

The NMR Task Force of the worldwide PDB

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The worldwide PDB



wwPDB was founded in 2003; members are:

- RCSB PDB (Rutgers Un. & UC San Diego)
- EBI – MSD (European Bioinformatics Inst.
Cambridge, UK)
- PDBj (Protein Data Bank Japan, Osaka)
- BMRB (BioMagResBank, Madison, Wisconsin,
since 2005)



About the NMR Task Force

- Established in 1999 shortly after the transition of the PBD from Brookhaven to the RCSB (renewed in 2005)
- Represents the biomolecular NMR community and provides advice to the wwPBD on NMR related issues
- Recent meetings held in Keystone (January, 2006), Goettingen (August, 2006), and Snowbird (January, 2007)
- Made recommendations on nomenclature, representation of NMR structures, and deposition of experimental NMR data

Members of the NMR Task Force

- Rob Kaptein (chair)
- Ad Bax
- Marc Baldus
- Andy Byrd
- Marius Clore
- Michael Nilges
- Peter Domaille
- Juli Feigon
- Peter Guentert
- Ernest Laue
- Guy Montelione
- Peter Wright

Ex-Officio:

- Helen Berman (PDB)
- Judy Flippen-Andersen (PDB)
- Monica Sundd (PDB)
- John Markley (BMRB)
- Eldon Ulrich (BMRB)
- Wim Vranken (MSD-EBI)
- Hideo Akutsu (PDBj)

NMR Task Force: discussion topics

- Data submission
 - One-stop deposition
 - What is required from depositors?
 - What is recommended?
 - Experimental NMR data (PDB-EXTRACT)
- Atom nomenclature (PDB vs. IUPAC)
- Data conversion
 - Formats (mmCIF, NMRSTAR)
 - Data dictionaries (BMRB and CCPN projects)
 - Data conversion routines e.g. AQUA

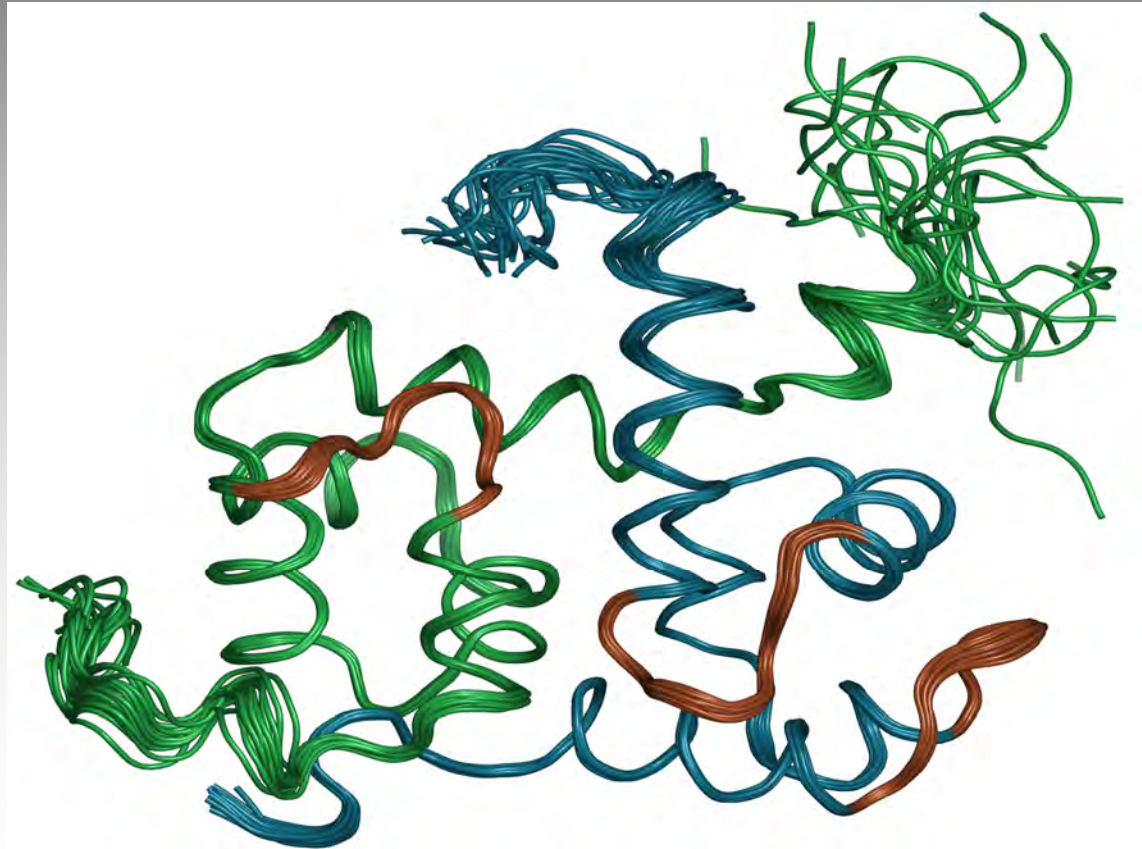
NMR Task Force: discussion topics cont'd

- Structure representation
 - How to deal with ensembles of structures?
 - Representative structure
 - Coordinate uncertainty (rmsd, other?)
 - Ordered vs. disordered regions

Ordered vs. disordered regions

Human ERCC1/XPF
heterodimer

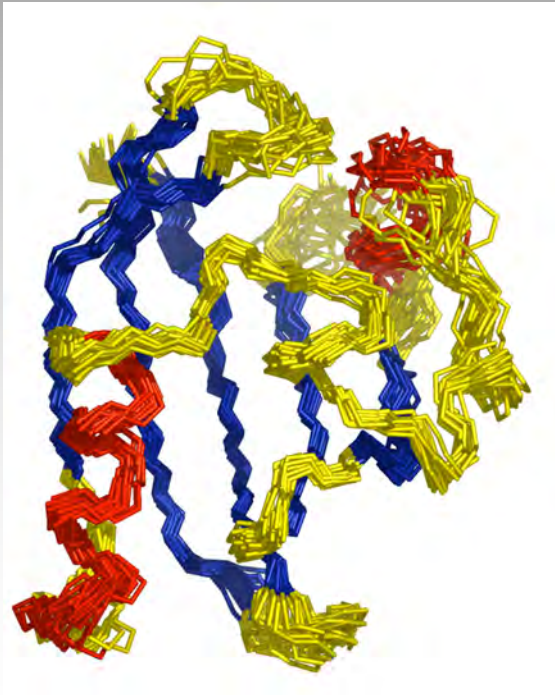
(DNA repair protein)



Ordered vs. disordered regions (2)

Photoactive Yellow Protein

dark



light



Recent recommendations to wwPDB

- H-atom nomenclature
 - use IUPAC (1998) instead of “PDB”
brings PDB in line with BMRB
- Representation of NMR structures
 - submitter defines regions that are well-defined or not well-defined (on residue and atom basis)
- Representative structure (from ensemble)
 - conformer closest to the average
 - minimized averaged structure
 - conformer with lowest energy

Recent recommendations to wwPDB cont'd

- Deposition of experimental NMR data
 - PDB should support and user is recommended to submit:
 - assigned chemical shift values
 - scalar and/or residual dipolar coupling data
 - restraint list for final structure calculation
 - NOESY peak lists with intensities
 - raw FID data for NOESY spectra

Acta Cryst. F discussion points

- Update IUPAC 1998 recommendations
- Validation issues
- Role of journal vs. database

Apart from coordinates what supporting data must be deposited in the PDB / BMRB?

For instance:

- chemical shifts
- scalar and residual couplings
- restraint lists