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Supplemental information

Systemwide disassembly and assembly

of SCF ubiquitin ligase complexes

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Document S1: Tables S1-S3

Table S1. Cryo-EM statistics for WT CAND1-SCF complexes, related to Figure 1, Figure 2, and Figure S2.

WT CAND1	no	Rolling-1	Rolling-2	Rolling-2	engaged	no	Rolling-1	Rolling-2	engaged	engaged
	SCF ^{FBXW7}	SCF ^{FBXW7}	SCF ^{FBXW7}	SCF ^{SKP2}	SCF ^{SKP2}	SCF ^{FBXO6}	SCF ^{FBXO6}	SCF ^{FBX06}	SCF ^{FBXO6}	SCF ^{FBXO6}
WT SCF	engaged	engaged	engaged	engaged	rocked	engaged	engaged	engaged	rocked	No SKP1-Fbp
	EMD- 16579	EMD- 16580	EMD- 16581	EMD- 16583	EMD- 16584	EMD- 16585	EMD- 16586	EMD- 16587	EMD- 16588	EMD- 16589
Data collection and processing										
Microscope		Glacios		Gla	cios			Glacios		
Magnification		22,000		22,	000			22,000		
Voltage (kV)		200		20	00			200		
Electron exposure (e–/Å ²)		~60		~1	60			~60		
Defocus range (µm)		-1.5~-3.0		-1.5	~-3.0			-1.5~-3.0		
Automation software		SerialEM		SerialEM SerialEM						
Pixel size (Å)		1.885		1.8	385	1.885				
Symmetry		C1		C	:1	C1				
Movies collected		2,167		2,0)24			1,989		
Initial particle (no.)		1,813,242		1,562	2,889			1,594,691		
Final particle (no.)	26,641	18,810	60,666	53,356	53,334	11,999	31,652	21,642	49,764	24,955
Map resolution(Å) FSC threshold	8.15 (0.143)	8.37 (0.143)	6.85 (0.143)	6.7 (0.143)	5.29 (0.143)	9.13 (0.143)	7.35 (0.143)	7.93 (0.143)	7.54 (0.143)	6.3 (0.143)

WT CAND1	Rolling-2a	Rolling-2b	Rolling- 2c	Rolling- 2d	Rolling- 1a	Rolling- 1b	little	no	no	CAND1 (2x) no	CAND1 (2x) Rolling-1	CAND1 (2x) Rolling-2	CAND1 (2x) engaged
WT SCF ^{FBXW7}	engaged	engaged	engaged	rocked									
Data collection and processing	EMD- 14603	EMD- 14604	EMD- 14601	EMD- 14602	EMD- 14599	EMD- 14600	EMD- 14605	EMD- 14606	EMD- 14607	EMD- 14615	EMD- 14616	EMD- 16577	EMD- 16578
Microscope	Krios										Gla	icios	
Magnification	105,000								22,000				
Voltage (kV)	300								200				
Electron exposure (e–/Å ²)		~68							~60				
Defocus range				-	0.5 ~ -2.0						-1.5	~ -3.0	
Automation software	SerialEM								SerialEM				
Pixel size (Å)					0.8512					1.885			
Symmetry imposed					C1					C1			
Movies collected	14,006									1,971			
Initial particle (no.)	4,250,310								1,59	4,265			
Final particle (no.)	31,620	63,774	21,628	13,085	13,416	9,913	7,362	5,385	5,420	28,057	42,006	102,99 6	33,454
Map resolution(Å) FSC threshold	3.9 (0.143)	3.8 (0.143)	4.7 (0.143)	4.8 (0.143)	4.5 (0.143)	6.5 (0.143)	6.6 (0.143)	7.2 (0.143)	6.5 (0.143)	8.15 (0.143)	7.54 (0.143)	6.7 (0.143)	7.18 (0.143)

Table S2. Cryo-EM statistics for Glacios data for mutant CAND1-SCF assemblies and substrate complex bound CAND1-SCF^{SKP2}, related to Figure 3, Figure S3, Figure 5, Figure S5, and Figure S7.

CAND1	engaged	rolling	engaged	rolling	no	∆β-hairpin partly engaged	∆β-hairpin Rolling-1	∆β-hairpin Rolling-2	
SCF ^{SKP2}	rocked	engaged	rocked	engaged	engaged	no	no	no	
Phospho-p27 +CKSHS1 +CyclinA-CDK2	p27- CKSHS1- CyclinA- CDK2	p27- CKSHS1- CyclinA- CDK2	(p27)- CKSHS1	(p27)- CKSHS1	p27- CKSHS1- CyclinA- CDK2				
	EMD- 16617	EMD- 16621	EMD- 16622	EMD- 16623	EMD- 16625	EMD- 16764	EMD- 16765	EMD- 16766	
Data collection and processing									
Microscope			Glacios				Glacios		
Magnification			22,000				22,000		
Voltage (kV)			200				200		
Electron exposure (e–/Ų)			~60		~60				
Defocus range (µm)			-1.5 ~ -3.0				-1.5 ~ -3.0		
Automation software			SerialEM			SerialEM			
Pixel size (Å)			1.885			1.885			
Symmetry imposed			C1		C1				
Movies collected			840				2131		
Initial particle (no.)			675,469				1,683,753		
Final particle (no.)	13,968	11,607	16,540	28,965	43,334	38,030	12,020	27,998	
Map resolution(Å) FSC threshold	7.73 (0.143)	8.6 (0.143)	7.35 (0.143)	9.4 (0.143)	7.73 (0.143)	6.1 (0.143)	9.1 (0.143)	7.73 (0.143)	

CAND1	engaged	engaged	∆β-hairpin partly engaged	∆β-hairpin Rolling-2a	∆β-hairpin Rolling-2b	∆β-hairpin Rolling-2c	∆β-hairpin Rolling-2d			
SCF ^{FBXW7}	No SKP1-Fbp	SKP1∆∆ rocked	Partially engaged rocked		engaged	engaged	engaged			
	EMD-14608	EMD-14609	EMD-14610	EMD-14614	EMD-14613	EMD-14612	EMD-14611			
Data collection and processing										
Microscope	Gla	cios			Glacios					
Magnification	22,0	000	22,000							
Voltage (kV)	200		200							
Electron exposure	~60		~60							
(e–/A ⁻) Defocus range (µm)	-1.5 ~	3.0		-1.5 ~ -3.0						
Automation software	Seria	aIEM		SerialEM						
Pixel size (Å)	1.8	85		1.885						
Symmetry imposed	С	1		C1						
Movies collected	2,2	.08		2,355						
Initial particle (no.)	1,759,987			1,979,155						
Final particle (no.)	50,363	34,667	113,745	44,926	73,155	19,053	20,378			
Map resolution(Å) FSC threshold	5.8 (0.143)	6.1 (0.143)	5.9 (0.143)	7.0 (0.143)	6.7 (0.143)	8.4 (0.143)	8.6 (0.143)			

Table S3. Cryo-EM statistics for Krios data for CAND1-CUL1-RBX1 and CAND1-SCF^{SKP2} complexes, related to Figure 4, Figure S4, Figure 5, Figure 5, Figure 6, and Figure S6.

CAND1	engaged	engaged	Rolling-2	Rolling-1	engaged	∆β-hairpin partly engaged	∆β-hairpin rolling	β- hairpin++ partly engaged	β- hairpin++ rolling
SCF ^{SKP2}	-	rocked	engaged	engaged	SKP1∆∆ rocked	Partly rocked	engaged	Partly rocked	engaged
	EMD- 14561	EMD- 14563	EMD- 14594	EMD- 16582	EMD- 14595	EMD- 14597	EMD- 14598	EMD- 16576	EMD- 16575
	PDB- 7Z8R	PDB- 7Z8T	PDB- 7ZBW		PDB- 7Z8V	PDB- 7ZBZ		PDB- 8CDK	PDB- 8CDJ
Data collection and processing									
Microscope					Krios				
Magnification	105,000		105,000		105,000	105	,000	105	,000
Voltage (kV)	300		300		300	30	00	30	00
Electron exposure (e–/Å ²)	~68		~68		~68	~1	68	~1	68
Defocus range	-0.5 ~ -2.0		-0.5 ~ -2.0		-0.5 ~ -2.0	-0.5 ·	~ -2.0	-0.5 ·	~ -2.0
Automation	SerialEM		SerialEM		SerialEM	Seria	alEM	Seria	alEM
software Pixel size (Å)	0.8512		0.8512		0.8512	0.8	512	0.8	512
Symmetry	C1		C1		C1	C	21	C	:1
Movies collected	11,695		15,953		13,710	9,3	325	12,	142
Initial particle	4,439,065	7,261,156		6,709,071	1,466,331		3,560,642		
Final particle (no.)	351,565	215,132	122,155	13,857	485,905	196,974	10,667	62,554	124,721
Map resolution(Å) FSC threshold	2.7 (0.143)	3.0 (0.143)	3.5 (0.143)	4.5 (0.143)	2.7 (0.143)	3.1 (0.143)	6.8 (0.143)	3.32 (0.143)	3.4 (0.143)
Refinement		6TTU	6TTU		6TTU	6TTU		6TTU	6TTU
Initial model used (PDB code)	6TTU, 1U6G	1U6G, 1LDK	1U6G, 1LDK		1U6G, 1LDK	1U6G, 1LDK		1U6G, 1LDK	1U6G, 1LDK
Model resolution (Å) FSC threshold	2.7 (0.143)	3.0 (0.143)	3.5 (0.143)		2.7 (0.143)	3.1 (0.143)		3.32 (0.143)	3.4 (0.143)
Map sharpening <i>B</i> factor (Ų) Model	Deep- EMhancer (local <i>B</i> factor)	Deep- EMhancer (local <i>B</i> factor)	Deep- EMhancer (local <i>B</i> factor)		Deep- EMhancer (local <i>B</i> factor)	Deep- EMhancer (local <i>B</i> factor)		Deep- EMhancer (local <i>B</i> factor)	Deep- EMhancer (local <i>B</i> factor)
composition -Non-	15124	18077	14784		18313	18156		16905	13629
atoms -Protein residues	1950 3	2395 3	2014 0		2417 3	2394 3		2392 3	2001 0
-Ligands <u>B factors (Å²)</u> -Protein -Ligand	60.63 84.74	72.13 77.15	81.54 -		68.98 76.43	65.06 78.18		89.5 86.92	78.28
<u>R.m.s. deviations</u> -Bond lengths (Å) -Bond angles (°)	0.002 0.520	0.002 0.500	0.003 0.536		0.003 0.507	0.003 0.519		0.003 0.566	0.003 0.563
<u>Validation</u> -MolProbity score -Clashscore -Poor rotamers (%)	1.22 4.29 0.06	1.26 4.88 0.05	1.46 5.46 0.07		1.20 4.21 0.00	1.22 4.38 0.00		1.25 4.76 0.00	1.26 4.9 0.00
<u>Ramachandran</u> <u>plot</u> -Favored (%) -Allowed (%) -Disallowed (%)	97.98 2.18 0.00	97.97 2.03 0.00	97.06 2.94 0.00		98.33 1.67 0.00	98.31 1.69 0.00		98.22 1.78 0.00	98.57 1.43 0.00