

# Supplement Figures S1-S6

## Figure S1 - CD8aa - Protodomain alignment and Quaternary Symmetric Arrangements - Coloring Scheme

**A)** CD8a monomer (PDBid: 1CD8) colored by protodomain - blue for protodomain 1 - magenta for protodomain and colored by Sheet A (A|B||E|D) in green (in front in that order) and Sheet B (C|C' ||G|F) in orange. CDR1 and CDR2 in grey.

**B)** Dimer forming a symmetric central barrel from two Sheets B seen with the axis orthogonal to the plane of the paper. Q-Q self complementarity through H-bonding, as in many homo and heterodimeric. (conserved in Human CD8AB while Q-E in mouse)

**C)** Sequence using the both coloring schemes and strand definitions and Link to iCn3D visualization

<https://d55qc.app.goo.gl/bmCQRj7DWcmqsmna6>

## Figure S2 - FN3 Ig domains - The cation-pi ladder

**A)** **FN3**, second domain of the cytokine-binding homology region (CHR) of the cell surface receptor gp130 (Structure 3HHR) ( IL-21 Receptor). The symmetric sequence patterns(see matched in structure forming a cation-pi ladder  $W^*R^*W^*R^*W$  from both (W)SxWS, the so called "WS motif" (see text). Aromatic residues (Trp) in green, cationic residues (Arg) in orange.

**B)** FN3 domain in the Homologous Growth hormone receptor (Structure 3HHR).

**C-D)** Structure based Sequence alignment of both receptor structures and their individual protodomain alignments. The orange hydrophilic residues a zipper mechanism for central strands C||F. The aromatic residues in the **WSxWS** motif in protodomains 2 of IL21 Receptor is not strictly conserved when analyzing the Growth Hormone Receptor (GHR), as it is replaced by **YGEFS** while the symmetric motif in protodomain 1 **SxWS** conserves **W** (see highlights in green/yellow). Both receptors share a conserved architecture with an antiparallel hydrophilic beta zipper (strands C/F). The aromatic residues Y/F and W from strands G and C' respectively, intercalate to form an extended cation-pi ladder. Y and F are structurally equivalent to the two vs W/W in protodomain 2, and W is conserved in protodomain 1. (PDBid: 3HHR, 1BQU) Link to iCn3D <https://d55qc.app.goo.gl/mLUJSMkanUhb74my1>

### Figure S3 - Pseudo symmetry and protodomains of Hfq

**A)** Domain and strand definitions.

**B and C)** Superimposed protodomains - optimizing symmetry match leads to an RMSD of 2.1Å. Symmetry matching of residues.

**D and E)** A shift of 2 residues on the first 2 strands of the protodomains leads to an RMSD of 1.6Å and a higher sequence match, yet symmetry match is not exact. (PDBid: 1KQ2)

### Figure S4 - Quaternary Topology of Hfq hexamer

Sheets NC and M of consecutive Hfq domains through strands b5 and b4 form inter-domains 6 stranded blades (see text and Figure 8) (PDBid: 1KQ2)

### Figure S5 - P53 vs. IgV an FN3 domains Ig-fold

Parallel Visualization of Topology/Sequence maps between IgV (PDBids: VH domain from Structure 5ESV; FN3 from Structure 1BQU domain 2 and P53 from Structure 1TUP). P53 belongs to the Common fold of diphtheria toxin/transcription factors/cytochrome f (b.2 in SCOP). It can be aligned in 3D to Ig domains and topology maps show a much more elaborate fold. Yet it can be decomposed in protodomains that may be aligned in 3D. It is however a much more complex fold with complex loops and insertions forming secondary structural elements that extend sheets in different ways. 3 strands protodomains, the best agreement is with FN3. Topology/Sequence maps can capture complexities and parallels in topology as one can obtain thorough domain and protodomains structural alignments. Link to iCn3D <https://d55qc.app.goo.gl/ktx3uZg4adpBRRUy2>. The chain B (P53) is colored accordingly and for example mutations can be mapped on structure 1TUP (chain B). Mapping of disease causing mutations from ClinVar can be done on top of the domain as in Topology Maps.

### Figure S6 - DNA Nucleosome Symmetry shared by a histone assembly and its DNA

**A)** 3 levels of C2 symmetry relate histones within a nucleosome assembly Chains A-H)

**B)** The vertical axis of symmetry matching both strands of DNA within a nucleosome

**C)** Structure based DNA sequence alignment of DNA Strands (chains I and J) (PDBid: 3C1B)

Figure S1

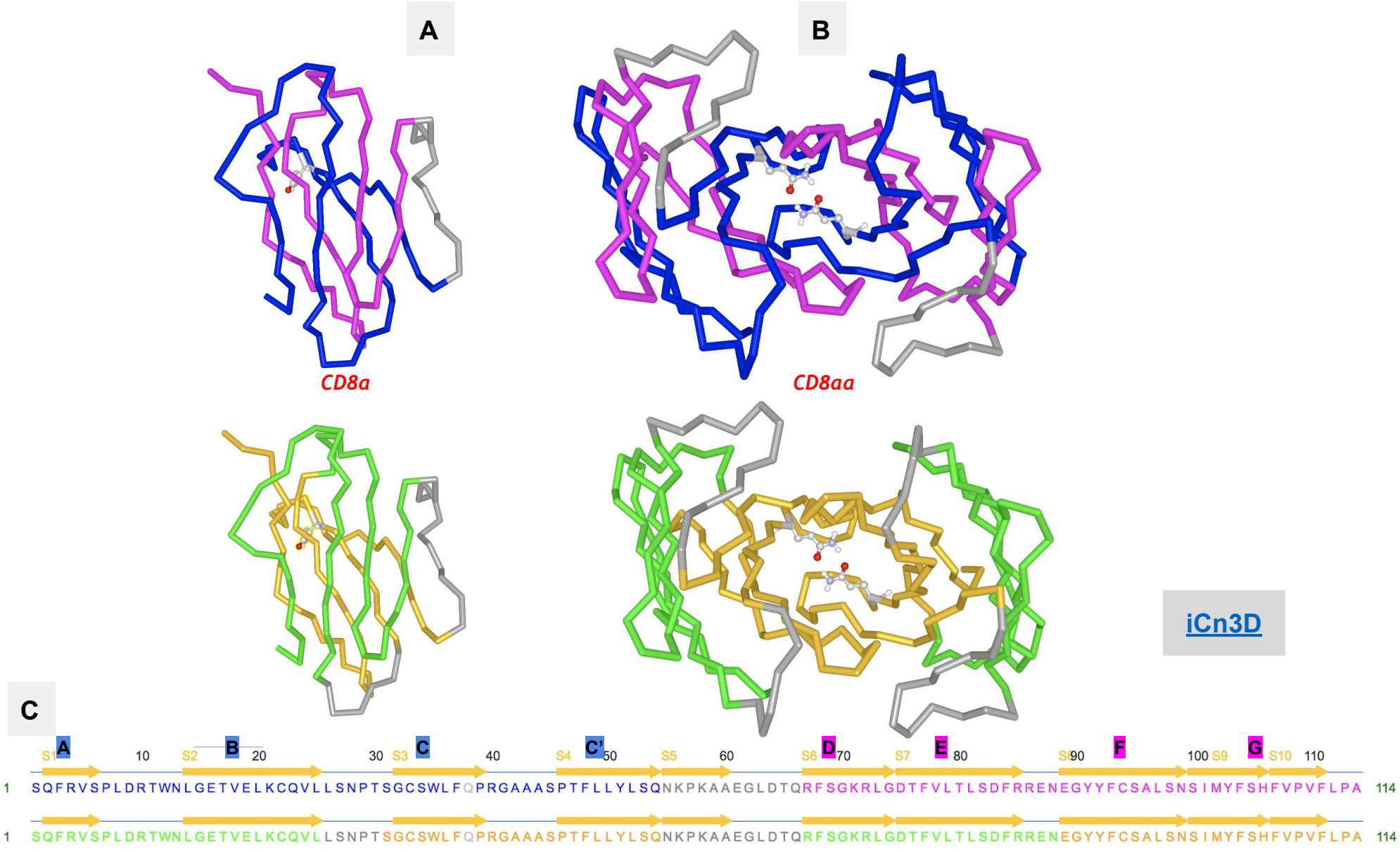


Figure S2

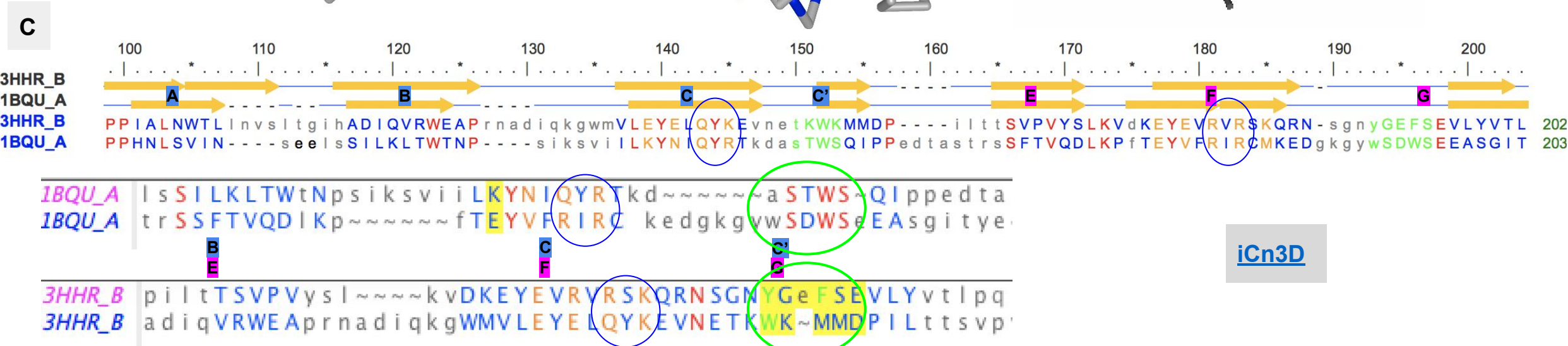
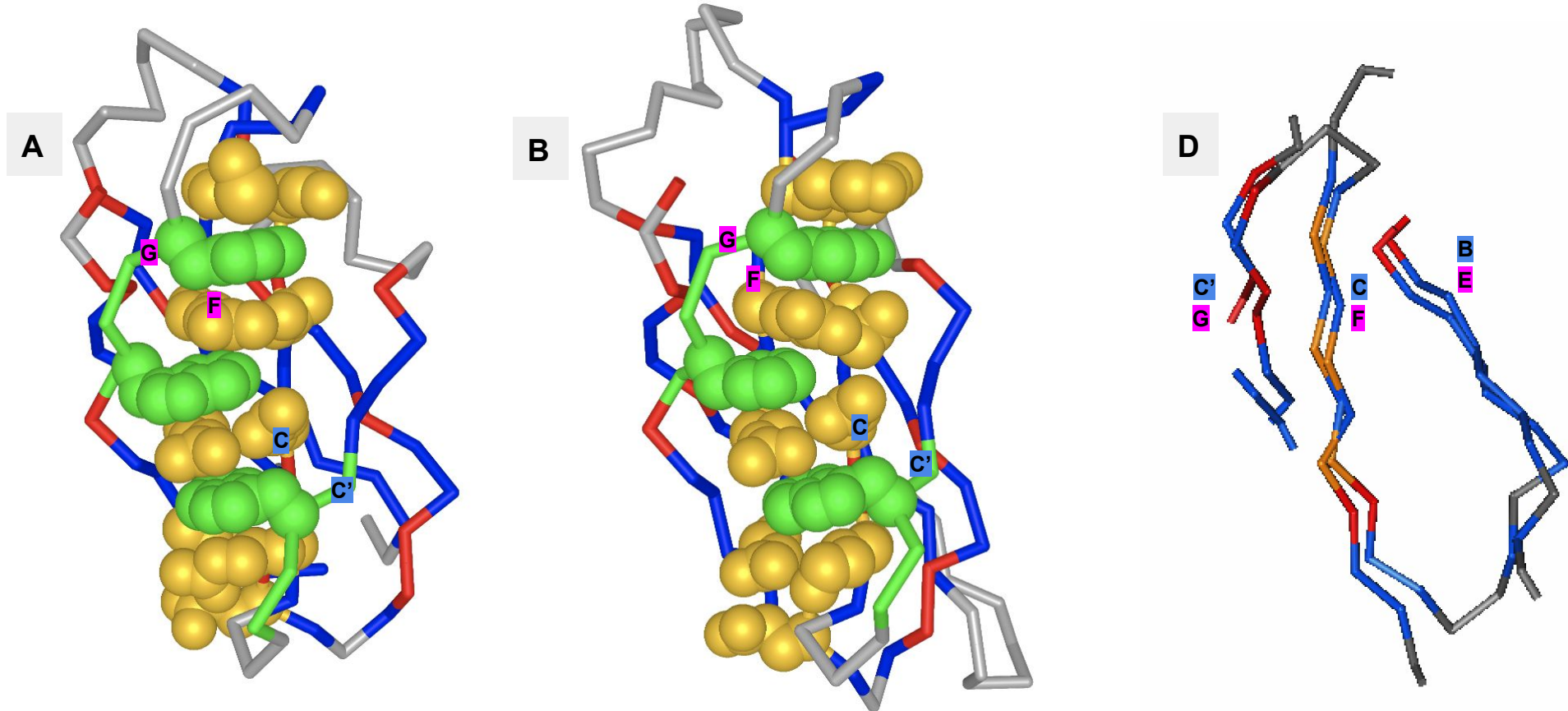


Figure S3

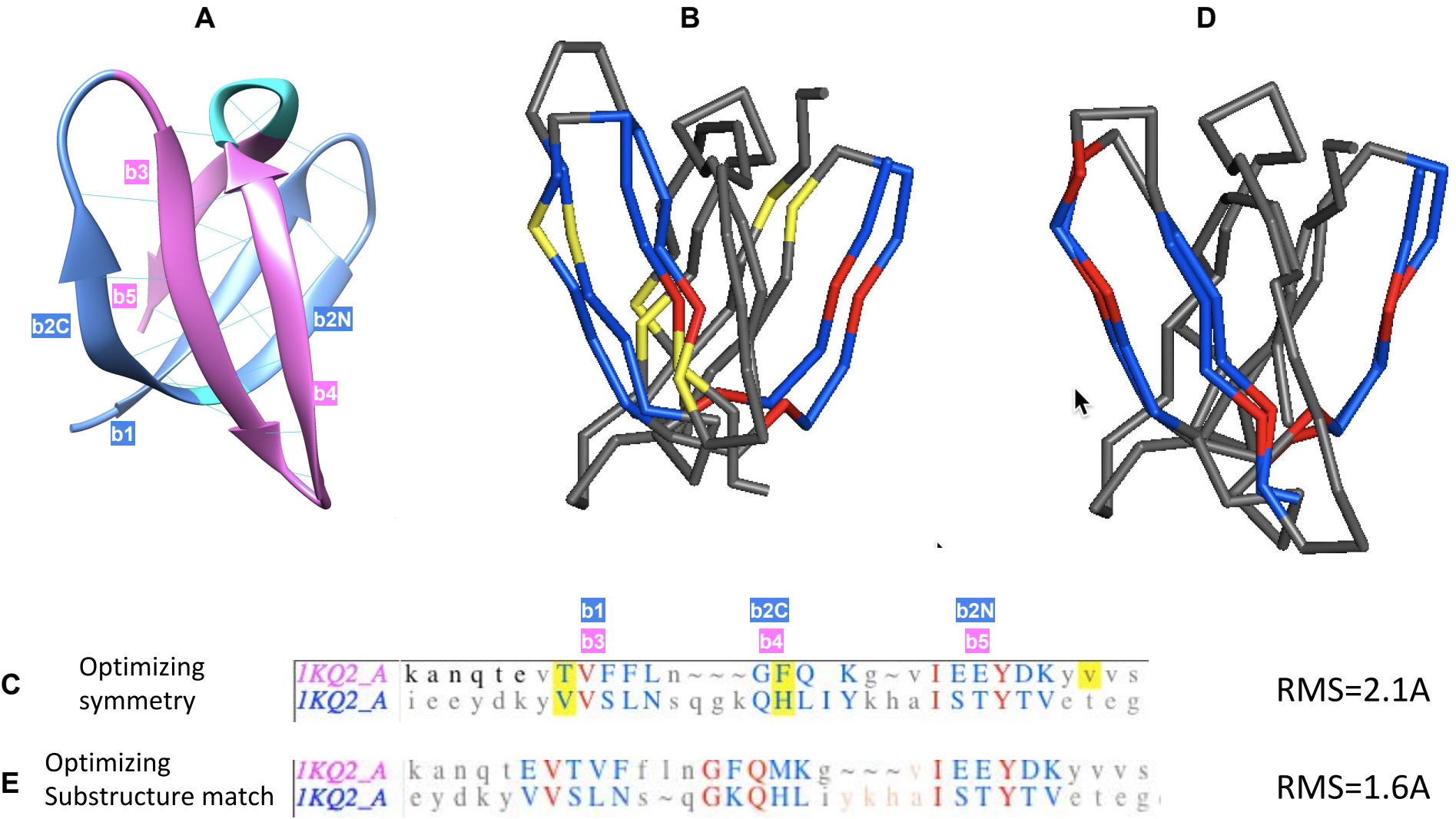


Figure S4

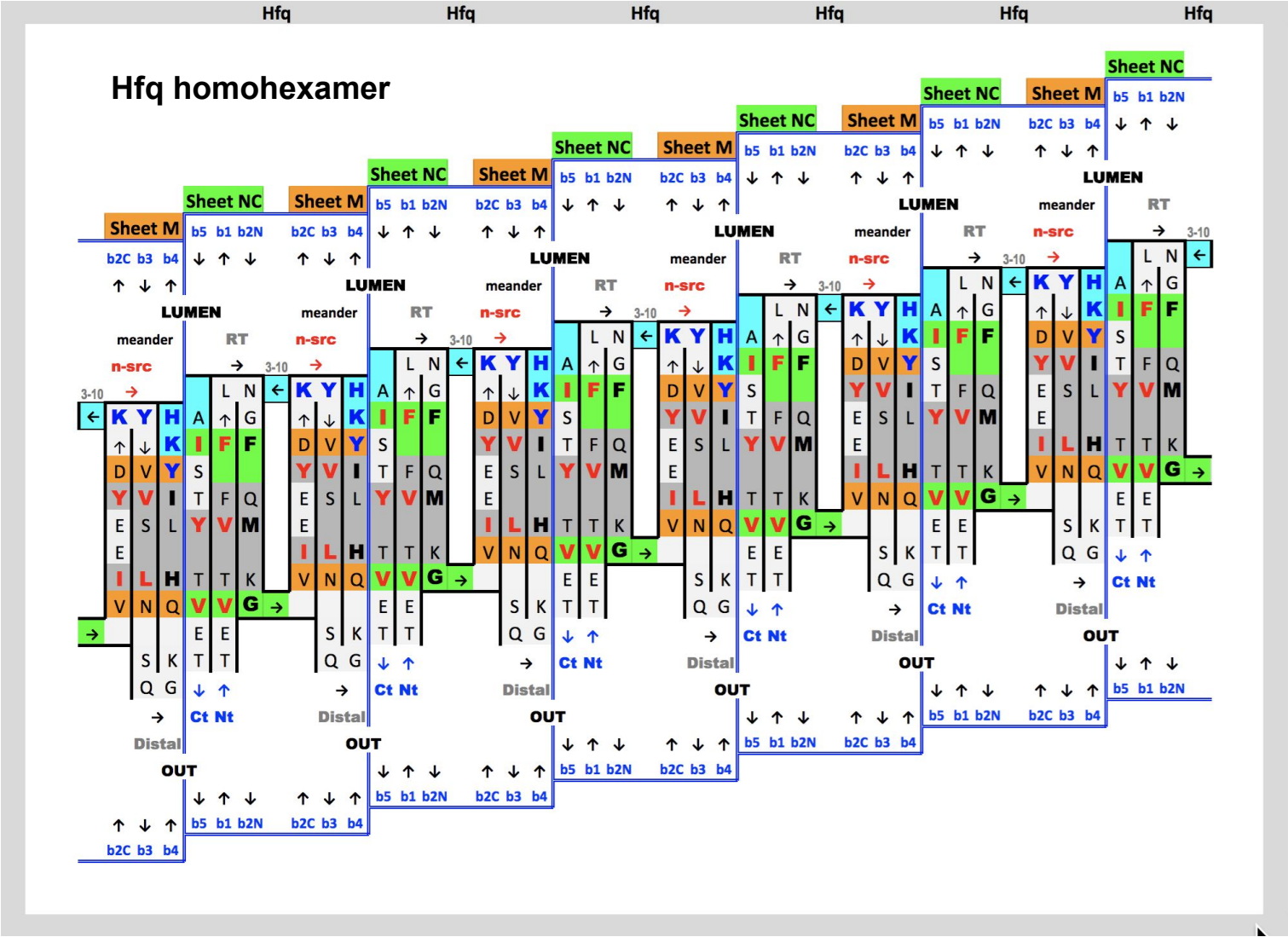
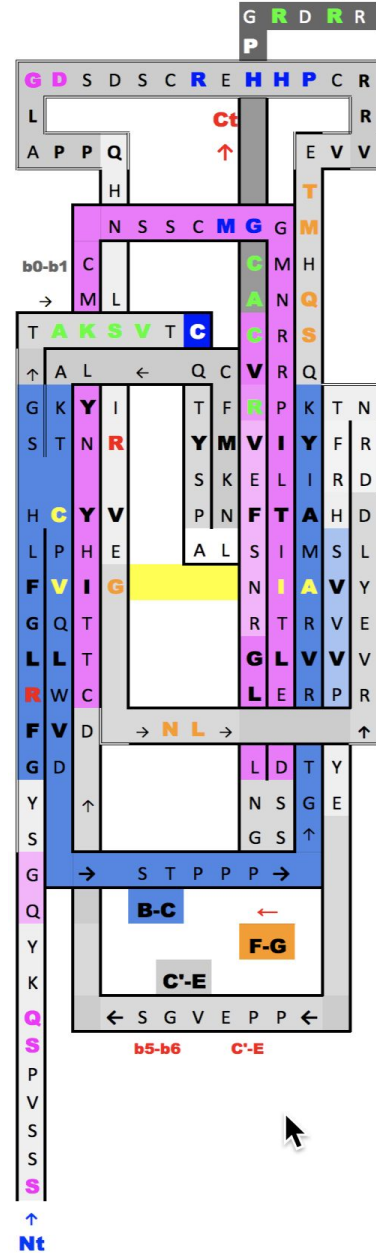
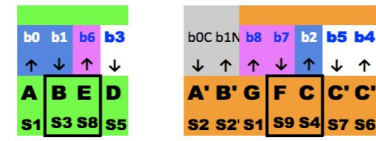
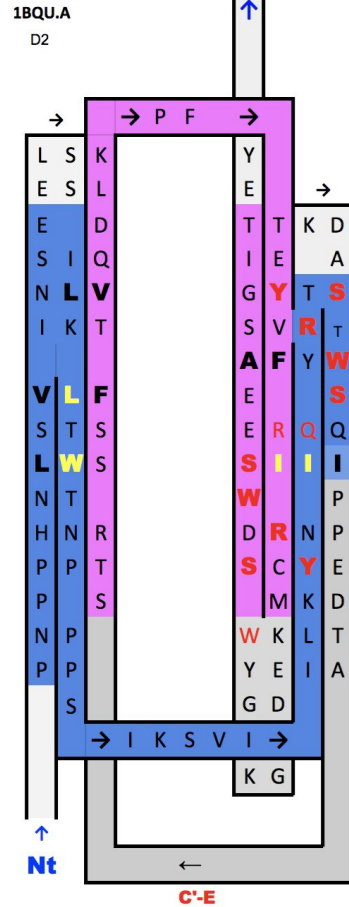
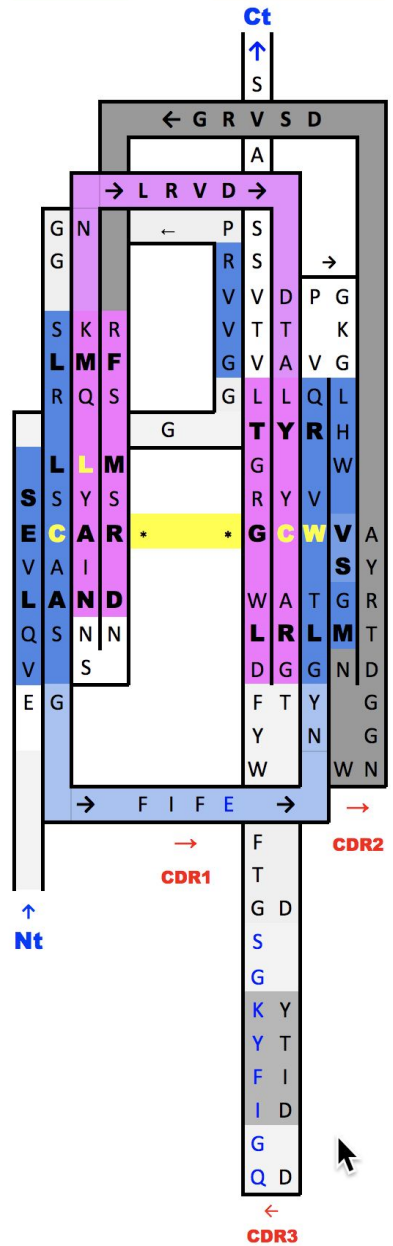
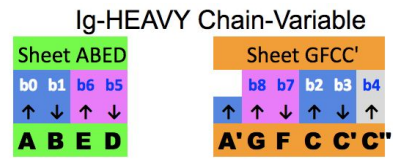


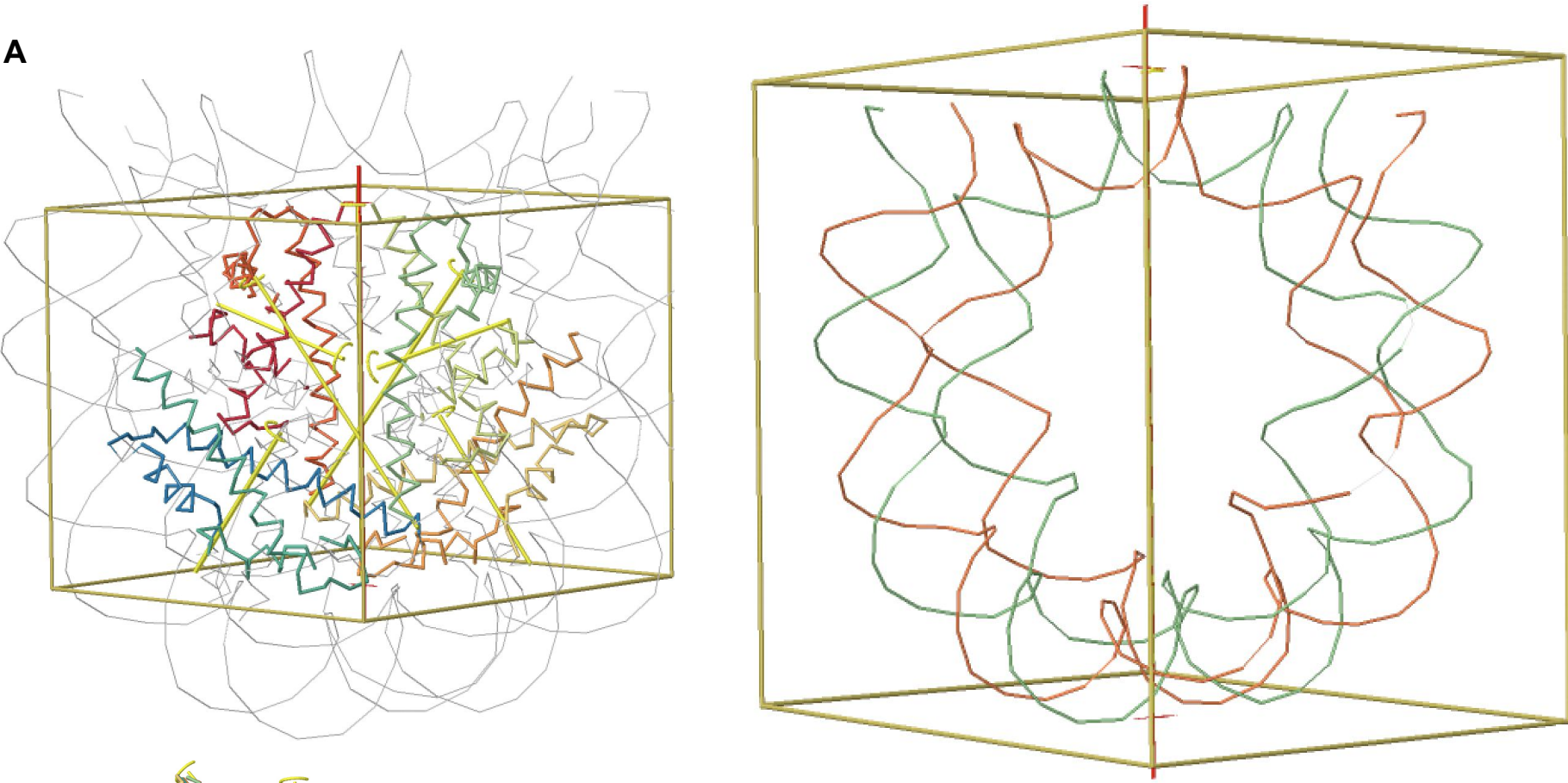
Figure S5



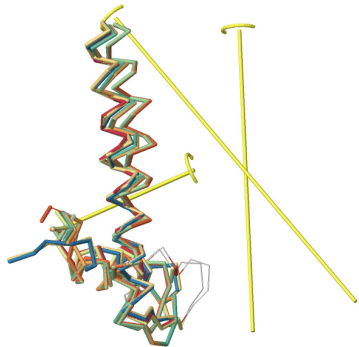
[iCn3D](http://iCn3D.com)

Figure S6

**A**



**B**



**C**

RMSD 2.68A

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148:J TCAATATCCACCTGCAGATTCTACCAAAAGTGTATTTGGAAACTGCTCCATCAAAA g GCATGTTTCAGCGG 217:J

71:I  GAATTCGCTGAACATGCCCTTTTGA t GGAGCAGTTTCCAAATACACTTTTGGTAGAATCTGCAGGTGGAT 140:I
218:J AATTCGCTGAACATGCCCTTTTGTAT - GGAGCAGTTTCCAAATACACTTTTGGTAGAATCTGCAGGTGGAT 286:J

141:I  ATTGAT 146:I
287:J  ATTGAT 292:J
    
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