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Fig.1S Hubs from PSN analysis of the MD ensemble of Ubc7. The hubs identified from the PSN analysis of the MD ensemble of $Ubc7_{XRay\text{-}OPEN}$ (A) and $Ubc7_{XRay\text{-}CLOSED}$ (B) are show in red.

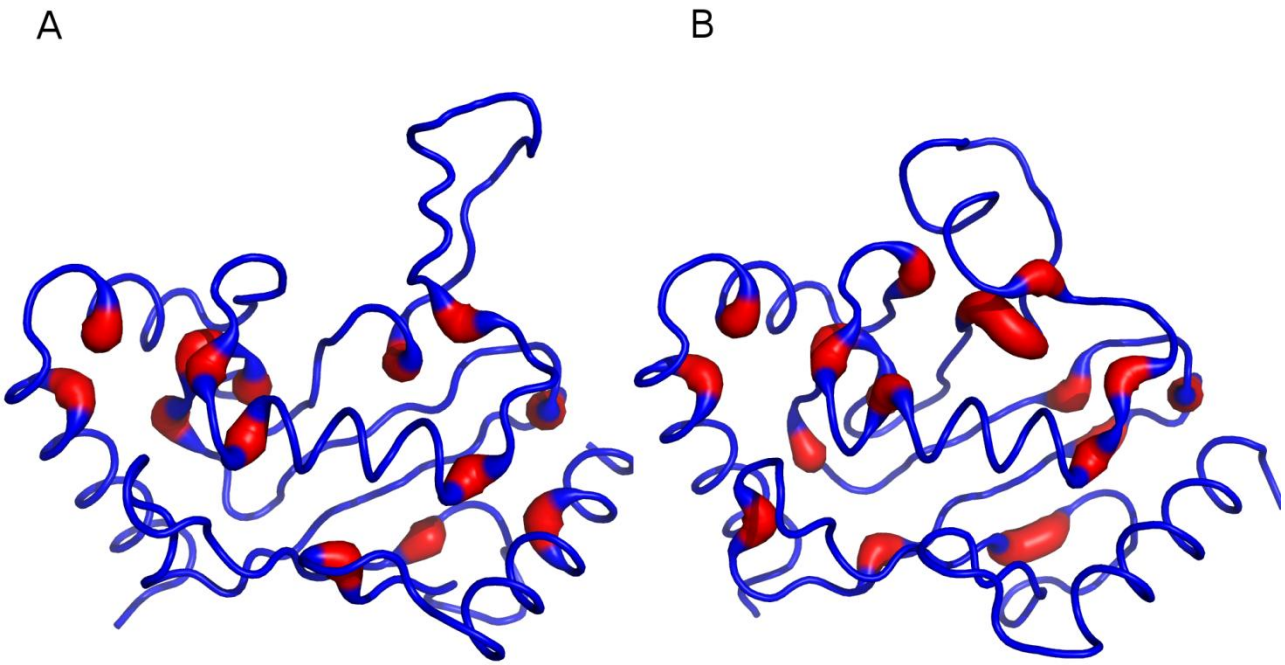

Table 1S. Comparison of the different shortest communication paths in Ube2g2$_{XRay-OPEN}$ and Ube2g2$_{XRay-CLOSED}$. The hub residues identified by PSN analysis are indicated in bold, whereas the conserved residues depicted in figure 1 are underlined. The common paths between the two forms were excluded by this analysis for sake of clarity. Occurrence Probability (O.P.) is indicated for each of them.

	Ube2g2$_{XRay-OPEN}$	**O.P.**	**Ube2g2$_{XRay-CLOSED}$**	**O.P.**
L6-P68	L6->F35->**L9**->F60->P69-**W110**->P72	43.05	/	/
L6-**Q114**	L6->F35->**L9**-> F60 ->P69->**W110**-> Q114	31.56	/	/
L6-S115	L6->F35->**L9**->**Y64**->E12->S115	15.96	/	/
L9-P130	**L9->W37**->L58->M71->V88->**I82**->H79->**P130**	42.17	/	/
L9-N131	**L9**->F60->P69->L93->**I90**->N81->N131	12.21	/	
L9-S111	/	/	**L9**->F60->P69->**W110**->**Q114**->S111	40.00
L9-V124	/	/	**L9**->F60->P69->**W110**->**Q114**->V214	25.54
E12-**Q114**	E12->**V116**->F60->P69->**W110**->**Q114**	31.59	/	/
I24-S111	/	/	I24->L120->**V116**->F60->P69->**W110**->**Q114**->S111	17.25
I24-K118	/	/	I24->L120->**V116**-> E12->S115->K118	20.94
I24-**P80**	I24->I41->**F73**->**I82**->H79->**P130**->**P80**	14.46	/	/
I24-R148	I24->I41->**F73 I82**->H79->**P130->W144**->R148	14.43	/	/
P28-V88	/		P28->**W37**->F60->P69->L93->**I90**->**I82**->V88	14.91
P28-**Y103**	/		P28->**W37**->F60->P69->L93->**I90**->M126->N81->S134-**Y103**	13.51
P28-Y152	/		P28->->**W37**->F60->P69->L93->**I90**->**I82**->H83->**P130**-> **W144**-> Y152	13.91
P44-R148			P44->L127->H79->**P130**->**W144**->R148	38.96
F49-I154	/		**F49**->H79->**P130**->**F151**->**F78**->I154	12.91
A56-**P80**	A56->**F73**->**I82**->H79->**P130**->**P80**	49.26	/	/
L58-**P80**	L58->M71->V88->**I82**->H79->**P130**->**P80**	70.81	/	/
L58-S115	/		L58->P69->F60->**V116**->E12->S115	16.77
L58-R148	L58->M71->V88->**I82**->H79->**P130**->**W144**->R148	70.40		
L58-Y152	L58->M71->V88->**I82**->H69->**P130**->**W144**->Y152	32.96		
F60-P44	/	/	F60->P69->L93->**I90**->**I82**->L127->P44	13.82
F60-**F73**			F60->P69->L93->**I90**->**I82**->**F73**	26.65
F60-Y83			F60->P69->L93->**I90**->**I82**->H79->**P130**->**P80**->A140->N137->Y83	16.22
F60-V88			F60->P69->L93->**I90**->**I82**-> V88	16.11
F60-H94			F60->P69->L93->**I90**->M126->N81->C89->H94	12.77
F60-**Y103**			F60->P69->L93->**I90**->M126->N81->S134->**Y103**	14.37
F60-S124			F60->P69->**W110**->**Q114**->I92->S124	35.53
F60-N137			F60->P69->L93->**I90**->**I82**->H79->**P130**->**P80**->A140->N137	19.05
P68-S114	P68->**W110**->P69->F60->**V116**->S114	31.12		
P68-S134	P68->**W110**->L93->**I90**->N81->S134	31.20	/	/
P69-R148			P68->L93->**I90**->**I82**->H79->**P130**->**W144**->R148	25.25
F73-P28			**F73**->**I82**->**I90**->L93->P69->F60->**W37**->P28	22.42
F73-N137			**F73**->**I82**->H79->**P130**->**P80**->A140->N137	57.84
C75-R148			C75->**F54**->V159->**F49**->H79->**P130**->**W144**->R148	16.37
M77-Y152	**M77**->**I82**->H79->**P130**->**W144**->Y152	37.31		
F78-P44			**F78**->A140->**P80**->**P130**->H79->L127->P44	12.77
F78-V88			**F78**->A140->**P80**->**P130**->H79->**I82**->V88	23.08
F78-L93			**F78**->A140->**P80**->**P130**->H79->**I82**->**I90**->L93	17.17
F78-L127			**F78**-> A140->**P80**->**P130**->H79->L127	17.99
H79-**L9**	H79->**I82**->V88->M71->L58->**W37**->**L9**	42.49	/	/
I82-L9	**I82**->V88->M71->L58->**W37**->**L9**	72.63	/	/
I82-N137	/	/	**I82**->H79->**P130**->**P80**->A140->N137	63.90
P84-R148	P84->N137->**F78**->**F151**->**W144**->R148	24.99	/	/
P84-Y152	P84->N137->**F78**->**F151**->**W144**->Y152	35.45	/	/
R87-**W110**			R87->**Y103**->H94->R109->P96->**W110**	12.51

V88-**W37**			V88->**I82**->**I90**->L93->P69->F60->**W37**	15.22
V88-**W110**			V88->**I82**->**I90**->L93->P69->**W110**	12.20
V88-**Q114**			V88->**I82**->**I90**->S122->I92->**Q114**	13.08
C89-P28			C89->N81->M126->**I90**->L93->P69->F60->**W37**->P28	20.71
C89-**F73**			C89->N81->M126->**I90**->**I82**->**F73**	20.31
C89-**P80**			C89->N81->M126->**I90**->**I82**->H79->**P130**->**P80**	14.08
C89-**Q114**			C89->N81->M126->**I90**->S122->I92->**Q114**	13.42
C89-**V116**			C89->N81->M126->**I90**->L93->P69->F60->**V116**	14.71
C89-I119			C89->N81->M126->**I90**->L93->I119	24.96
C89-L127			C89->N81->M126->**I90**->**I82**->L127	15.00
C89-R148			C89->N81->M126->**I90**->**I82**->H79->**P130**->**W144**->R148	13.97
I90-S106			**I90**->M126->N81->C89->**Y103**->S106	12.23
I90-N137			**I90**->**I82**->H79->**P130**->**P80** ->A140 ->N137	37.19
I90-R148			**I90**->**I82**->H79->**P130**->**W144**->R148	47.70
I90-Y14	**I90**->L93->P69->F60->**W37**->Y14	12.15	/	/
I92-P28	/	/	I92->**Q114**->**W110**->P69->F60->**W37**->P28	49.44
I92-**P80**			I92->S122->**I90**->**I82**->H79->**P130**->**P80**	15.91
I92-**Y103**			I92->S124->**I90**->M126->N81->**S134**->**Y103**	12.14
I92-L120			I92->**Q114**->**W110**->P69->F60->**V116**->L120	14.88
I92-R148			I92->S122->**I90**->**I82**->H79->**P130**->**W144**->R152	15.77
L93-N137			L93->**I90**->**I82**->H79->**P130**->**P80**->A140->N137	33.93
L93-R148			L93->**I90**->**I82**->H79->**P130**->**W144**->R148	43.30
H94-P28			H94->C89->N81->M126->**I90**->L93->P69->F60->**W37**->P28	12.17
H94-V88			H94->C89->N81->M126->I92->**I82**->V88	13.14
H94-S111			H94->R109->P96->**W110**->**Q114**->S111	14.02
H94-I119			H94->C89->N81->M126->**I90**->L93->I119	16.40
H94-V123			H94->C89->N81->M126->**I90**->V123	20.62
H94-**P130**			H94->C89->N81->M126->**I90**->**I82**->H79->**P130**	12.05
D99-P28			D99->**Y103**->**S134**->N81->M126->**I90**->L93->P69->F60->**W37**->P28	12.23
D99-**I82**			D99->**Y103**->**S134**->N81->M126->**I90**->**I82**	13.65
D99-S122			D99->**Y103**->S134->N81->M126->**I90**->**S122**	12.37
D99-V123			D99->**Y103**->S134->N81->M126->**I90**->V123	21.68
E104-P69			E104->D99->**Y103**->S134->N81->M126->**I90**->L93->P69	12.40
E104-**I82**			E104->D99->**Y103**->S134->N81->M126->**I90**->**I82**	12.57
E104-I119			E104->D99->**Y103**->S134->N81->M126->**I90**->L93->I119	14.34
E104-V123			E104->D99->**Y103**->S134->N81->M126->**I90**->V123	19.51
S106-V123			S106->S134->N81->M126->**I90**->V123	13.94
S111-V123			S111->**Q114**->I92->S122->I92->V123	25.76
Q114-T17	**Q114**->**W110**->P69->F60->**W37**->Y13->T17	31.65		
Q114-V124			**Q114**->**W110**->P69->F60->**V116**->L120->I24->V124	12.23
Q114-R148			**Q114**->I92->S122->**I90**->**I82**->H79->**P130**->**W144**->R148	15.40
S115-V123			S115->E12->**V116**->F60->P69->L93->**I90**->V123	12.74
S115-V124			S115->E12->**V116**->L120->I24->V124	29.48
S115->T17	S115->**V116**->**W37**->Y13->T17	25.13		
K118->**L9**	K118->**Q114**->**W110**->P69->F60->**L9**	27.53		
K118->M10	K118->S115->E12->**V116**->**W37**->P28->**F34**->M10	14.32		
K118->Y13	K118-> **Q114**->**W110**->P69->F60->**W37**->Y13	17.43		
L120-**I90**			L120->**V116**->F60->P69->L93->**I90**	16.85
L120-S111			L120->**V116**->F60->P69->**W110**->**Q114**->S111	19.74

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L120-M10	L120->**V116**->**W37**->P28->**F34**->M10	17.26		
V123-**W144**	V123->M126->**I82**->H79->**P130**->**W144**	14.82		
M126-**Y64**			M126->**I90**->L93->P69->F64->**Y64**	21.68
M126-S111			M126->**I90**->S124->I92->**Q114**->S111	23.48
M126-S115			M126->**I90**->L93->P69->F60->**V116**->E12->S115	16.31
L127-R148	30.00 L127->**F49**->H79->**P130**->**W144**->R148	30.00		
L127-N137			L127->H79->**P130**->**P80**->A140->N137	37.59
P130-M71			**P130**-> H79->**I82**->**F73**->A56->M71	13.60
N131-R148			N131->M126->**I90**->**I82**->H79->**P130**->**W144**->R148	15.88
D132-**F54**			D132->**W144**->**P130**->H79->**I86** ->**F54**	48.19
D132-**M77**			D132->**W144**->**P130**->H79->**I82**->**M77**	27.53
D132-V159			D132->**W144**->**P130**->H79->**F49**->V159	25.79
S134-**W37**	S134->N81->**I90**->L93->P69->F60->**W37**	12.23		
S134-V88			S134->N81->M126->**I90**->**I82**->V88	14.74
S134-**W144**			S134->N81->M126->**I90**->**I82**->H79->**W144**	15.48
N137-S122			N137->A140->**P80**->**P130**->H79->**I82**->**I90**->S122	12.51
N137-V123			N137->A140->**P80**->**P130**->H79->**I82**->**I90**->V123	18.99
N137-V159			N137->A140-> **P80**->**P130**->H79->**F49**->V159	27.51
A140-P28			A140->**P80**->**P130**->H79->**I82**->**I90**->L93->P69->F60->**W37**->P28	17.48
A140-I41			A140->**P80**->**P130**->H79->**F49**->P44->I41	13.17
A140-T47			A140->**F78**->**F151**->**W144**->Y152->T47	20.94
A140-A56			A140->**P80**->**P130**->H79->**I82**->**F73**->A56	42.10
A140-P68			A140->**P80**->H79->**I82**->**I90**->L93->P69->**W110**->P68	13.17
A140-C75			A140->**P80**->**P130**->H79->**F49**->V159->**F54**->C75	12.54
A140-N81			A140->**P80**->**P130**->H79->**I82**->**I90**->M126->N81	18.11
A140-L93			A140->**P80**->**P130**->H79->**I82**->L93	35.62
A140-**Q114**			A140->**P80**->**P130**->H79->**I82**->**I90**->**Q114**	12.23
A140-I119			A140->**P80**->**P130**->H79->**I82**->**I90**->L93->I119	13.08
A140-V123			A140->**P80**->**P130**->H79->**I82**->**I90**->V123	20.25
A140-N131			A140->**P80**->**P130**->H79->**I82**->**I90**->M126->N131	12.71
A140-L163			A140->**P80**->**P130**->H79->**F49**->V159->**F54**->L163	17.62
R148-**W110**			R148->**W144**->**P130**->H79->**I82**->**I90**->L93->P69->**W110**	16.80
F151-L58	**F151**->**P130**->H79->**I82**->V88->M69->L58	40.88		
I154-L127			I154->**F78**->**F151**->**P130**->H79->L127	14.20
A155-L58	A155->**F49**->H79->**I82**->V88->M71->L58	33.38		
L163-R148			L163->**F54**->V159->**F49**->H79->**P130**->**W144**->R148	23.22
L163-Y152			L163->**F54**->V159->**F49**->H79->**P130**->**W144**->Y152	16.68

Table 2S. Main differences in the shortest communication paths with probability of occurrence higher than 30% between the open (Ube2g2$_{Xray-OPEN}$) and closed (Ube2g2$_{Xray-CLOSED}$) states. The paths that featured differences between open and closed simulations lower than 5% were excluded for sake of clarity. Occurrence Probability (O.P.) for each path is indicated.

Ube2g2$_{XRay-OPEN}$			**Ube2g2$_{XRay-CLOSED}$**		
pair	**O.P.**	**Path**	**pair**	**O.P.**	**path**
L6-P68	43.05	L6->F35->**L9**->F60->**P69**-**W110**->P72			
L6-**Q114**	31.56	L6->F35->**L9**-> F60 ->**P69**->**W110**-> **Q114**			
L9-P130	42.17	**L9->W37->**L58->M71->V88->**I82->**H79->**P130**			
			L9-S111	50.01	**I90**->**I82->**H79->**P130**->**W144**->R148
E12-P68	47.70	E12->**V116**->F60->**P69**->**W110**->P68	E12-P68	35.19	E12->**V116**->F60->**P69**->**W110**->P68
E12-**Q114**	31.59	E12->**V116**->F60->**P69**->**W110**->**Q114**			
P28-P68	60.00	P28->**W37**->F60->**P69**->**W110**->P68	P28-P68	38.92	P28->**W37**->F60->**P69**->**W110**->P68
			P44-R148	38.96	P44->L127->H79->**P130**->**W144**->R148
F49-P80	43.72	**F49**->H79->**I82->**V88->M71->P68			
			F60- S124	35.53	F60->**P69**->**W110->Q114**->I92->S124
A56-**P80**	49.26	A56->**F73**->**I82**->H79->**P130**->**P80**			
			A56-N137	39.05	A56->**F73**->**I82**->H79->**P130**->**P80**->A140->N137
L58-**P80**	70.81	L58->M71->V88->**I82**->H79->**P130**->**P80**			
L58-R148	70.40	L58->M71->V88->**I82**->H79->**P130**->**W144**->R148			
L58-Y152	32.96	L58->M71->V88->**I82**->H69->**P130**->**W144**->Y152			
P68-S114	31.12	P68->**W110**->**P69**->F60->**V116**->S114			
P68-**S134**	31.20	P68->**W110**->L93->**I90**->N81->**S134**			
M71-R148	75.98	M71->V88->**I82**->H69->**P130**->**W144**->R148	M71-R148	30.36	M71->V88->**I82**->H69->**P130**->**W144**->R148
F73-R148	63.18	**F73**->**I82**->H69->**P130**->**W144**->R148	**F73**-R148	49.50	**F73**->**I82**->H69->**P130**->**W144**->R148
			F73-N137	57.84	**F73**->**I82**->H79->**P130**->**P80**->A140->N137
M77-R148	79.55	**M77**-> **I82**->H69->**P130**->**W144**->R148	**M77**-R148	30.00	**M77**->**I82**->H79->**P130**->**W144**->R148
M77-Y152	37.31	**M77**->**I82**->H79->**P130**->**W144**->Y152			
H79-**L9**	42.49	H79->**I82->**V88->M71->L58->**W37->L9**			
I82-L9	72.63	**I82**->V88->M71->L58->**W37**->**L9**			
			I82-N137	63.90	**I82**->H79->**P130**->**P80**->A140->N137
P84-Y152	35.45	**P84**->N137->**F78**->**F151**->**W144**->Y152			
			I90-N137	37.19	**I90**->**I82**->H79->**P130**->**P80** ->A140 ->N137
			I90-R148	47.70	**I90**->**I82->**H79->**P130**->**W144**->R148
			L93-N137	33.93	L93->**I90**->**I82**->H79->**P130**->**P80**->A140->N137
			L93-R148	43.30	L93->**I90**->**I82**->H79->**P130**->**W144**->R148
			E104-M126	36.82	E104->D97->**Y103**->**S134**->N81->M126
Q114-T17	31.65	**Q114**->**W110**->**P69**->F60->**W37->**Y13->T17			
L127-R148	30.00	L127->**F49**->H79->**P130**->**W144**->R148			
			L127-N137	37.59	L127->H79->**P130**->**P80**->A140->N137
			D132-**F54**	48.19	D134->**W144**->**P130**->H79->**I82**->**F54**
A140-V88	31.35	A140->**P80**->**P130**->H79->I84->V88	A140-V88	50.73	A140->**P80**->**P130**->H79->**I82**->V88
			A140-A56	42.10	A140->**P80->P130->**H79**->I82->F73**->A56
			A140-L93	35.62	A140->**P80**->**P130**->H79->**I82**->L93
R148-Y83	87.49	R148->**W144->P130->**H79->Y83	R148-Y83	35.08	R148->**W144->F151->F78->**N137->Y83
R148-V159	31.63	R148->**W144**->**P130**->H79->**F49**->V159	R148-V159	43.33	R148->**W144**->**P130**->H79->**F49**->V159
F151-L58	40.88	**F151**->**P130**->H79->**I82**->V88->M69->L58			
A155-L58	33.38	A155->**F49**->H79->**I82**->V88->M71->L58			