Figure S1

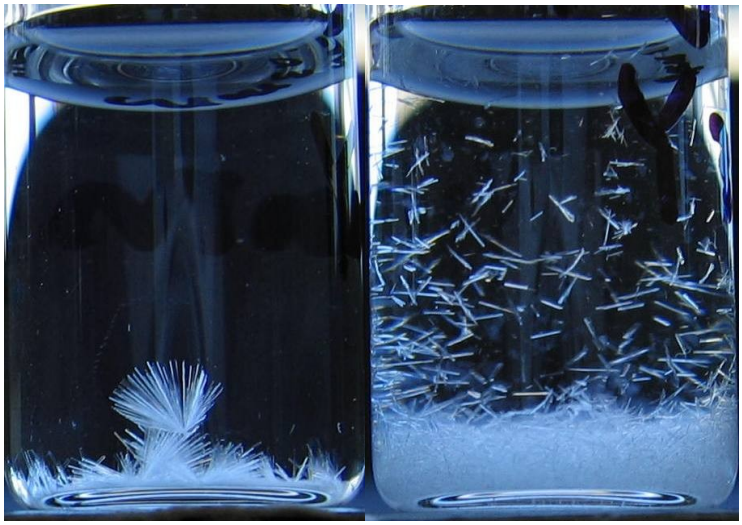

Figure S1: High quality single crystals grown from BLG 6.7 mg/mL with 0.3 and 3.0 mM YCl_3, corresponds to Regimes IIa and IIb, respectively.

Table S1. Data-collection statistics [a,b]

	BLG-4.0	BLG-3.0	BLG-0.3
Source	PX-III	home source	home source
Wavelength λ [Å]	1.82	1.54	1.54
Detector	MAR225	MAR345	MAR345
unit cell	41.09 63.69 134.53	40.80 63.57 134.03	41.06 63.71 134.16
Resolution [Å]	30 – 2.30 (2.36 – 2.30)	25 – 2.40 (2.46 – 2.40)	25 - 2.53 (2.58 - 2.53)
Spacegroup		$P2_12_12_1$	
No. of reflections			
Measured	364204 (18218)	144244 (10386)	166238 (9783)
Unique	29710 (2192)	26250 (1930)	21458 (1522)
R_{meas} [%]	6.3 (53.3)	7.4 (57.8)	9.7 (65.0)
Completeness [%]	98.1 (96.8)	99.8 (99.9)	95.0 (92.4)
Multiplicity	12.3 (8.3)	5.5 (5.3)	7.7 (6.4)
$\langle I \rangle / \langle \sigma(I) \rangle$	28.6 (3.9)	19.1 (3.0)	17.0 (3.0)
Wilson Factor [$Å^2$]	42.7	42.5	42.4
Crystal Mosaicity [°]	0.15	0.41	0.43
Subunit / ASU		2	

[a] Values in parentheses are for the highest shell

[b] The model resulting from this data set was used to establish an initial structure. It was not fully refined. Thus, no refinement statistics are given below.

Table S2: Refinement statistics

	BLG-3.0	**BLG-0.3**
Resolution range [Å]	20 – 2.40	20 – 2.53
R_{cryst}	22.2	24.2
R_{free}	26.4	28.1
No. of non-H atoms		
Protein	2450	2456
Yttrium	4	4
Chloride	1	1
Water	39	43
Average isotropic B-factor [Å^2]		
Main chain A / B	37.9 / 45.2	37.7 / 43.1
Side chain A / B	39.5 / 47.3	38.6 / 44.7
Water	37.3	36.8
Yttrium	56.6	47.3
Chloride	54.4	56.0
Rmsd for bond lengths [Å]	0.006	0.007
Rmsd for bond angles [°]	0.993	1.006
Ramachandran regions		
Most favorable [%]	97.1	94.6
Allowed [%]	2.3	4.8
Outliers [%]	0.6	0.6

Table S3: Anomalous peak heights of different yttrium sites calculated from Bijvoet differences

Yttrium site	peak height BLG-3.0	peak height BLG-0.3
1	11.5	10.8
2	11.0	10.5
3	10.7	10.2
4	5.3	2.9
C106C119	4.7 / 5.0	4.5 / 5.0

Experimental Procedure

Structure determination, refinement and substrate modeling

Data collection information for three typical crystals are listed in Table 1. One crystal grown in 4.0 mM yttrium solution was used for phase determination by SAD protocol with wavelength of 1.82 Å at the PXIII (swiss light source, Villigen, Switzerland). Freshly prepared crystals were utilized for collecting the data sets at copper K_α wavelength of the lab source. Data sets of BLG grown under different yttrium concentrations were collected on a rotating anode generator equipped with a Mar345 imaging plate detector. Data reduction of all data sets was performed using XDS and XSCALE.[1] For phase determination the yttrium positions were located using SHELXD [2] and used for phasing and density modification as implemented in SHARP/autoSHARP.[3] The final experimental electron density map was of decent quality (phasing power 0.761, figure of merit 0.307) and allowed chain tracing. A partial model was placed manually and served as starting point of automatic chain tracing performed by ARP/wARP.[4] The resulting model was completed by several cycles of manual building with COOT [5] and refinement with REFMAC5.[6] Water molecules were placed using ARP/wARP SOLVENT and checked manually with COOT. The final refinement steps involved TLS group refinement using one TLS group per polypeptide chain and resulted in models of reasonable quality (Table 2). Phasing of the remaining data sets were performed by molecular replacement procedure using rigid body refinement procedure of REFMAC5. Model bias was avoided by performing several cycles of simulated annealing using PHENIX.[7] The following refinement procedure was similar as described above. The structure factor amplitudes were scaled using SCALEIT. Anomalous difference maps using the Bijvoet differences ($|F^+|-|F^-|$) as coefficients were calculated with FFT.[8] All structures were validated using RAMPAGE [9] and SFCHECK (Table 3). Figures were generated using POVscript+ [10] and POVRAY (www.povray.org).

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