Supporting Information

The structure of the cataract causing P23T mutant of HgD crystallin exhibits distinctive local conformational and dynamic changes.

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Supporting information: Figures S1 –S4 that present NMR spectra illustrating differences between the wild-type, P23T, P23V and P23S HgD and similarities between His-tagged and non-His-tagged mutant P23T HgD.

Supporting information
Fig. S1.

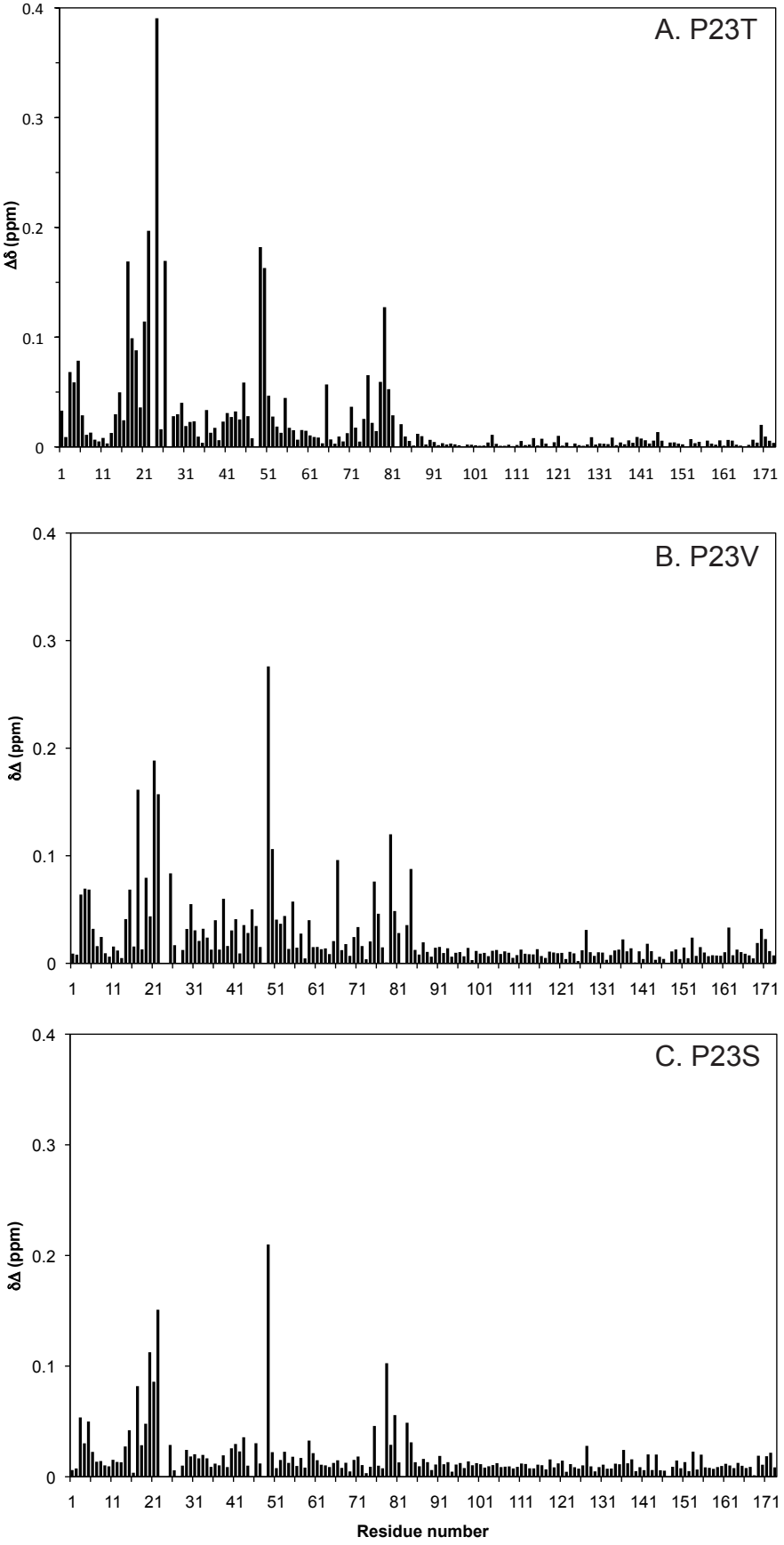

Figure S1. Backbone chemical shift difference between the mutant and wild-type HgD proteins. (A) P23T (B) P23V and (C) P23S. No values are plotted for prolines and unassigned residues.

Supporting information
Fig. S2.

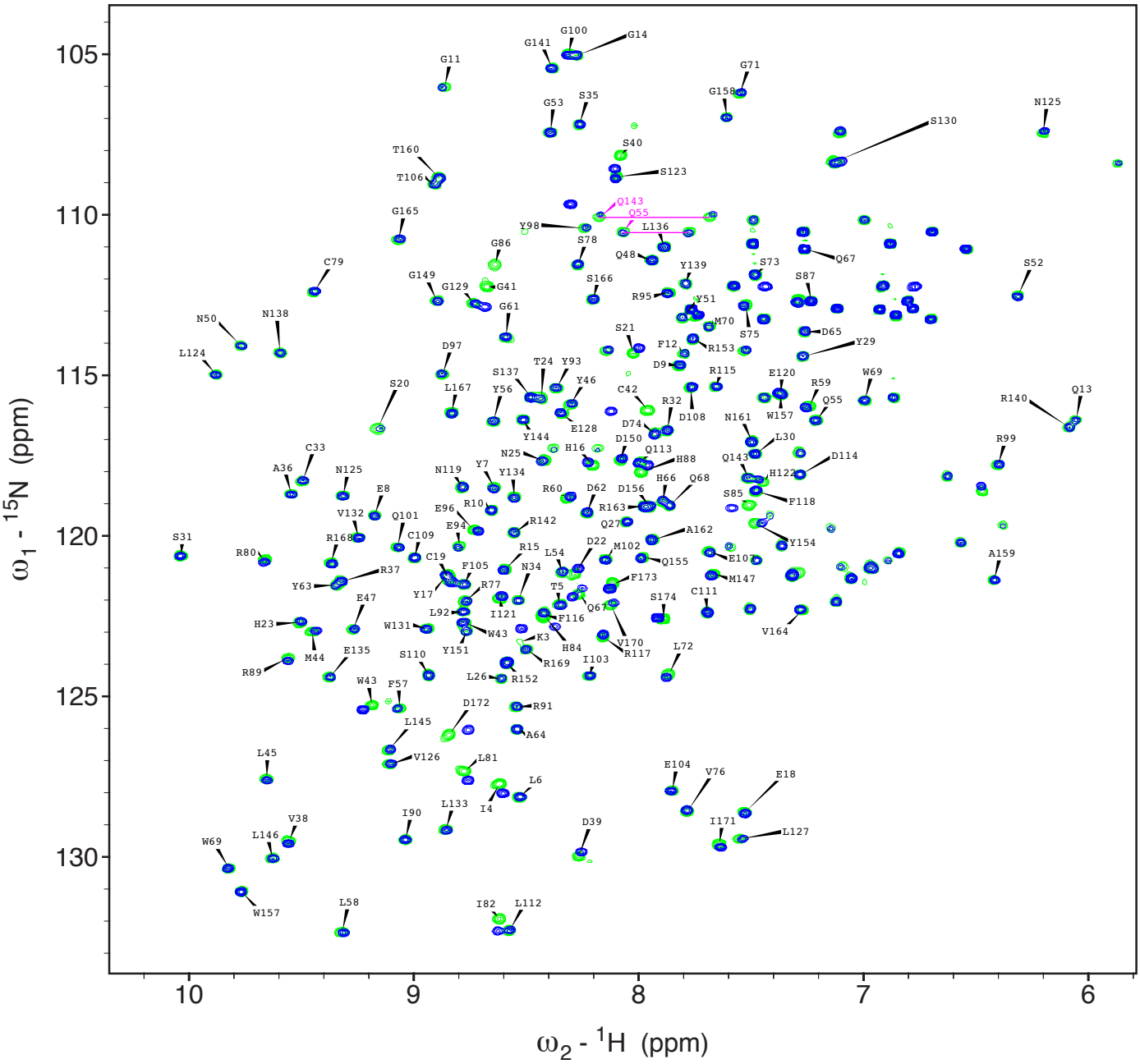

Figure S2. Superposition of the ^{1}H-^{15}N HSQC spectra of the His-tagged and non-His-tagged P23T HgD mutant proteins. Spectra were collected for samples in 20mM sodium phosphate buffer, 5mM DTT, 0.02% NaN_3, pH 6.2 at 700MHz. Resonances for the His-tagged and non-His-tagged proteins are plotted in blue and green, respectively, and assignments are marked with residue names and numbers. All residue numbers are shifted as +1 from numbering in Figure 2.

Supporting information
Fig. S3.

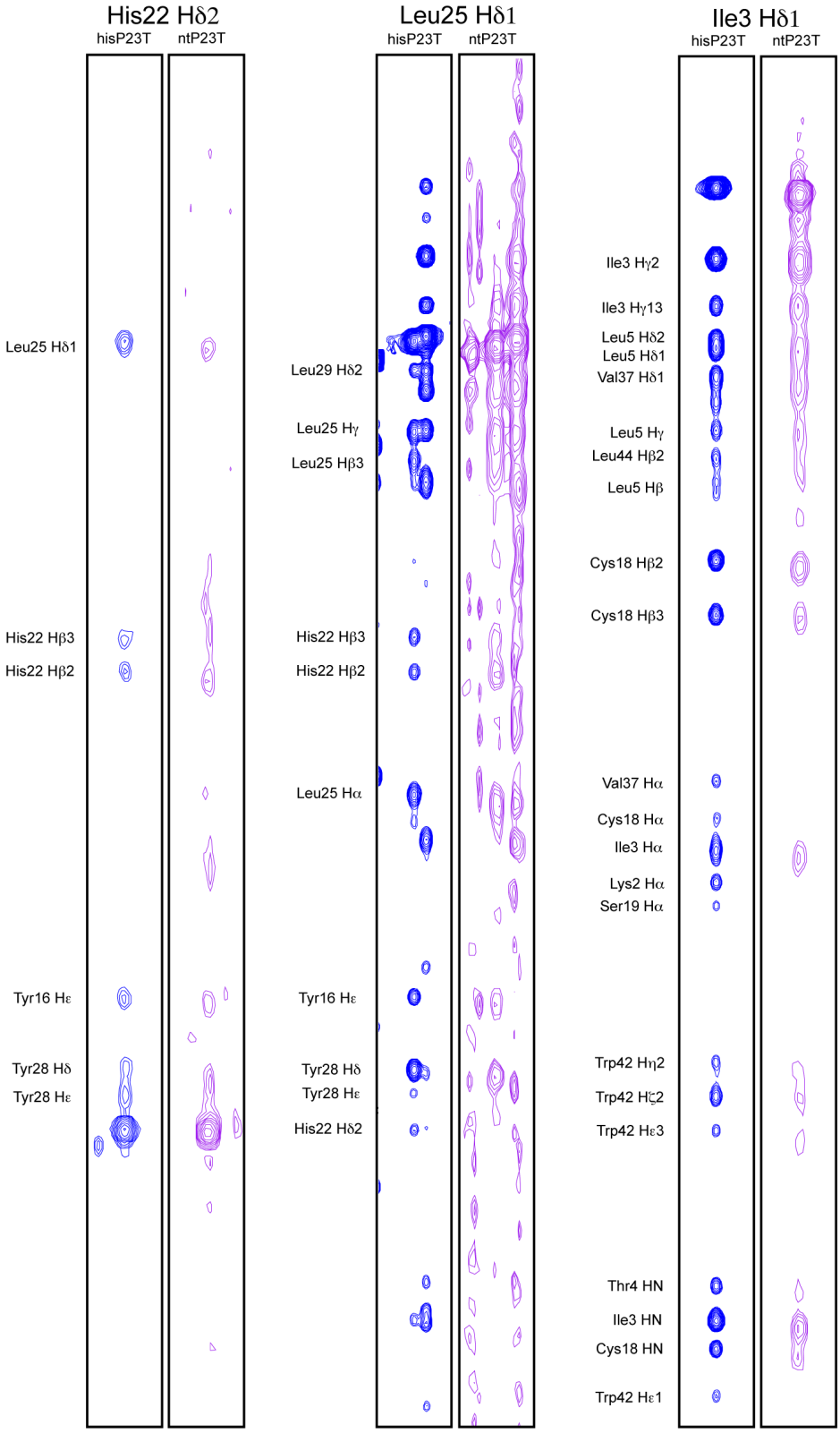

Figure S3. Selected strips from the ^{13}C-edited NOESY spectra recorded for the His-tagged (blue) and non-His-tagged (purple) P23T HgD mutant proteins. Three strips are shown for His22 Hδ2, Leu25 Hδ1 and Ile3 Hδ1 protons, respectively. Assignments of the NOEs are labeled at the left side of the strips.

Supporting information
Fig. S4

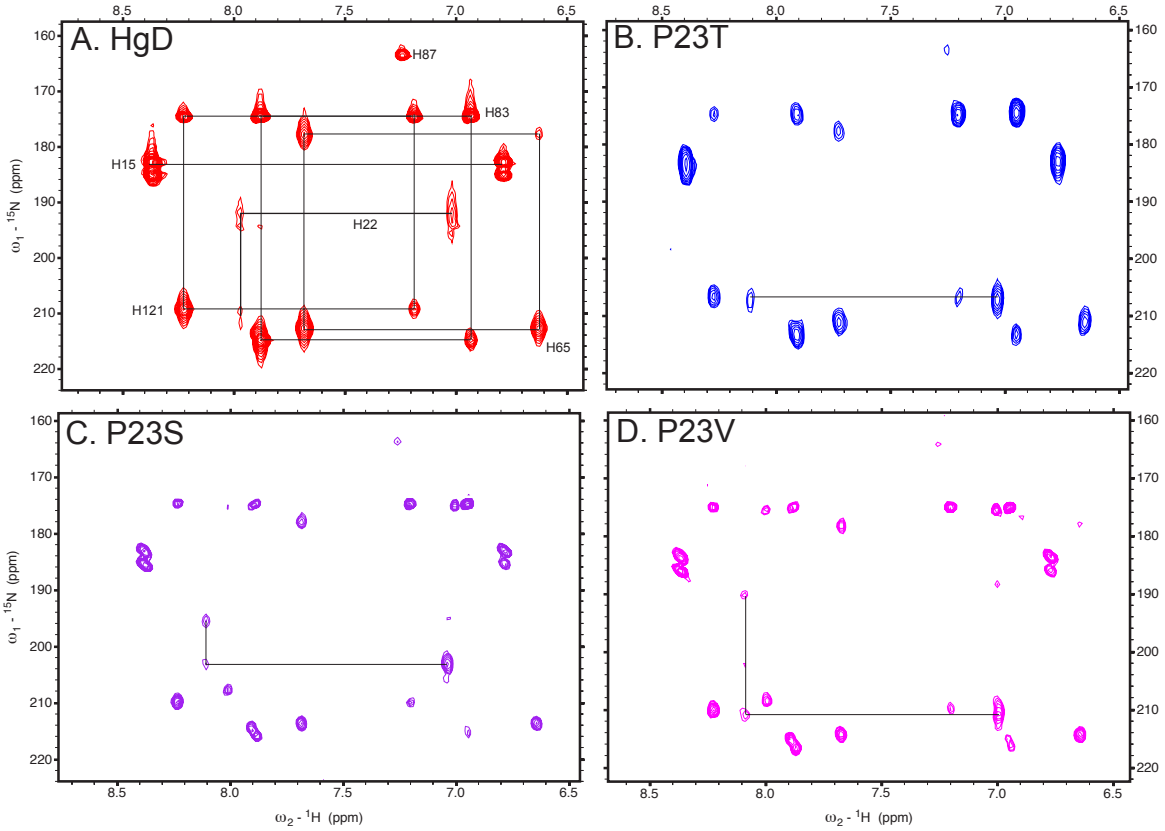

Figure S4. ^{1}H-^{15}N HMBC spectra of wild-type and mutant HgD proteins. All spectra were recorded at 600 MHz for protein samples in 20mM sodium phosphate buffer, 5mM DTT, 0.02% NaN_3, pH 6.2 except the spectrum in (A) that was collected at 800MHz. In (A) all resonances that belong to the same imidazole ring are connected, whereas in (B)-(D) only those resonances that arise from the imidazole ring of His22 are connected.