Supplementary Material

for

The Structure of Urease Activation Complexes Examined by Flexibility Analysis, Mutagenesis, and Small-Angle X-Ray Scattering

by

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Table S1

Polar Interactions of Region 1 (UreB residues 2 – 8)

Residue 1	**Donor Atom**	**Residue 2**	**Acceptor Atom**	**Energy (Kcal/mol)**
UreB Gly4	N	UreC Ala24	O	-2.73
UreC Lys20	N	UreB His7	O	-3.62
UreB His7	N	UreC Lys20	O	-4.58
UreC Arg22	N	UreB Glu5	O	-6.52
UreC Arg22	NH1	UreB Glu5	OE2	-8.11

Table S2

Hydrophobic Interactions of Region 1 (UreB residues 2 – 8)

Residue 1	**Atom 1**	**Residue 2**	**Atom 2**
UreB Glu5	CG	UreC Trp29	CH2
UreB Tyr6	CD1	UreC Val21	CG2
UreB His7	CB	UreC Trp29	CZ3
UreB Val8	CG1	UreC Arg6	CB
UreB Val8	CG2	UreC Ala10	CB

Table S3

Polar Interactions of Region 2 (UreB residues 11 – 19)

Residue 1	Donor Atom	Residue 2	Acceptor Atom	Energy (Kcal/mol)
UreC Arg6	N	UreB Gly11	O	-3.45
UreC Ile4	N	UreB Ile13	O	-4.53
UreB Leu15	N	UreC Ser2	O	-4.73
UreB Asn16	N	UreC Tyr39	O	-4.87
UreB Ile13	N	UreC Ile4	O	-7.18
UreB Arg19	NH2	UreC Glu41	OE2	-7.34
UreB Arg19	NH1	UreC Glu41	OE2	-8.88

Table S4

Hydrophobic Interactions of Region 2 (UreB residues 11 – 19)

Residue 1	Atom 1	Residue 2	Atom 2
UreB Ile13	CB	UreC Ile4	CG2
UreB Ile13	CG2	UreC Tyr39	CG

Table S5

Polar Interactions of Region 3 (UreB residues 20 – 101)

Residue 1	**Donor Atom**	**Residue 2**	**Acceptor Atom**	**Energy (Kcal/mol)**
UreB His39	NE2	UreC Glu41	OE2	-1.03
UreB Arg60	NH2	UreC Glu41	OE1	-1.43
UreB Arg60	NE	UreC Glu41	OE2	-1.84
UreC Lys49	NZ	UreB Gly66	O	-2.11
UreB His87	N	UreC Pro102	O	-2.20
UreB Ala85	N	UreC Ile104	O	-2.84
UreB Ala89	N	UreC Asp103	O	-3.09
UreB His87	ND1	UreC Asp103	OD1	-4.27
UreB His39	NE2	UreC Glu41	OE1	-8.55
UreB Arg60	NH2	UreC Glu41	OE2	-8.98

Table S6

Hydrophobic Interactions of Region 3 (UreB residues 20 – 101)

Residue 1	Atom 1	Residue 2	Atom 2
UreB Tyr40	CD2	UreC Met55	CE
UreB Phe84	CG	UreC Ile104	CG2
UreB Phe84	CD1	UreC Ile104	CB
UreB Phe84	CE1	UreC Ile104	CD1
UreB Phe91	CB	UreC Gln59	CG
UreB Phe93	CE1	UreC Met55	CE
UreB Phe93	CE1	UreC Met55	SD
UreB Phe93	CE1	UreC Met55	CG
UreB Phe93	CZ	UreC Met55	CG

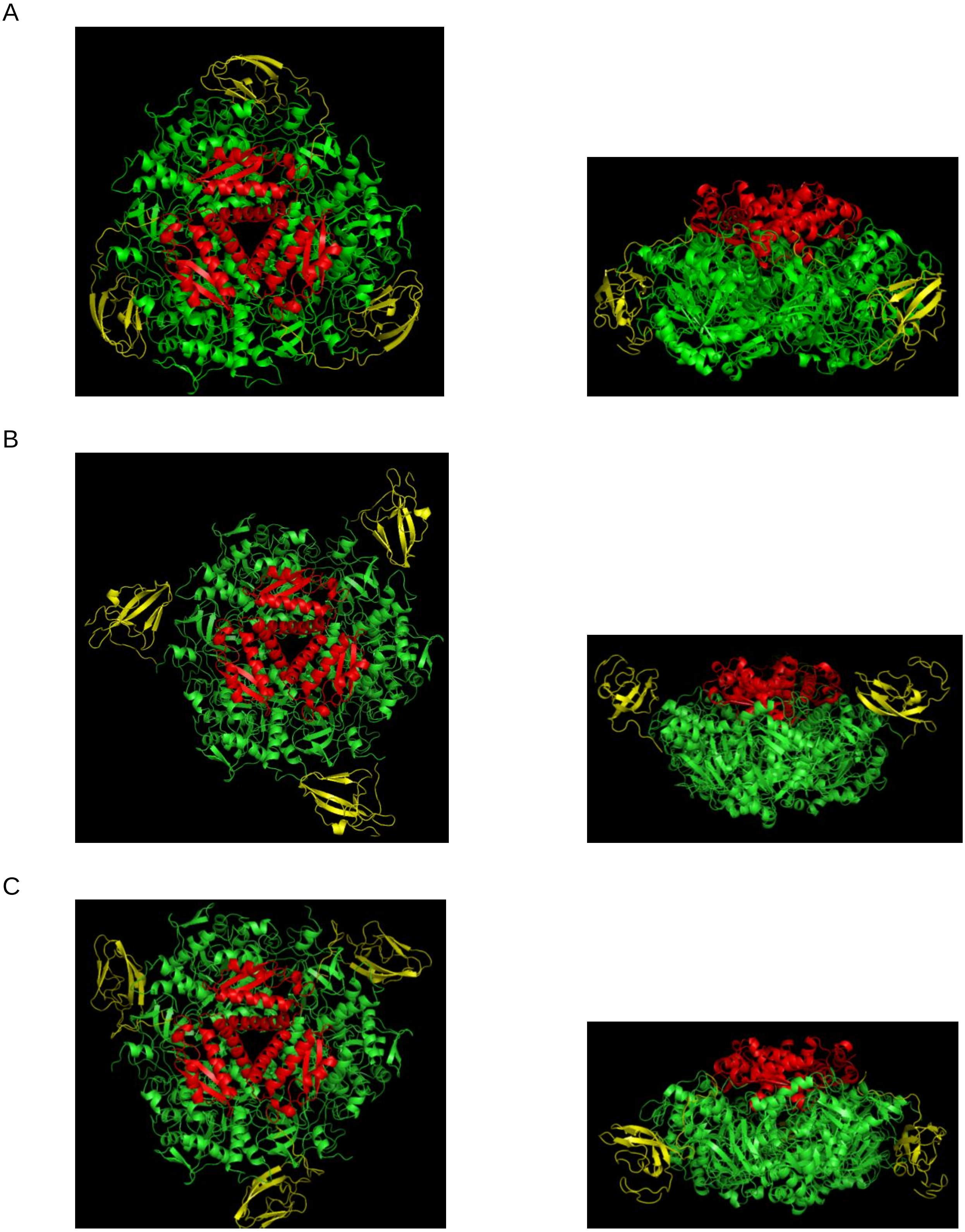

Fig. S1. Two views of (A) the native conformation of urease, (B) UreB conformation 1 (torsionally adjusted UreB Gly11 and Gly18 residues), and (C) UreB conformation 2 (severed linker, docked domain, and reconnected linker). UreA is depicted in red, UreB in yellow, and UreC in green.

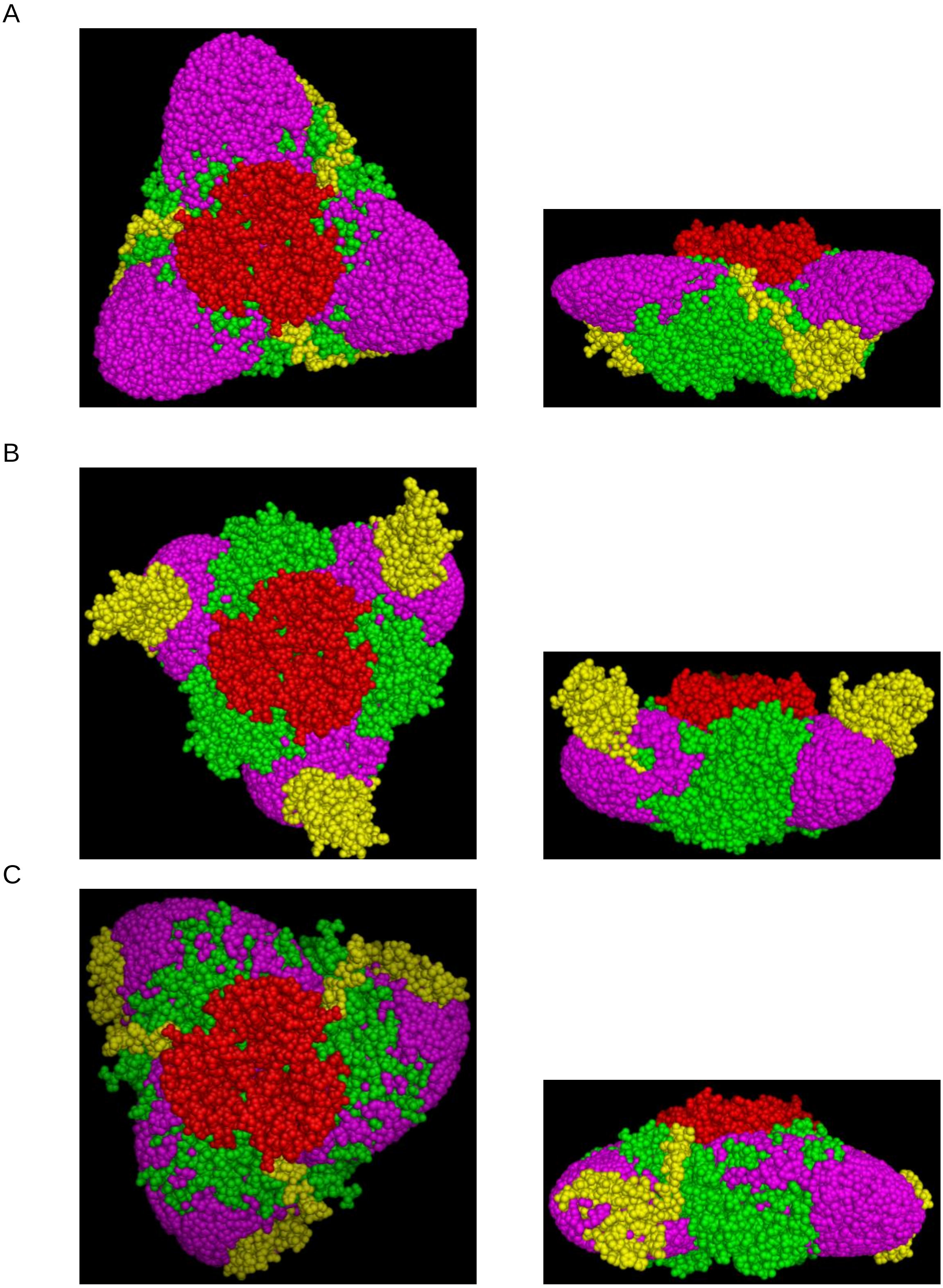

Fig. S2. Two views in space-filling representation of the best models of (UreABC-UreD)$_3$ generated by adding ellipsoids for UreD to the (A) native urease conformation, (B) UreB conformation 1, and (C) UreB conformation 2. UreA is depicted in red, UreB in yellow, UreC in green, and UreD in magenta.

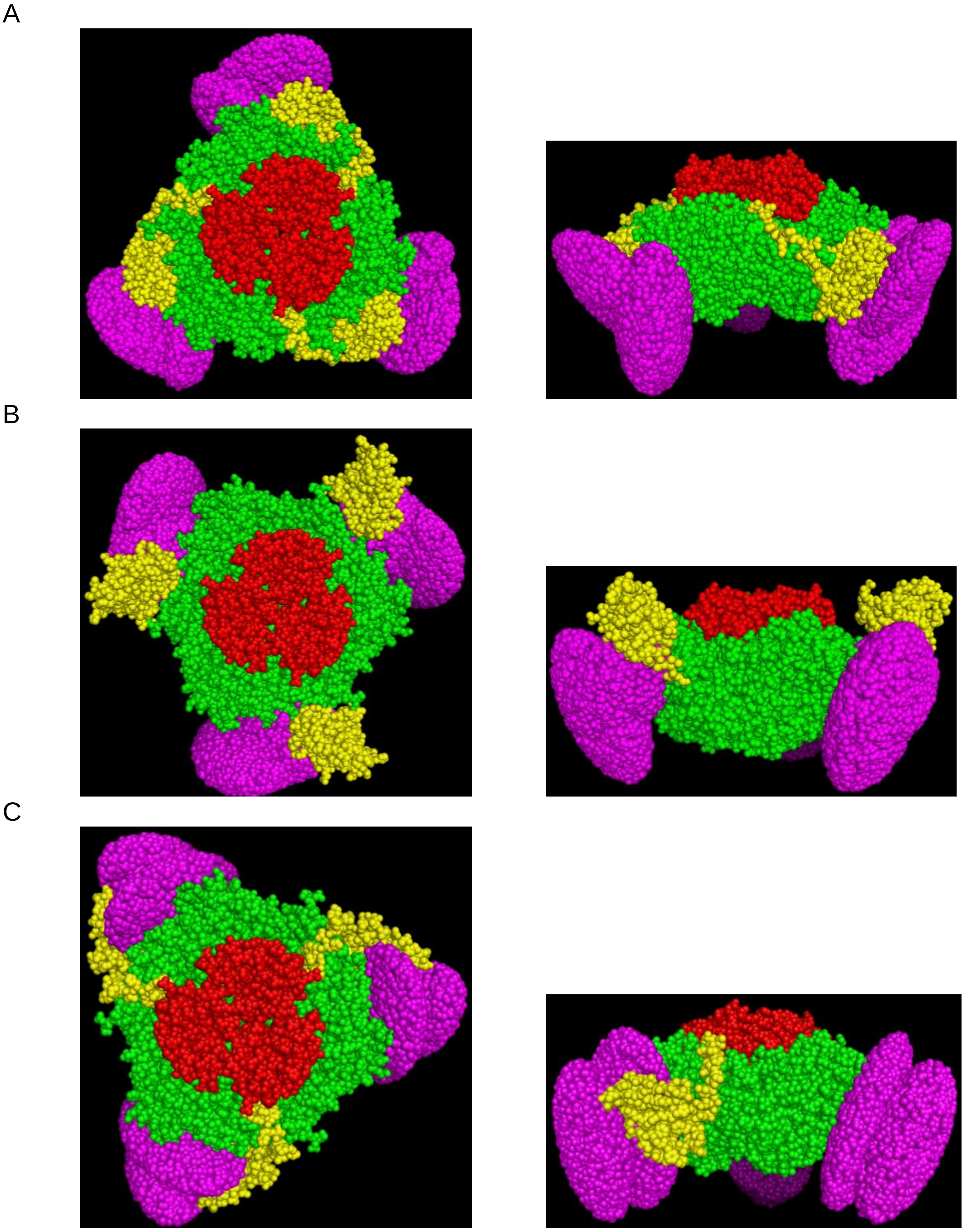

Fig. S3. Two views of space-filling representation of the best models of (UreABC-UreDF)$_3$ generated by adding ellipsoids for UreD and UreF to the (A) native urease conformation, (B) UreB conformation 1, and (C) UreB conformation 2. UreA is shown in red, UreB in yellow, UreC in green, and both UreD and UreF (because the shapes cannot be distinguished by SAXS) are shown in magenta.