SUPPORTING INFORMATION

Strains and vectors. *Escherichia coli* strain DH5α (Promega) was used as a cloning host for all DNA manipulations. Plasmid pTTc9[1] was the source of the *cel6A* cDNA and pSP73 (Promega) was used for making the mutations. The fungal expression vector was pUJ10, a derivative of pBR322 containing the *lacZ* gene linked to the *cel7A* promoter and terminator sequences (Airaksinen, U. and Penttilä, M., unpublished). The phleomycin selection plasmid pAN8-1[2] was used in the selection of the *Trichoderma* transformants. The Cel6A D221A mutant was expressed in the *cel6A* negative *T. reesei* strain ALKO 2721 and the Cel6A D175A mutant in the *cel6A/cel5A* double negative strain ALKO2877[3] Cel6A wt protein was purified from the *T. reesei* Rut C-30.

Construction of the Mutant Clones. The *Eco*RI-*Bam*HI fragment of pTTc9, containing the *cbh2* cDNA, was first cloned into pSP73 and the D175A (GAT→GCT) and D221A (GAC→GCC) mutations were introduced using the PCR overlap extension method of Ho *et al.*[4]. Nucleotide sequences of the fragments subjected to PCR were confirmed. The mutated Cel6A cDNAs were then cloned under the *cel7A* promoter in pUJ10 as described earlier[5].

Transformation and Screening of the Fungal Transformants. Fungal transformation was carried out using standard procedures[6,7] and screening of the best producing transformants as described by[8].

Protein purification. The mutant proteins were produced on cellulase inducing media and purified as described earlier[3,8] In brief, mycelia was separated from the culture supernatant by centrifugation and subsequent filtration. After concentration and desalting, the protein solution was run through DEAE-Sepharose FF (Pharmacia, Sweden) equilibrated in 50mM sodium acetate buffer pH 5.6. The flow-through fraction containing Cel6A was further purified using p-aminobenzyl 1-thiocellobioside-based affinity chromatography[9] and immunoaffinity chromatography[3]. Catalytic domains of the two mutant proteins were produced for structure determination by papain digestion (Sigma) as described in[5]. The purity of the mutant preparations was verified by SDS-PAGE and Western blot as described[5]. The presence of contaminating cellulases was excluded by measuring the activities against HEC and small chromogenic substrates[3]. The Cel6A wild-type protein was purified as described by[10] and its purity checked as described above.

Protein Concentration. Absorbance values at 280nm were used to measure Cel6A concentration using $\varepsilon = 80{,}500\ M^{-1}cm^{-1}$ for both the Cel6A wild type and mutated proteins.

Cellobiosyl fluorides. α- and β-Cellobiosyl fluorides were made essentially as described before[11], although HF/pyridine 70:30[12,13] rather than liquid HF was used to convert octaacetyl cellobiose to heptaacetyl α–cellobiosyl fluoride. An impurity of up to 2% of the β-anomer was always present in α–cellobiosyl fluoride, as estimated by complete hydrolysis with *T. reesei* cel7A, which acts on the β- but not the α-anomer. ^{19}F-NMR spectra were recorded at 282 MHz using $FCCl_3$ as external reference.

Synthesis of 1,5-anhydro 4-O-(β–D-glucopyranosyl)-1,1-difluoro-D-glucitol (hereinafter 1-fluorocellobiosyl fluoride)

(Z)-2,3,6-Tri-O-benzyl-4-O-(2,3,4,6-tetra-O-benzyl-β-D-glucopyranosyl)-D-glucono hydroximo-1,5-lactone (I) A methanolic solution (200 mL) of hydroxylamine hydrochloride (2.3 g) and sodium methoxide (1.8 g) was cooled to 0°, filtered, and added to 2,3,6-tri-*O*-benzyl-4-*O*-(2,3,4,6-tetra-*O*-benzyl-β-D-glucopyranosyl)-D-glucopyranose (4.1 g) [14]. The mixture was heated under reflux for 1.5 h, cooled, and taken to dryness (rotavapor). The residue was taken up in water and extracted with dichloromethane. The dichloromethane extracts were filtered (cotton pad) and evaporated (rotavapor). A solution of the dried (high vacuum) crude product (4.1 g) in absolute dichloromethane (60 mL) was cooled under argon to –78°, treated with DBU (0.73 mL) and then, portionwise, with NCS (648 mg). After 15 min at –78°, the reaction mixture was warmed to 25° and poured into water. The water was extracted with dichloromethane, and the dichloromethane extracts were filtered (pad) and evaporated (rotavapor). The residue was purified by flash chromatography (pentane/acetone 7:3 to yield the title compound (2.6 g, 62%).

IR ($CHCl_3$): 3586*m*, 3445*w*, 3350*w*, 3067*m*, 2869*m*, 1951*w*, 1868*w*, 1733*w*, 1669*m*, 1653*w*, 1497*m*, 1454*s*, 1363*m*, 1279*m*, 1071*s*, 1028*s*, 932*m*.

^{1}H-NMR (200 MHz, $CDCl_3$): δ 7.37–7.16 (*m*, 35 arom. H); 6.91 (br. *s*, NOH); 4.93 (*d*, *J* = 11.2), 4.84 (*d*, *J* = 10.8), 4.82 (*d*, *J* = 10.8, 3 PhC*H*); 4.76–4.46 (*m*, H–C(5), H–C(1′), 10 PhC*H*); 4.39 (*d*, *J* = 12.4 PhC*H*); 4.19–4.13 (*m*, H–C(3), H–C(4)); 4.10 (br. *s*, H–C(2)); 3.78 (*m*, 2 H–C(6)); 3.74–3.53 (*m*, H–C(2′), H–C(4′), 2 H–C(6′)); 3.44 (*t*, *J* = 8.3, H–C(3′)); 3.37–3.33 (*m*, H–C(5′)).

^{13}C-NMR (75 MHz, $CDCl_3$): 151.13 (*s*, C(1)); 138.49, 138.24, 138.14, 137.92, 137.85, 137.16 (6 *s*, 7 C); 128.36–127.54 (many *d*); 104.17 (*d*, C(1′)); 84.65 (*d*, C(3′)); 82.14 (*d*, C(2′)); 79.73 (*d*, C(2)); 77.63 (*d*, C(4), C(4′)); 76.14 (*d*, C(3)); 75.60 (*d*, C(5′)); 75.00, 74.50, 73.61 (3 *t*); 73.22 (*d*, C(5)); 72.95, 72.59, 71.33, 70.25 (4 *t*); 68.56 (*t*, C(6′)); 67.70 (*t*, C(6)).

FAB-MS: 1972 (8, $[2M]^+$), 986 (90, M^+), 984 (10), 878 (10), 554 (17), 464 (20), 271 (11), 181 (100), 154 (32), 138 (22), 136 (30).

(Z)-2,3,6-Tri-O-benzyl-4-O-(2,3,4,6-tetra-O-benzyl-β-D-glucopyranosyl)-N-[(methylsulfonyl)oxy]-D-gluconimido-1,5-lactone (II). To a solution of (I) (2.6 g) and triethylamine (0.64 mL) in absolute dichloromethane (20 mL), under argon at 0° was added methanesulfonyl chloride (0.73 mL). After 20 min at 0°, the reaction mixture was poured into saturated aqueous $NaHCO_3$. Extraction with dichloromethane, filtration (pad), and rotary evaporation afforded the crude material, which was purified by flash chromatography (pentane/acetone 7:3). The pure product (2.6g, 92%) was crystallized from pentane/ether, mp 63–64°.

IR ($CHCl_3$): 3076*w*, 3009*m*, 2869*m*, 1951*w*, 1878*w*, 1811*w*, 1654*m*, 1497*m*, 1369*s*, 1326*m*, 1178*m*, 1071*s*, 1028*m*, 969*m*, 909*m*, 845*m*.

^{1}H-NMR (200 MHz, $CDCl_3$): 7.37–7.14 (*m*, 35 arom. H); 4.90 (*d*, *J* = 10.9), 4.81 (*d*, *J* = 10.9), 4.80 (*d*, *J* = 10.9, 3 PhC*H*); 4.72–4.44 (*m*, H–C(5), 9 PhC*H*); 4.48 (*d*, *J* = 7.8, H–C(1′)); 4.44 (*d*, *J* = 12.1), 4.38 (*d*, *J* = 12.1, 2 PhC*H*); 4.21 (*t*, *J* ≈ 2.3, H–C(3)); 4.16 (*dd*, *J* = 1.9, 9.9, H–C(4)); 4.13 (*d*, *J* = 2.5, H–C(2)); 3.73 (br. *d*, 2 H–C(6)); 3.69–3.60 (*m*, H–C(2′), 2 H–C(6′)); 3.57 (*t*, *J* ≈ 9.0, H–C(4′)); 3.42 (*t*, *J* ≈ 8.5, H–C(3′)); 3.37–3.33 (*m*, H–C(5′)); 3.06 (*s*, MsO).

^{13}C-NMR (75 MHz, $CDCl_3$): 157.57 (*s*, C(1)); 138.56, 138.18, 137.94, 137.85, 137.65, 137.57 (6 *s*, 7 C); 128.61–127.65 (many *d*); 104.49 (*d*, C(1′)); 84.65 (*d*, C(3′)); 82.11 (*d*, C(2′)); 79.09 (*d*, C(2)); 77.50 (*d*, C(4), C(4′)); 76.97 (*d*, C(3)); 75.66, 74.98, 74.93 (3 *t*); 74.74 (*d*, C(5′)); 73.32,

73.14 (2 *t*); 72.94 (*d*, C(5)); 71.71, 71.16 (2 *t*); 68.56, 66.94 (2 *t*, C(6), C(6´)); 35.94 (*q*, MsO).

FAB-MS: 2128 (1, $[2M]^+$), 2033 (1), 1156 (16), 1155 (40), 1154 (45), 1066 (10), 1065 (31, $[M + H]^+$), 1064 (50), 1063 (40), 1062 (61), 986 (14), 972 (20), 971 (20), 970 (32), 956 (19), 848 (33), 632 (100), 542 (59), 181 (70).

1,5-Anhydro-2,3,6-tri-O-benzyl-4-O-(2,3,4,6-tetra-O-benzyl-β-D-glucopyranosyl)-1-hydrazi-D-glucitol (III). To a solution of oxime mesylate (II) (200 mg) in CH_2Cl_2 (1.0 ml) was added saturated methanolic ammonia (3.0 mL). The solution was stirred in a sealed flask for 50 h at 25°, and then evaporated at 0°C (rotavapor). Purification of the crude product by flash chromatography (pentane/acetone 7:3) and recrystallization in ether afforded the title product (150mg, 81%), m.p. 93-97°.

IR ($CHCl_3$): 3271*w*, 3090*w*, 3067*w*, 3007*m*, 2870*w*, 1951*w*, 1879*w*, 1812*w*, 1746*w*, 1606*w*, 1497*m*, 1454*m*, 1399*w*, 1361*m*, 1316*w*, 1275*m*, 1072*s*, 1028*m*, 909*s*.

^{1}H-NMR (200 MHz, $CDCl_3$): 7.42–7.13 (*m*, 35 arom. H); 5.12 (*d*, *J* = 11.2), 4.88 (*d*, *J* = 11.2), 4.83 (*d*, *J* = 10.6), 4.79 (*d*, *J* = 10.9, 4 PhC*H*); 4.76–4.74 (*m*, 2 PhC*H*); 4.71 (*d*, *J* = 11.5), 4.66 (*d*, *J* = 10.6), 4.58 (*d*, *J* = 12.1), 4.56 (*d*, *J* = 10.9, 4 PhC*H*); 4.52–4.38 (*m*, H–C(1´), 4 PhC*H*); 4.25 (*dd*, *J* = 9.0, 9.9, H–C(4)); 4.02 (*d*, *J* = 9.0, H–C(2)); 3.91 (*dd*, *J* = 2.8, 11.2, H–C(6)); 3.73 (*dd*, *J* = 1.9, 11.2, H´–C(6)); 3.69–3.53 (*m*, 5 H); 3.49 (*t*, *J* ≈ 9.0, H–C(4´)); 3.37 (*dd*, *J* = 7.8, 9.0, H–C(3´)); 3.32–3.29 (*m*, H–C(5´)); 2.67 (*d*, *J* = 9.6, NH); 2.32 (*d*, *J* = 9.4, N´H).

^{13}C-NMR (75 MHz, $CDCl_3$): 139.20, 138.67, 138.58, 138.37, 137.89, 137.73 (6 *s*, 7 C); 128.57–127.31 (many *d*); 102.49 (*d*, C(1´)); 84.86 (*d*, C(3´)); 83.03 (*s*, C(1)); 82.64 (*d*, C(2´)); 82.59 (*d*, C(2)); 77.98 (*d*, C(4´)); 76.74 (*d*, C(4)); 75.76 (*d*, C(5), C(3)); 75.64 (*t*); 75.59 (*t*); 75.26 (*t*); 75.10 (*d*, C(5´)); 74.96 (*t*); 74.76 (*t*); 73.32 (*t*); 73.27 (*t*); 68.94 (*t*, C(6´)); 67.19 (*t*, C(6)).

FAB-MS: 1970 (41, $[2M]^+$), 1955 (40), 1025 (17), 986 (64, $[M + H]^+$), 985 (100, M^+), 181 (25).

1,5-Anhydro-1-azi-2,3,6-tri-O-benzyl-4-O-(2,3,4,6-tetra-O-benzyl-β-D-glucopyranosyl)-D-glucitol (IV). A solution of iodine (180 mg) in absolute dichloromethane (10 mL) was added dropwise under argon to a cooled (–78°) solution of the diaziridine (700 mg) and trimethylamine (0.5 mL) in absolute dichloromethane (10 mL) over 1.5 h. The reaction mixture was then warmed to 0°, filtered through silica, and evaporated at 0° under vacuum. A further two hours' drying under high vacuum at –78° afforded the product (663 mg, 95%) as a yellow foam.

UV (MeOH): λ_{max} 350nm ($\varepsilon = 45$).

IR ($CHCl_3$): 3090*w*, 3066*w*, 3006*w*, 2926*m*, 2856*m*, 1951*w*, 1877*w*, 1810*w*, 1755*w*, 1651*w*, 1605*w*, 1563*w*, 1497*w*, 1454*m*, 1362*m*, 1317*w*, 1261*m*, 1071*s*, 1028*s*, 909*s*.

^{1}H-NMR (200 MHz, $CDCl_3$, –25°): 7.39–7.15 (*m*, 35 arom. H); 5.01–4.81, 4.75–4.43, 4.37–3.38 (*m*, 27 H).

1,5-Anhydro-2,3,6-tri-O-benzyl-4-O-(2,3,4,6-tetra-O-benzyl-β-D-glucopyranosyl)-1,1-difluor-D-glucitol (heptabenzyl 1-fluoro-cellobiosyl fluoride) (V). To a solution of the diazirine (IV) (117 mg) in absolute dichloromethane (1.0 mL), maintained at –78° under argon in a Teflon reaction vessel, was added xenon difluoride (154 mg). The sealed reaction vessel was allowed to warm slowly to 25° C over twelve hours, and the excess pressure was carefully released. The mixture was poured into saturated $NaHCO_3$ solution, and the product was

extracted with dichloromethane. The dichloromethane extracts were filtered through a filter pad, and evaporated in a rotavapor. Separation of the products by preparative HPLC (Spherisorb-SW, 5 μm, flow rate 7.5 mL/min) using isocratic elution with hexane/ethyl acetate 4:1 gave the title compound (t_R 12.2 min, 13 mg, 11%), heptabenzyl β-cellobiosyl fluoride (t_R 13.0 min, 50 mg, 43%) and heptabenzyl α-cellobiosyl fluoride (t_R 20.6 min, 17 mg , 14%).

Data for heptabenzyl 1-fluoro-cellobiosyl fluoride

IR ($CHCl_3$): 3090*w*, 3067*w*, 3008*w*, 2918*w*, 2871*w*, 1951*w*, 1870*w*, 1811*w*, 1750*w*, 1605*w*, 1497*m*, 1455*m*, 1400*w*, 1363*m*, 1308*w*, 1153*m*, 1076*s*, 1028*m*, 912*w*, 832*w*.

^{1}H-NMR (300 MHz, $CDCl_3$): 7.37–7.17 (*m*, 35 arom. H); 5.07 (*d*, *J* = 11.2), 4.89 (*d*, *J* = 10.9), 4.83 (*d*, *J* = 11.2), 4.81 (*d*, *J* = 10.6), 4.76 (*d*, *J* = 11.2), 4.71 (*d*, *J* = 11.5), 4.70 (*d*, *J* = 10.9), 4.59 (*d*, *J* = 11.8), 4.55 (*d*, *J* = 10.9, 9 PhC*H*); 4.44 (*d*, *J* = 7.8, H–C(1′)); 4.43 (*d*, *J* = 12.1), 4.39 (*s*, 5 PhC*H*); 4.16 (br. *t*, *J* = 9.9, H–C(4)); 3.88 (br. *d*, *J* = 10.9, 1 H); 3.76–3.55 (*m*, 7 H); 3.51 (*t*, *J* = 9.0, H–C(4′)); 3.36 (*t*, *J* = 8.1, H–C(2′)); 3.32–3.29 (*m*, H–C(5′)).

^{19}F-NMR (282 MHz, $CDCl_3$): –78.68 (br. *d*, *J* = 149.5, F_{eq}); –87.12 (*dd*, *J* = 17.1, 147.4, F_{ax}).

The ^{19}F chemical shifts and $J_{F,H}$ agree well with the data of glucopyranosylidene difluorides[15,16].

Heptabenzyl β-cellobiosyl fluoride: ^{19}F-NMR (282 MHz, $CDCl_3$): –135.50 (*dd*, *J* = 12.8, 53.4, F_{eq}).

Heptabenzyl α–cellobiosyl fluoride: ^{19}F-NMR (282 MHz, $CDCl_3$): –149.37 (*dd*, *J* = 25.6, 53.4, F_{ax}).

The ^{19}F chemical shifts and $J_{F,H}$ of Heptabenzyl β-cellobiosyl fluoride and Heptabenzyl α-cellobiosyl fluoride agree well with the data of glucopyranosyl fluorides[17].

1-Fluorocellobiosyl fluoride. The fluoride (V) (10 mg) was protected by stirring its solution in a mixture of methanol (5 mL) and ethyl acetate (1 mL), with 10% Pd/C (25 mg) under a hydrogen pressure of 3.5 bar for 17 h at 25°. Filtration, evaporation, and flash chromatography (AcOEt/MeOH/H_2O 6:3:2) gave the title compound (3.7 mg, 98%)

^{1}H-NMR (300 MHz, CD_3OD): δ 4.43 (*d*, *J* = 7.8, H–C(1′)); 3.95 (br. *d*, *J* ≈ 12.4, 1 H); 3.89–3.62 (*m*, 7 H); 3.59 (*dd*, *J* = 4.7, 9.7, 1 H); 3.40–3.27 (*m*, 2 H); 3.23 (*t*, *J* ≈ 8.3, irradiation at 4.43 → *d*, *J* = 8.7, H–C(2′)).

^{13}C-NMR (75 MHz, CD_3OD):δ 104.6 (*d*, C(1′)); 78.5 (*d*, C(4)); 78.1 (*d*, C(5′)); 77.9 (*d*, C(3′)); 77.4 (*m*, $J_{C,F}$ ≈ 2.9, C(5)); 74.9 (*d*, C(2′)); 74.2 (*dd*, $J_{C,F}$ = 9.8, C(3)); 73.1 (*ddd*, $J_{C,F}$ = 28.1, 31.7, C(2)); 71.3 (*d*, C(4′)); 62.4 (*t*, C(6)); 60.5 (t, C(6)); signal of C(1) not observed. (only noise, signal expecetd [15,16] as a *dd* ($J_{C,F}$ = 272 and 256 Hz at ca. 120 ppm).

^{19}F-NMR (282 MHz, CD_3OD): –82.68 (*dd*, *J* = 4.3, 149.5, F_{eq}); –89.64 (*dd*, *J* = 18.2, 150.6, F_{ax}). (data in agreement with of glugopyranosylidene difluoride [15,16].

FAB-MS: 385 (10, $[M + Na]^+$), 363 (3, $[M + H]^+$), 329 (5), 289 (16), 176 (10), 163 (4).

X-ray crystallography of the D175A mutant. Crystals of the Cel6A D175A mutant core were prepared as described[18] with small modifications. High-quality crystals were obtained with microseeding using wild-type Cel6A crystals as seeds. The crystals were grown in 20% polyethylene glycol monomethyl ether (mPEG) 5000, 20mM morpholinoethane sulfonic acid (MES) buffer (pH 6.0) and 10mM $CoCl_2$ at room temperature. One crystal was soaked in the cryo-protectant solution containing 25% mPEG5000, 20mM MES buffer pH 6.0, 10mM $CoCl_2$ and 15% glycerol for one minute before flash freezing in liquid nitrogen stream. The crystal belongs to space group $P2_1$ and is isomorphous with the wild-type Cel6A crystal with two molecules per asymmetric unit, related by an almost pure translation operator. The diffraction data set was collected at a temperature of 100 K on an RAXIS II image-plate scanner using CuKα radiation from a Rigaku rotating-anode generator. The images were integrated and scaled with the HKL program suite[19] and further processed with programs included in the CCP4 software package[20].

Since the D175A mutant crystal is isomorphous to the wild-type protein, refinement was started from a model of the wild-type enzyme that had been refined at 1.8Å (GJK, unpublished results). Residue 175 was replaced by an alanine and all water molecules were removed from the model. Five percent of the reflections were put aside for calculating free R-values[21]. The initial model was improved using alternating cycles of refinement with X-PLOR[22] and rebuilding with O[23]. Waters, glycosylation moieties, and ions were added based on the electron density and hydrogen bonding patterns. In the final rounds of refinement, the CNS program[24] was used, and all data between 20.0 and 2.1 Å resolution were included. The final model contains residues 85 to 447, 9 glycosylation entities in each chain and a total of 450 water molecules. Data collection and refinement statistics are listed in Tables S1 and S2.

X-ray crystallography of the D221A mutant. Crystals of the Cel6A D221A mutant were obtained using 20% PEG6000 as precipitant and buffered by 10mM MES pH 6.0. The quality of the crystals was improved by macroseeding. The crystals thus obtained diffracted up to 2.1 Å resolution. Diffraction data were collected at room temperature from a single crystal on an SDMS multiwire area detector[25]. The raw images were processed using the program MADNES[26,27]. The space group was determined to be P1 , which was later confirmed by measurements on a precession camera. The structure was solved by the molecular replacement method using the program AMORE[28] and with two molecules in the asymmetric unit. The initial model was improved using alternating cycles of refinement with X-PLOR and rebuilding with O. The two molecules in the asymmetric unit were restrained to have similar conformations. There was no density for residue 221 after Cβ, confirming that it was indeed mutated to alanine. Water molecules and other entities were gradually added based on 2Fo-Fc and Fo-Fc density maps. The final model contains residues 85 to 447, 9 glycosylation entities in each chain, a total of 186 water molecules and 2 glucoses in the B chain of the molecule. Data collection and refinement statistics are listed in Tables S1 and S2.

Table S1. Crystallographic data collection and processing statistics

Protein	D175A	D221A
Temperature	100 K	Room temperature, 20° C
Space group	$P2_1$	P1
Cell parameters	a=48.6Å, b=74.7Å, c=91.4Å,	a=49.6Å, b=67.5Å, c=53.8Å,
Resolution range (Å)	80.0-2.10 (2.18-2.10)[a]	8.0-2.13 (2.29-2.13)
No. of unique reflections	37,025	31,767
Average multiplicity	2.8 (2.8)	2.3 (1.3)
Completeness (%)	99.5 (99.9)	80.3 (48.1)
R_{merge}[b]	0.049 (0.118)	0.080 (0.158)
I/σ(I)	19.8 (7.8)	8.8 (1.9)

[a]The values in parentheses correspond to the outer resolution shell.
[b]$R_{merge}= \Sigma_h\Sigma_i |I_{hi}-\langle I_h\rangle| / \Sigma_h\Sigma_i |I_{hi}|$

Table S2. Crystallographic refinement and model statistics for the mutant protein structures.

Protein	D175A	D221A
Resolution range (Å)	20.0-2.1	8.0-2.2
No. of reflections	36,964	26,776
R value, free R value	0.183, 0.225	0.198, 0.258
No. of non-hydrogen atoms	6144	5908
No. of solvent waters	446	186
No. of glycosylation sites	18	18
<B-factor> protein main-chain atoms ($Å^2$)	14.5	21.7
<B-factor> protein side-chain atoms ($Å^2$)	15.3	22.0
<B-factor> solvent atoms ($Å^2$)	19.4	25.8
<B-factor> glycosylation atoms ($Å^2$)	28.3	43.6
<B-factor> ligand atoms ($Å^2$)	N/A	44.9
<B-factor> protein main-chain atoms	28.3, 23.7	30.8, 49.0
<B-factor> protein side-chain atoms	30.7, 28.7	35.5, 50.7
Main-chain RMSD ΔB, between bonded atoms	1.1	1.3
Side-chain RMSD ΔB, between bonded atoms ($Å^2$)	1.9	1.9
Ramachandran plot outliers (%)[a]	3.0	3.6
RMSD from ideal bond lengths (Å)[b]	0.005	0.006
RMSD from ideal bond angles (°) [(b)]	1.3	1.3
RMSD NCS, on Cα atoms (Å)	0.57	0.60
RMSD NCS, on all atoms (Å)	0.83	0.74

[a] 29
[b] 30

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