

Supplementary material:

Table 1: Ramchandran plot and Z-score of the models

Model	Ramachandran plot	Prosa2003
AGPase Large subunit	88.4	-9.54
AGPase Small subunit	89.3	-8.17
Template (1YP2)	87.5	-8.76

Table 2: Hydrogen bonding pattern in complex

Donor	Acceptor	Distance(Å)
THR A* 422	MET B* 138	2.11
ARG A* 420	GLY B* 47	1.98
SER B* 306	SER A* 259	3.17
ILE B* 311	GLU A* 241	3.14
GLN A* 113	GLU B* 286	1.96
LYS B* 291	GLN A* 70	3.31

*A- Small subunit; *B- Large subunit

Table 3: Hydrophobic contacts in the complex

Total contacts	*SS amino acids	*LS amino acids	Distance(Å)
10	Tyr30	Lys 291	2.72-3.80
2	Trp111	Asp289	3.71-3.87
5	Gln113	Glu286	2.34-3.77
4	Glu192	Pro302, Pro303	3.40-3.82
6	Lys193	Tyr300	3.35-3.76
4	Phe243	Ser306, Cys309	3.13-3.63
11	Pro244	Ile311, Lys312	2.83-3.72
3	Gly245	Ala314, Ile315	2.84-3.83
3	Ser251	Pro303	3.40-3.77
4	Ser259	Lys305	2.59-3.59
2	Ala413	Thr78	3.35-3.89
6	Val415	Thr78	2.09-3.85
5	Ala419	Asn45, Gly47	3.38-3.57
2	Glu421	Met138	3.25-3.65
8	Thr422	Met138	2.89-3.87

*SS- Small subunit; *LS- Large subunit

Table 4: Accessible surface area values for AGP-S amino acids in unbound and bound stage

SS* Amino acids	Uncomplex	Complex
Tyr30	75.88	28.04
Trp111	89.44	33.41
Gln113	109.75	17.85
Glu192	89.97	33.02
Lys193	102.56	51.7
Phe243	50.89	6.16
Pro244	70.32	17.79
Gly245	63.04	15.07
Ser251	40.8	14.78
Ser259	96.06	13.41
Ala413	102.1	65.39
Val415	65.94	28.25
Ala419	62.7	33.05
Glu421	41.9	12.1
Thr422	103.87	69.52

*SS- Small subunit

Table 5: Accessible surface area values for AGP-L amino acids in unbound and bound stage

LS* Amino acids	Uncomplex	Complex
Asn45	59.41	21.49
Gly42	5.2	4.63
Gln70	19.17	17.05
Thr78	109.51	30.17
Met138	95.99	20.27
Glu286	69.69	10.06
Asp289	26.29	4.64
Lys291	167.82	36.53
Thr300	203.15	104.67
Pro302	70.93	41.6
Pro303	120.86	20.94
Lys305	118	85.79
Ser306	50.81	12.61
Cys309	33.28	6.89
Ile311	61.78	3.34
Lys312	141.95	134.54
Ala314	26.08	2.6

*LS- Large subunit