Table 1. Data collection, refinement statistics, and structural characteristics of InlA-mutant/hEC1 complexes

	$InlA_{WT}$/hEC1†	**$InlA_{Y369A}$/hEC1**	**$InlA_{G194S+S}$/hEC1**	**$InlA_{S192N}$/hEC1**‡	**$InlA_{S192N-Y369S}$/hEC1**‡	**$InlA_{S192N-G194S+S}$/hEC1**	**$InlA_{G194S+S-Y369S}$/hEC1**
Data collection*							
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P1$	$P1$
Cell constants							
a, *b*, *c* (Å)	55.4, 86.8, 110.7	55.3, 84.6, 108.3	55.2, 88.5, 110.5	55.5, 68.9, 132.4	55.4, 87.4, 111.0	44.9, 54.1, 68.6	45.0, 54.3, 68.6
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	74.7, 80.7, 67.7	75.0, 80.8, 67.4
Resolution, Å	25-1.8 (1.86-1.80)	40-1.6 (1.63-1.60)	40-2.0 (2.1-2.0)	40-1.7 (1.76-1.70)	50-1.9 (1.97-1.90)	50-1.7 (1.77-1.70)	50-1.8 (1.86-1.80)
R_{merge} (%)	6 (39)	5 (29)	12 (37)	6 (28)	8 (42)	6 (52)	6 (51)
I/σ_I	14 (3)	29 (6)	9 (4)	20 (4)	17 (3)	16 (2)	12 (2)
Completeness (%)	92 (84)	99 (95)	96 (92)	99 (95)	97 (86)	91 (77)	94 (75)
Redundancy	6 (5)	8 (8)	5 (4)	6 (6)	12 (4)	5 (4)	5 (4)
Refinement							
Resolution, Å	1.8	1.6	2.0	1.7	1.9	1.7	1.8
No. reflections	41618	60684	37285	50104	43193	56061	47450
R_{work}/R_{free} (%)	17 /22	15 / 19	19 / 28	16 / 21	15 / 22	17 / 22	16 / 22
No. atoms							

	$InlA_{WT}$/hEC1[†]	**$InlA_{Y369A}$/hEC1**	**$InlA_{G194S+S}$/hEC1**	**$InlA_{S192N}$/hEC1**[‡]	**$InlA_{S192N-Y369S}$/hEC1**[‡]	**$InlA_{S192N-G194S+S}$/hEC1**	**$InlA_{G194S+S-Y369S}$/hEC1**
Protein	4577	4645	4524	4704	4630	4797	4691
Ca^{2+}/Cl^-	2 /3	0 / 0	1 / 1	2 / 4	2 / 2	1 / 1	1 / 1
Water	541	801	605	697	845	723	783
B-factors mean	24	11	18	10	18	14	18
Wilson	23	16	23	14	21	19	15
rmsd							
Bond lengths, Å	0.018	0.022	0.024	0.025	0.022	0.024	0.022
Bond angles, °	1.8	1.8	2.1	2.0	1.7	2.0	1.9
Analysis[§]							
rmsd (InlA)	-	0.43	0.39	0.59	0.30	0.32	0.24
rmsd (hEC1)	-	0.47	0.28	0.46	0.24	0.42	0.41
rmsd (complex)	-	0.64	0.30	0.61	0.31	0.50	0.57

[*]Numbers in parentheses indicate values corresponding to the shell of highest resolution.

[†] Schubert WD, Urbanke C, Ziehm T, Beier V, Machner MP, Domann E, Wehland J, Chakraborty T, Heinz DW (2002) *Cell* 111:825-836.

[‡]Wollert T, Pasche B, Rochon M, Deppenmeier S, van den Heuvel J, Gruber AD, Heinz DW, Lengling A, Schubert WD (2007) *Cell* 129:891-902.

[§] rmsd values were calculated using main chain atoms.