Supplementary Materials

Mechanism of self/nonself-discrimination in *Brassica* self-incompatibility

Murase et al.

Supplementary Figures 1–11 Supplementary Table 1 Supplementary References а

S₈-eSRK



b

m1,2,4



Mutations

m3: F159S

m4: L180R

m5: F190S

m1: P79S, Y80E, I81R

m2: F108V, L110R

m6: L239S

m7: L214Q

m8: I228N

m9: F264S

m10: V286G, V287A

Supplementary Fig. 1

(S₈-meSRK)

m1,2,3,6

H B1 W 11 M B1



Supplementary Fig. 1 S₈-meSRK expression and recognition of S₈-SP11. a, Left, schematic diagram of S_8 -eSRK constructs. Arrowheads show the positions of mutations used in S_8 -meSRK. Right, list of mutations used for screening of S_8 -eSRK expression shown in b. b, Screening of S_8 -eSRK constructs for stable overexpression in Sf9 cells. Numbers in the construct names indicate that the constructs have the corresponding mutations listed in a. Asterisk shows non-specific bands. c, Gel-filtration analysis of S_8 meSRK, S₈-SP11, and S₈-meSRK-S₈-SP11 proteins using a calibrated Superdex 200 column. Upper panel shows the merged chromatogram of the samples. Arrows show the calculated molecular size of each peak. Lower panel shows a Coomassie blue-stained SDS-PAGE gel of the separated fractions from chromatography of S_8 -meSRK– S_8 -SP11 proteins. **d**, Chemical shift perturbation analysis of S_8 -SP11. The signal intensities of the ¹H-¹⁵N HSQC spectrum of S₈-SP11 were reduced upon addition of unlabeled S₈meSRK. Signal reduction versus amino acid residue is shown for S_8 -SP11. The data are represented by the intensity ratio Iper/Iref; Iper and Iref were measured in the presence and absence of S_8 -meSRK, respectively. The error bars were calculated based on the signal-to-noise ratios. e, Selected region of overlay of 2D ¹H–¹⁵N HSQC spectra of the ¹⁵N-labeled S₈-SP11 in the presence (red) and absence (blue) of S_8 -meSRK. The representative drastically perturbed (i.e., reduced) signals are marked by dotted circles. The S₈-SP11 and S₈-meSRK concentrations were 70 µM and 35 µM, respectively. The spectra were recorded at 900 MHz at the ¹H frequency.







rmsd = 0.34 Å



Supplementary Fig. 2 Structural features of S_8 -meSRK– S_8 -SP11 complex. a, Superimposition of the two S_8 -meSRK molecules in the heterotetramer of S_8 -meSRK– S_8 -SP11, colored in pink and yellow. Dashed lines show disordered regions. b, Superimposition of two S_8 -SP11 molecules in the heterotetramer of S_8 -meSRK– S_8 -SP11, colored in cyan and green. Eight cysteine side chains forming disulfide bonds are represented by stick models. c, Domain organization of S_8 -meSRK. Lectin 1, Lectin 2, EGF-like, and PAN domains are colored in cyan, purple, green, and magenta, respectively. Cysteines forming disulfide bonds and sugar chains are represented as stick models. d, HV regions forms an SP11 binding surface on S_8 -meSRK. HV regions are shown in purple (HV I), salmon pink (HV II), and yellow (HV III). S_8 -SP11 molecules are colored in cyan and green.

b







rmsd = 2.29 Å



S₈-meSRK

6°





S₉-eSRK











Supplementary Fig. 3 Comparison of S₈-meSRK–S₈-SP11 and S₉-eSRK–S₉-SP11 complexes. a, b, S₈meSRK-S₈-SP11 (cyan) and S₉-eSRK-S₉-SP11 (purple) complexes are superimposed using C_{α} atoms of whole complexes (a) and single eSRK molecules (b). eSRK molecules used for superimposition are enclosed by a circle. c, S_8 -SP11 (cyan) is superimposed on S_9 -SP11 (purple). d, Molecular surfaces of S_8 meSRK (cyan) and S_9 -eSRK (purple). SP11 binding sites 1 and 2 are colored in yellow and blue, respectively. e, Electrostatic potential surfaces of S_8 -meSRK (left) and S_9 -eSRK (right). S_8 -SP11 is shown in cyan. **f**, Close-up view of the center of the S_8 -meSRK– S_8 -SP11 complex. S_8 -meSRK is shown in pink, and S_8 -SP11 molecules in cyan and green. g, Close-up view of HV III regions of S_8 -meSRK (pink) and S_9 eSRK (silver). S_8 -SP11 and S_9 -SP11 are shown in green and orange, respectively. h, i, Differences in ligand-receptor interaction between the two heterodimers in the S_8 -meSRK- S_8 -SP11 complex. The heterodimers are superimposed based on the C_{α} atoms of each S₈-meSRK. S₈-meSRK–S₈-SP11 pairs are shown in pink–cyan and yellow–green, respectively. The side chain of Arg29 in S_8 -SP11, shown in cyan, is disordered. g-i, Dotted lines represent hydrogen bonds. Water molecules are shown in small cyan spheres. j, Conservation profile of Brassica eSRK proteins. Conservation scores, calculated with the ConSurf program using 30 B. rapa SRK sequences, are shown in color on the molecular surface of S₈-meSRK. S₈-SP11 molecules are shown in yellow.

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S ₈ -SRK 59 GFFTPGSSSRWYLGIWYKKLPYITYVWVANRDNPLSNSTGTLKI	ISGNNIFLIGDSNKSIW
S ₉ -SRK 57 GFFRTNSRWYLGMWYKKLSGRTYVWVANRDNPLSNSIGTLKI	ISNMNLVLLDHSNKSVW
S_{12} -SRK 61 GFFKNTLNSRWYLGIWYKNLSDRTYVWVANRDSSLSNAIGTLKF	SGSNLVLRGRSNKFVW
Sra-SRK 48 GFFTTNSSSRWYLGTWYKKLTDRTYVWVANRDNPLSSSTGTLKT	SGNNLVIEGHSNKSVW
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S12-SRK 121 STNLTRGNERSPVVAELLANGNFVIRYSYNNDASGFLWQSFDFF	PTDTLLPEMKLGYYLKT
S52-SRK 108 STNLTIGNERSPVVAELLANGNFVMRDPNNNEASGFLWQSFDYF	PTDTLLPEMKLGYDLKT
S ₆₀ -SRK 121 STNLTRENVRSPVIAELLPNGNFVMRYSNNKDSSGFLWQSFDFF	PTDTLLPEMKLGYDFKT
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S_{2} - SRK 179 CUNRELTSSRNEDDPSSCDYSYKLEPRR-LPEFYLICCDV	VREHRSGPWNGTOFSGT
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$S_{12}-SRK 181 GLNRFLTSWRNFDDPSSGEFSYKLETR-LPEFYLLKNGS S_{52}-SRK 168 GLNRFLISWRSSDDPSSGEITYKLEPRR-FPEFYIFSDDF S_{60}-SRK 181 GRNRFLTSWRSYDDPSSGKFTYELDIQTGLPEFILINRFINORY HVI 240 260 HVI S_{9}-SRK 234 PEDQKLBYMVYNFTENSEEVAYTFRMTNNSFYSRI TINSEGYLH S_{9}-SRK 236 PEDQLSYMVYNFTENSEEVAYTFRMTDNSIYSRI S_{22}-SRK 236 PEDQLSYMVYNFTENSEEVAYTFRMTDNSIYSRI S_{52}-SRK 241 PEVQGLNYMVYNFTENSEEVAYSFRMTNSIYSRI S_{60}-SRK 241 PEVQGLNYMVYNTENSEE IAYSFQMTNQSIYSRI S_{9}-SRK 294 SPN-HQCDMYRMCGPYSYCDVNTSPSCNCIQGFNPGNVQQWALF S_{9}-SRK 296 SPN-HQCDMYRMCGPYSYCDVNTSPSCNCIQGFNPGNVQQWALF S_{9}-SRK 296 SPN-HQCDMYRMCGPYSYCDVNTSPSCNCIQGFNPGNVQQWALF S_{22}-SRK 296 SPN-HQCDMYRCGPYSYCDVNTSPVCNCIQGFMPFDNQQWALF S_{22}-SRK 300 DFTRMKNIKLPDTRMIVDRSIGLKECEKRCLSDCNCTAFAMZ S_{9}-SRK 353 DGFTRMKNIKLPDTRMAIVDRSIGLKECEKRCLSDCNCTAFAMZ S_{9}-SRK 356 DGFTRMKNIKLPDTRMAIVDRSIGVKECEKRCLSDCNCTAFAMZ S_{22}-SRK 343 DGFTRMKNMKLPETTMATVDRSIGVKECEKRCLSDCNCTAFAMZ S_{22}-SRK 343 DGFTRMKNMKLPDTTTAIVDRSIGVKECEKRCLSDCNCTAFAMZ S_{22}-SRK 343 DGFTRMKNMKLPDTTTAIVDRSIGVKECEKRCLSDCNCTAFAMZ S_{60}-SRK 413 EDMRNYAEGQDLYVRLAAADUVKKRTANGKIISLI S_{9}-SRK 413 EDMRNYAEGQDLYVRLAAADUVKKRTANGKIVSLI S_{9}-SRK 416 DDMRNYAVSGQDLYVRLAAADUVKKRTANGKIVSLI S_{10} DMRNYAVSGQDLYVRLAAADUVKKRTANGKIVSLI S_{10} DMRNYANGFNAADU$	SPG DRSGPWNGVQFSGI FRVHRIGPWNGIGFIGI ZWDQRSGPWNGIGFIGI 280 ERLTWAPSSVVWNVFWS ERLTWTPSLVIWNPIWS ERLTWTPTSGTWNLFWS DRLMWTPSTEIWQVFWS NFTRIPPSWGWSLFWS NFTRIPPSWGWSLFWS HVII 340 RNQISGCKRRTRLSCNG RDHTRGCIRRTRLSCSG CIRRTRLSCSG SCHGCVRTTQMSCSG 400 ADIRNRVTGCVIWTGEL ADIRDGGTGCVIWTGEL ADIRNGGTGCVIWTGEL ADIRNGGTGCVIWTGEL ADIRNGGTGCVIWTGEL ADIRNGGTGCVIWTGEL
$S_{12} - SRK$ $S_{12} - SRK$ $S_{12} - SRK$ $S_{16} - SRK$ S_{1	SPG PRSGPWNGVQFSGI FRVHRIGPWNGIGFIGI ZWDPRSGPWNGIGFIGI 280 ERLTWAPSSVVWNVFWS ERLTWTPSLVIWNPIWS ERLTWTPTSGTWNLFWS ORLMWTPSTEIWQVFWS IRFTRIPPSWGWSLFWS INFTRIPPSWGWSLFWS INFTRIPPSWGWSLFWS INFTRIPS INFTRIPSWGWSLFWS INFTRIPSWGWSLFWS
$S_{12} - SRK 181 GLNRFLTSWRNFDDPSSGEFSYKLETR-LPEFYLLKNGS S_{52} - SRK 168 GLNRFLISWRSSDDPSSGEITYKLEPR-FPEFYIFSDDF S_{60} - SRK 181 GRNRFLTSWRSYDDPSSGKFTYELDIQCLPEFILINRFLNORY HVI S_{60} - SRK 234 PEDQKLBYMVYNFTENSEEVAYTFRMTNNSFYSRITINFSGFFI S_{12} - SRK 236 PEDQVLSYMVYNFTENSEEVAYTFRMTNNSIYSRIDLSPEGLLE S_{52} - SRK 236 PEDQVSTYIVYNFTENSEEVAYTFRMTNNSIYSRIDLSPEGLLE S_{52} - SRK 241 PEVQGLNYMVYNTENSEEVAYFRMTNNSIYSRITISEGYFC S_{60} - SRK 294 SPN-HQCDMYRMCGPYSYCDVNTSPSCNCIQGFNPGNVQQWALF S_{12} - SRK 296 SPN-HQCDMYRMCGPYSYCDVNTSPSCNCIQGFNPGNVQQWALF S_{12} - SRK 296 SPN-HQCDMYRMCGPYSYCDVNTSPSCNCIQGFNPGNVQQWALF S_{52} - SRK 294 SPNSLQCDPYMICGPSYCDVNTSPVCNCIQGFMPFDMQQWALF S_{52} - SRK 353 DGFTRMKNIKLPDTMAIVDRSIGLKECEKRCLSDCNCTAFANF S_{60} - SRK 353 DGFTRMKNMKLPETTMATVDRSIGVKECEKKCLSDCNCTAFANF S_{60} - SRK 353 DGFTRMKNMKLPDTTAIVDRSIGVKECEKKCLSDCNCTAFANF S_{52} - SRK 353 DGFTRMKNMKLPDTTAIVDRSIGVKECEKKCLSDCNCTAFANF S_{60} - SRK 413 EDMRNYAEGGQDLYVRLAAADLVKKRNGNWKIISLI S_{9} - SRK 416 EDIRNYIGNGQDLYVRLAAADLVKKRANGKIVSLI S_{12} - SRK 416 EDIRNYIGNGQDLYVRLAAADLVKKRANGKIVSLI$	SPG DRSGPWNGVQFSGI FRV HRIGPWNGIGFIGI ZWDQRSGPWNGIGFIGI 280 ERLTWAPSSVVWNVFWS ERLTWTPSLVIWNPIWS ERLTWTPSGTWNLFWS QRLMWTPSTEIWQVFWS NFTRIPPSWGWSLFWS HVII 340 RNQISGCKRRTRLSCNG RDHTRGCIRRTRLSCSG CIRRTRLSCSG CIRRTRLSCSG CIRRTRLSCSG CIRRTRLSCSG CIRRTRLSCSG CIRRTRLSCSG CIRRTRLSCSG CIRCUTTQMSCSG 400 ADIRNRVTGCVIWTGEL ADIRDGGTGCVIWTGEL ADIRNGGTGCVIWTGEL ADIRNGGTGCVIWTGEL ADIRNGGTGCVIWTGEL



Supplementary Fig. 4 Sequence alignments of *Brassica* SRK and SP11. a, Sequence alignment of *B. rapa* SRK ectodomains. Contact amino acids against the cognate SP11 are shown as magenta (S_8) and cyan (S_9) circles. The black boxes indicate three HV regions. Cysteine residues forming disulfide bonds are connected by lines. Yellow arrowheads and upper numbers show the positions of S_8 -SRK. The positions of the 11 amino acid mutations in S_8 -meSRK are indicated by blue boxes. b, Sequence alignment of *B. rapa* SP11 proteins. Amino acids contacting with eSRK are shown by purple (S_8) and green (S_9) circles. Arrowhead shows the endpoint of the signal peptide. Arrows and cylinder indicate the β -strands and α -helix of S_8 -SP11, respectively. Dotted line shows the disordered region in the crystal structure of the S_8 -meSRK– S_8 -SP11 complex.



916.1 Å² b b e





S₉-eSRK



1	

	1 7 0	
S8-SKK	170	GLNRFLTSSRNFDDPSSGDISIKLEPRR-LPEFILLLGDVREHRSGPWNGIQFSGI
S9-SKK	1 0 1	
S ₁₂ -SRR	101	GLNRFLISWRNFDDPSSGEFSIKLEIRR-LPEFILLKNGSPGDRSGPWNGVQFSGI
S ₅₂ -SRK	100	
S_{60} -SRK	181	GRNRFLTSWRSYDDPSSGKFTYELDIQ <mark>UGLPEFTLINRFLNQRVVMD</mark> RSGPWNGIEFSGI HVI
a apr	004	
S ₈ -SRK	234	PEDQKLSYMVYNFTENSEEVAYTFRMTNNSFYSRITINSEGYLERLTWAPSSVVWNVFWS
$S_9 - SRK$	226	PEEQQLSYMVYNFTENSEEVAYTFLVTNNSIYSRITINFSGFFERLTWTPSLVIWNPIWS
S_{12} -SRK	236	PEDQTLSYMVYNFTENSEEVAYTFRMTDNSIYSRIQLSPEGLLERLTWTPTSGTWNLFWS
S_{52} -SRK	223	PEDQNSTYIVYNFTENSEEVAYSFRMTNNSIYSRLIITSEGYFQRLMWTPSTEIWQVFWS
S_{60} -SRK	241	PEVQGLNYMVYNYTENSEEIAYSFQMTNQSIYSRL <u>TVS-DYTLNRFTRIPPSWGWSLFWS</u>
S ₈ −SRK	294	SPN-HQCDMYRMCGPYSYCDVNTSPSCNCIQGFNPGNVQQWALRNQISGCKRRTRLSCNG
S_9 -SRK	286	SPASFQCDPYMICGPGSYCDVNTLPLCNCIQGFKPLNVQEWDMRDHTRGCIRRTRLSCRG
S_{12} -SRK	296	APVDIQCDVYMTCGPYAYCDVNTSPVCNCIQGFMPFDMQQWALRDGTGGCIRRTRLSCSS
S_{52} -SRK	283	SPMSLQCDPYRICGPYAYCDESTSPMCICIQGFDPKNRQQWDLRSHASGCIRRTRLRCSG
S_{60} -SRK	300	LP-TDVCDSLYFCGSYSYCDLNTSPYCNCIRGFVPKNRORWDLRDGSHGCVRTTQMSCSG
		360 <u>380</u> 400
$S_8-{ m SRK}$	353	DGFTRMKŇIKLPDTRMAIVDRŠIGLKEČEKRCLSDCNČTAFANADIRŇRVTGCVIWTĠEL
S₀-SRK	346	DGFTRMKNMKLPETTMATVDRSIGVKECEKKCLSDCNCTAFANADIRDGGTGCVIWTGRL
S_{12} -SRK	356	DGFTRMKNMKLPDTKMAIVDRSIDVKECEKRCLSDCNCTAFANADIRNGGTGCVTWTGEL
S_{52} -SRK	343	DGFTRMKNMKLPDTTTAIVDRSIGVKECEKRCLSDCNCTAFANADIRNGGTGCVIWTGEL
$S_{60}-SRK$	359	DGFLRLNNMNLPDTKTASVDRTIDVKKCEEKCLSDCNCTSFATADVRNGGLGCVFWTGDL
		4 40
$S_8-{ m SRK}$	413	EDMRNYAĖG <mark>GQDLYVRLAAA</mark> DLVKKRNĠNWKIISL <mark>I</mark>
S_9 -SRK	406	D <mark>DMR</mark> NYAVS <mark>GQDLYVRLAAA</mark> DVVEKRTANGKIVSL <mark>I</mark>
S_{12} -SRK	416	EDIRNYIGNGQDLYVRLAAADLVKKRKANGKIISLI
S_{52} -SRK	403	EDIRTYVADGQDLYVRLAAADLVRKRNANGKIVSLI
S_{60} -SRK	419	VEIRKQAVVGQDLYVRLNAADLDFSSGEKRDRTGTI

Supplementary Fig. 5 Comparison of homodimerization interfaces between S_8 -meSRK and S_9 eSRK. a, Molecular surfaces of S_8 -meSRK (left) and S_9 -eSRK (right). Dimerization surfaces are colored in yellow. Details of the interactions enclosed by boxes are shown in b and e. Box e' indicates the symmetrical region of box e in the S_8 -meSRK dimer. **b**–g, Close-up views of eSRK dimer interfaces. S_8 -meSRK is shown in pink and yellow, and S_9 -eSRK in silver and cyan. b, e, Homodimer interface of S_8 -meSRK. c, f, Superimpositions of S_8 -meSRK (pink) and S_9 -eSRK (silver). d, g, Snapshot of S_9 -eSRK homodimer interface, shown as in c and f. Dotted lines represent hydrogen bonds. Water molecules are shown as small cyan spheres. **h**, Sequence alignment of *B. rapa* SRK ectodomains. Amino acids involved in eSRK–eSRK interactions are shown in purple (S_8) and blue (S_9) circles. Three HV regions are shown in boxes. Yellow arrowheads and upper numbers show the positions of S_8 -SRK.



Supplementary Fig. 6 Modeling of various SP11 structures by aMD simulation. a, Structure of S_9 -eSRK modeled using the crystal structure of S_8 -meSRK (chain A). b, Initial structure of S_9 -SP11, generated by homology modeling with S_8 -SP11 as a template, is shown in black. Crystal structure of S_9 -SP11 is depicted in green. c, Converged S_9 -SP11 model obtained by aMD at 150 ns starting with the initial structure is shown in red (helix) and yellow (strand). d, Plots of rmsd over 150-ns aMD simulations. The aMD was conducted after 20-ns conventional MD simulations. The rmsd values were calculated for all C α atoms of the crystal structure of S_9 -SP11. e, Modeled SP11 structures (S_{32} , S_{36} , S_{46} , S_{47} , S_{61} , S_{29} , S_{40} , S_{44} , and S_{60}) after aMD improvement. Important residues for binding to the self-eSRK calculated by MM–GBSA are shown in red.





0.02



Supplementary Fig. 7 Phylogenetic trees of *Brassica SRK* and *SP11. S*-haplotypes categorized in the S_8 -, S_9 -, and class-II subgroups by MM–GBSA analysis are located in the same clades. White circles, black circles, and white triangles show the member of S_8 -, S_9 -, and class-II subgroups analyzed in this study, respectively. S_b -SRK and S_b -SP11 sequences from *Arabidopsis lyrata* were used as the root. Sequences and accession numbers used in these trees are listed in Supplementary Data 1. S_{61} -SP11 sequence was excluded from the tree because only a partial sequence was available.





Supplementary Fig. 8 eSRK–SP11 model structures in S_8 -subgroup. Modeled complex structures of S_8 - (a–c), S_{46} - (d–f), S_{47} - (g, h), and S_{61} - (i, j) haplotypes are shown. Cyan and green represent SP11, and yellow and pink represent eSRK. **a**, **d**, Overall structure of S_8 - (a) and S_{46} - (d) complex structures after 150-ns MD simulations. Mutated residues in S_8 -meSRK (a) and in S_{46} -eSRK (d) used for pull-down assays shown in Fig. 4b are indicated in orange. **b**, **e**, **g**, **i**, Top panels show close-up views of the interfaces around eSRK-HV III, SP11-CR I, and SP11-CR II in S_8 - (b), S_{46} - (e), S_{47} - (g), and S_{61} - (i) complexes, respectively. Ruby, marine, and bule represent HV III, CR I, and CR II, respectively. **c**, **f**, **h**, **j**, Left (c, f) and top (h, j) panels show close-up views of the interfaces where two eSRK and two SP11 molecules make contact in S_8 - (c), S_{46} - (f), S_{47} - (h), and S_{61} - (j) complexes, respectively. Important residues for ΔG calculated by MM–GBSA are shown in red (c, f, right; h, j, bottom). Subscripts to the right of residue numbers indicate chain ID in the complex (a, b, eSRK; c, d, SP11).



Supplementary Fig. 9 eSRK–SP11 complex structure models in S_9 -subgroup. Model structures of S_{32} - (a) and S_{36} - (b) complexes. Cyan and green represent SP11, whereas yellow and pink represent eSRK. Close-up views of the interfaces around eSRK-HV III, SP11-CR I, and SP11-CR II are shown in the left upper panels, and close-up views of the interfaces where two eSRK and two SP11 molecules make contact are shown in the right upper panels. Dotted lines represent hydrogen bonds. Important residues for ΔG calculated by MM–GBSA are shown in red (bottom). Subscripts to the right of residue numbers indicate chain ID in the complex (a, b, eSRK; c, d, SP11).



b

Supplementary Fig. 10 eSRK–SP11 complex structure models in the class-II subgroup. Model structures of S_{29} - (a), S_{40} - (b), S_{44} - (c), and S_{60} - (d) complexes. Cyan and green represent SP11, while yellow and light orange represent eSRK. Close-up views of the interfaces around eSRK-HV III, SP11-CR I, and SP11-CR II are shown in the left upper panels, while close-up views of the interfaces where two eSRK and two SP11 molecules make contact are shown in the right upper panels. Ruby, marine, and bule represent HV III, CR I, and CR II, respectively. Dotted lines represent hydrogen bonds. Important residues for ΔG calculated by MM–GBSA are shown in red (bottom). Subscripts to the right of residue numbers indicate chain ID in the complex (a, b, eSRK; c, d, SP11).

Fig. 1a

Fig. 1b

Fig. 2j

Fig. 4b

Supplementary Fig1. c CBB staining

Supplementary Fig. 11 Uncropped gel/blot images from Figures.

	S_8 -meSRK- S_8 -SP11	SeMet-S ₈ -meSRK-S ₈ -SP11			
Data collection					
Space group	$P4_{1}2_{1}2$	$P4_{1}2_{1}2$			
Cell dimensions					
<i>a</i> , <i>b</i> , <i>c</i> (Å)	143.56, 143.56, 194.40	142.69, 142.69, 194.76			
α, β, γ (°)	90.0, 90.0, 90.0	90.0, 90.0, 90.0			
Wavelength (Å)	0.9000	0.9791			
Resolution (Å)	50.0-2.60 (2.64-2.60)*	50.0-3.50 (3.56-3.50)			
No. of reflections					
Total	424,212	592,261			
Unique	59,763	48,219			
R _{merge}	0.10 (0.63)	0.14 (0.48)			
$I/\sigma I$	41.3 (5.38)	18.2 (4.23)			
Completeness (%)	94.9 (97.5)	100 (100)			
Redundancy	7.1 (7.7)	12.3 (12.4)			
CC1/2	†(0.87)				
Refinement					
Resolution (Å)	43.8-2.60 (2.69-2.60)				
$R_{\rm work}/R_{\rm free}$	0.220/0.251 (0.308/0.402)				
No. of atoms					
Protein	6,752				
Sugar	70				
Solvent	184				
Average B-factors (Å ²)					
Protein	61.7				
Sugar	87.2				
Solvent	50.6				
R.m.s deviations					
Bond lengths (Å)	0.012				
Bond angles (°)	1.17				
Ramachandran plot (%)					
Favored	94.0				
Allowed	6.0				
Outliers	0				

Supplementary Table 1 Statistics of the data collection and refinement.

*Values in parentheses are highest resolution shell

†HKL2000 does not calculate total value of CC1/2

Supplementary references

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