Table S1. Oligodeoxyribonucleotides used in this study.

Oligo	Sequence	Purpose
1	5′-GAG AAA TTA ACT ATG **GCG GCG GCG** TGT GAA ATG AAA CGC ACC ACA CTG-3′	Encodes DKD(2-4)-AAA mutation.
2	5′-GAG AAA TTA ACT ATG GAC **GCG GCG GCG** GAA ATG AAA CGC ACC ACA CTG-3′	Encodes KDC(3-5)-AAA mutation.
3	5′-G GAG AAA TTA ACT ATG GAC AAG **GCG GCG GCG** ATG AAA CGC ACC ACA CTG G-3′	Encodes DCE(4-6)-AAA mutation.
4	5′-G GAG AAA TTA ACT ATG GAC AAG GAT **GCG GCG GCG** AAA CGC ACC ACA CTG G-3′	Encodes CEM(5-7)-AAA mutation.
5	5′-G GAG 5′-GG CTA GCC **GCG GCG GCG** TGG CTT CTG GCC CAT G-3′	Encodes VKE(164-166)-AAA mutation.
6	5′-GGA GGG CTA GCC GTG **GCG GCG GCG** CTT CTG GCC CAT G-3′	Encodes KEW(165-167)-AAA mutation.
7	5′-G GGC 5′-TA GCC GTG AAG **GCG GCG GCG** CTG GCC CAT GAA GG-3′	Encodes EWL to AAA mutation.
8	5′-TA GCC GTG AAG GAA **GCG GCG GCG** GCC CAT GAA GGC CAC CG-3′	Encodes WLL(167-169)-AAA mutation.
9	5′-AGT CAG TCA GTC AGT CAG TCA GTC AG-3′	Binding substrate.
10	5′-CTG ACT GAC TGA CTG ACT GAC TGA CT-3′	Binding substrate.

Table S2. Circular dichroism secondary structure analysis[a]

AGT Protein	Algorithm	H(tot)[b]	S(tot)[b]	Turn[b]	UO[b]
Wild-type	Selcon 3	20	30	20	29
	Continll	23	25	19	32
KDC(3-5)-AAA	Selcon 3	18	30	19	27
	Continll	22	26	19	33
DCE(4-6)-AAA	Selcon 3	c	c	c	c
	Continll	5.7	39	21	35
CEM(5-7)-AAA	Selcon 3	19.2	25.5	18	25
	Continll	19.5	29	19	32
VKE(164-166)-AAA	Selcon 3	22	30	19	28
	Continll	23	25	20	32
KEW(165-167)-AAA	Selcon 3	13	36	17	23
	Continll	16.5	27.4	18	38
EWL(166-168)-AAA	Selcon 3	11	40	18	26
	Continll	17	29	18	36

a. Values obtained using Contin/LL and Selcon3 algorithms implemented in the CDpro program, using the SDP48 basis set (22,23).

b. Percent of residues in each conformation. H(tot) = H(R) + H(D), where H(R) is the percent in "regular" helix and H(D) is the percent in "distorted" helix estimated by the program. S(tot) = S(R) + S(D), where S(R) is the percent in "regular" sheet and S(D) is the percent in "distorted" sheet estimated by the program. Turn refers to the fraction in b-turn conformation; UO is the percent that cannot be assigned other major secondary structures. The normalized mean root square derivation between calculated and experimental spectra was in the range of 2.3-5.5 %.

c. Calculation failed to converge.

Figure S1

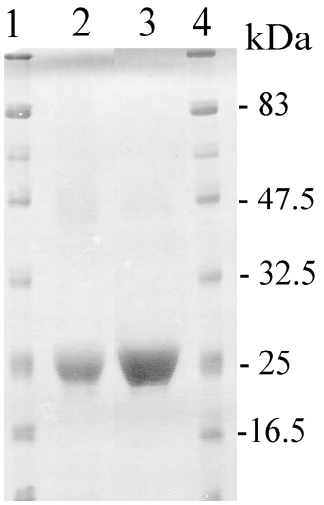

Figure S1. SDS-polyacrylamide gel electrophoresis of representative AGT preparations. SDS-PAGE gels (15% acrylamide) were prepared and run as described (29) and stained with coomasssie blue R-250. Lanes 1 and 4 contain molecular weight standards. Lane 2 contains wild-type AGT (20µg). Lane 3 contains AGT-mutant KDC(3-5)-AAA (35µg). Molecular weights of standards (in units of KDa) are given in the margin.

Figure S2

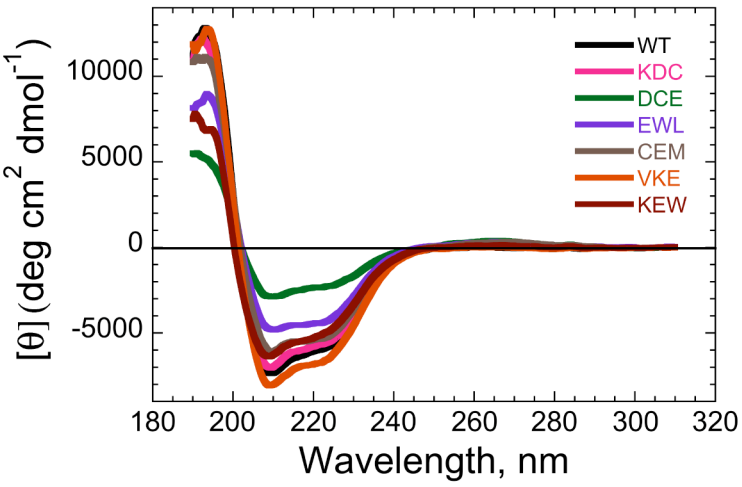

Figure S2. Circular dichroism spectra of wild-type and mutant AGT proteins. Spectra were obtained at 4°C, using a cell with a path length of 0.02 cm. Samples contained wild-type or mutant protein at concentrations of ~0.19 mg/ml (~9 µM) dissolved in 50 mM sodium phosphate (pH 7.5 at 4°C). Each spectrum is the average of twenty consecutive scans.