS) Conventional Hydrogen Bonds

Donor Residue	Donor Residue NO	Donor Atom	Acceptor Residue	Acceptor Residue NO	Acceptor Atom	Occupancy%
GLY	1	N	GLY	1	O	38.71
GLY	4	N	PRO	2	O	90.75
GLY	4	N	ARG	3	O	56.59
GLY	4	N	ASP	5	O	59.23
GLY	7	N	ASP	5	O	54.93
GLY	7	N	ASP	5	O	47.84
GLY	7	N	LYS	6	O	71.62
GLY	10	N	GLU	8	O	98.66
GLY	10	N	GLU	8	O	86.77
GLY	7	N	GLU	8	O	84.30
GLY	13	N	GLU	11	O	93.72
GLY	10	N	GLU	11	O	83.95
GLY	13	N	GLU	11	O	94.14
GLY	13	N	ALA	14	O	86.88
GLY	16	N	ALA	14	O	80.39
GLY	16	N	ALA	14	O	83.98
GLY	19	N	ILE	17	O	95.52
GLY	19	N	ILE	17	O	90.23
GLY	16	N	ILE	17	O	97.54
GLY	22	N	HIE	20	O	97.81
GLY	19	N	HIE	20	O	73.07
GLY	22	N	HIE	20	O	97.52
GLY	22	N	PHE	23	O	94.97
GLY	25	N	PHE	23	O	79.09
GLY	25	N	PHE	23	O	87.49
GLY	25	N	PRO	26	O	38.71

Table S4. MODEL-4 (TYPE1_AuNS) Conventional Hydrogen Bonds

Donor Residue	Donor Residue NO	Donor Atom	Acceptor Residue	Acceptor Residue NO	Acceptor Atom	Occupancy%
GLY	757	N	SER	758	O	93.77
GLY	757	N	GLU	755	O	65.76
GLY	760	N	ALA	761	O	94.51
GLY	760	N	PRO	758	O	86.44
GLY	760	N	SER	758	O	81.96
GLY	763	N	ALA	761	O	97.40
GLY	763	N	PRO	764	O	95.94
GLY	763	N	GLU	761	O	87.50
GLY	766	N	PRO	764	O	92.62
GLY	769	N	THR	770	O	85.68
GLY	769	N	ALA	767	O	80.43
GLY	769	N	PRO	767	O	51.99
GLY	772	N	THR	770	O	92.11
GLY	772	N	THR	770	O	82.29
GLY	772	N	PRO	773	O	76.04
GLY	775	N	ILE	776	O	95.58
GLY	775	N	PRO	773	O	95.05
GLY	775	N	PRO	773	O	92.06
GLY	778	N	GLN	779	O	93.61
GLY	778	N	LEU	776	O	71.79
GLY	778	N	ILE	776	O	53.80

Table S5. MODEL-1 (GPO) without_AuNS Conventional Hydrogen Bonds

Donor Residue	Donor Residue NO	Donor Atom	Acceptor Residue	Acceptor Residue NO	Acceptor Atom	Occupancy%
GLY	1	N	PRO	2	O	52.97
GLY	4	N	PRO	5	O	87.14
GLY	4	N	PRO	2	O	85.76
GLY	4	N	PRO	2	O	83.61
GLY	7	N	PRO	5	O	89.19
GLY	7	N	PRO	5	O	88.88
GLY	7	N	PRO	8	O	88.46
GLY	10	N	PRO	11	O	88.89
GLY	10	N	PRO	8	O	88.67
GLY	10	N	PRO	8	O	88.03
GLY	13	N	PRO	14	O	89.06
ALA	13	N	PRO	11	O	88.17
GLY	13	N	PRO	11	O	87.65
GLY	16	N	PRO	14	O	89.21
GLY	16	N	PRO	14	O	88.40
GLY	16	N	PRO	17	O	88.01
GLY	19	N	PRO	17	O	89.38
GLY	19	N	PRO	17	O	89.29
GLY	19	N	PRO	20	O	88.83
GLY	22	N	PRO	23	O	89.78
GLY	22	N	PRO	20	O	88.92
GLY	22	N	PRO	20	O	86.23
GLY	25	N	PRO	23	O	89.16
GLY	25	N	PRO	23	O	87.53

Table S6. MODEL-2 (GPP) without_ AuNS Conventional Hydrogen Bonds

Donor Residue	Donor Residue NO	Donor Atom	Acceptor Residue	Acceptor Residue NO	Acceptor Atom	Occupancy%
GLY	1	N	PRO	2	O	51.10
GLY	4	N	PRO	5	O	89.14
GLY	4	N	PRO	2	O	88.16
GLY	4	N	PRO	2	O	84.80
GLY	7	N	PRO	5	O	90.76
GLY	7	N	PRO	8	O	90.53
GLY	7	N	PRO	5	O	90.27
GLY	10	N	PRO	11	O	91.20
GLY	10	N	PRO	8	O	90.80
GLY	10	N	PRO	8	O	89.86
GLY	13	N	PRO	14	O	90.86
ALA	13	N	PRO	11	O	90.00
GLY	13	N	PRO	11	O	89.95
GLY	16	N	PRO	14	O	91.03
GLY	16	N	PRO	14	O	90.48
GLY	16	N	PRO	17	O	89.91
GLY	19	N	PRO	17	O	90.90
GLY	19	N	PRO	17	O	90.46
GLY	19	N	PRO	20	O	90.23
GLY	22	N	PRO	23	O	90.63
GLY	22	N	PRO	20	O	90.21
GLY	22	N	PRO	20	O	89.88
GLY	25	N	PRO	23	O	90.13
GLY	25	N	PRO	23	O	89.65

Table S7. MODEL-3 (TYPEIII) without_ AuNS Conventional Hydrogen Bonds

Donor Residue	Donor Residue NO	Donor Atom	Acceptor Residue	Acceptor Residue NO	Acceptor Atom	Occupancy%
GLY	1	N	PRO	2	O	71.45
GLY	4	N	ASP	5	O	98.98
GLY	4	N	PRO	2	O	98.36
GLY	4	N	PRO	2	O	97.03
GLY	7	N	ASP	5	O	99.36
GLY	7	N	ASP	5	O	99.32
GLY	7	N	GLU	8	O	98.90
GLY	10	N	GLU	11	O	99.27
GLY	10	N	GLU	8	O	98.96
GLY	10	N	GLU	8	O	98.45
GLY	13	N	GLU	11	O	99.11
ALA	13	N	GLU	11	O	99.07
GLY	13	N	ALA	14	O	98.23
GLY	16	N	ALA	14	O	95.66
GLY	16	N	ILE	17	O	95.52
GLY	16	N	ALA	14	O	95.20
GLY	19	N	HIE	20	O	98.02
GLY	19	N	ILE	17	O	97.86
GLY	19	N	ILE	17	O	97.34
GLY	22	N	HIE	20	O	98.31
GLY	22	N	PHE	23	O	94.61
GLY	22	N	HIE	20	O	94.37
GLY	25	N	PHE	23	O	95.41
GLY	25	N	PHE	23	O	93.40
GLY	25	N	PRO	26	O	88.06

Table S8. MODEL-4 (TYPEI) without_AuNS Conventional Hydrogen Bonds

Donor Residue	Donor Residue NO	Donor Atom	Acceptor Residue	Acceptor Residue NO	Acceptor Atom	Occupancy%
GLY	757	N	GLU	755	O	79.95
GLY	757	N	GLU	755	O	62.86
GLY	757	N	SER	758	O	89.52
GLY	760	N	PRO	758	O	93.14
GLY	760	N	SER	758	O	90.65
GLY	760	N	ALA	761	O	97.08
GLY	763	N	ALA	761	O	96.38
GLY	763	N	GLU	761	O	93.15
GLY	763	N	PRO	764	O	95.88
GLY	766	N	THR	764	O	95.48
GLY	766	N	PRO	764	O	95.26
GLY	766	N	ALA	767	O	96.90
GLY	769	N	ALA	767	O	96.04
GLY	769	N	PRO	767	O	94.40
GLY	769	N	THR	770	O	95.67
GLY	772	N	THR	770	O	95.95
GLY	772	N	THR	770	O	95.33
GLY	772	N	PRO	773	O	94.12
GLY	775	N	PRO	773	O	97.85
GLY	775	N	PRO	773	O	97.56
GLY	775	N	ILE	776	O	98.01
GLY	778	N	LEU	776	O	97.73
GLY	778	N	ILE	776	O	96.94
GLY	778	N	GLN	779	O	96.46

Conventional Hydrogen bonds for all the model systems are given in the Tables.

Table S1. MODEL-1 (GPO_AuNS) Table S2. MODEL-2 (GPP_AuNS) Table S3. MODEL-3 (TYPEIII_AuNS) Table S4. MODEL-4 (TYPEI_AuNS) Table S5. MODEL-1 (without_AuNS) Table S6. MODEL-2 (without_AuNS) Table S7. MODEL-3 (without_AuNS) Table S8. MODEL-4 (without_AuNS)