Group-A

Q1 current best practice

- Starting from some common molecular representation with bond orders, configuration on chiral centers (e.g. ChemDraw, SMILES)
- NEW! PDB should become resource for refinement dictionary
- PDB-provided dictionary should include citable sources
- Documentation with dictionary: source, date, alerts for chiral ambiguity, tautomers
- In case of ambiguities (unspecified chiral center(s), tautomers): produce all allowable options, make user consider all options
- Add annotation, such as unknown configuration
- ALLOW ligand IDs with > 3 characters
- Include all hydrogens if possible (include zero occupancy hydrogen)

Q2 Validation (see BUSTER report as a good template)

- Include density map (standard multiple orientations)
- NEW! Capture coeffs of depositor's final "2Fo-Fc", "Fo-Fc" maps
- Archive and make available depositor's map coefficients (from the refinement output mtz)
- Use correlation between depositor's and standard map as diagnostic statistic
- For journal review to see map
- NEW! Atom level RSR, RSCC
- Provide possible solution to fix problem(s)
- Ligand geometry vs both depositor's and PDB "Best Practices" dictionaries
- Do not include "strain energy" at this time, but do revisit inclusion in future

Q3 Information required for PDB depositions

- (a), (b), (d), (e) agreed, see Q1, Q2
- (c) not so much.
- (f) yes. But based on "standard" map, at atom level. see Q2
- Structure/segment/chain/residue/atom-level annotations
- Q == 0 "feels" different from "not observed"
- Allow alternative models (as opposed to just alternate conformers)

Q4

- Non-crystallographer's introduction to Validation Report on page 1.
 - "How to read this report?" same on each report
- Request to PDB: contact dictionary software developers to include all references inside dictionary file

Q5

- Generate reports on all structures
- Regeneration of reports as new features become available, and as archive expands
- Replace "obsolete" with versions

Q6 Ligand chemistry

- Agreed. See Q1, Q2.
- We agree on importance of hydrogen atoms in refinement.
- If observed ligand differs from added chemical component, chemical description of added component is required in addition to description of observed ligand

Additional Questions

Facilitate batch PDB depositions

- Introduce atom comments, make graphical programs display comments (just like any other string such as atom label)
- H atoms (all resolutions, but zero occupancy unless resolution demands it)
- Experimental phases if trouble with ligand, radiation damage. Biology view
- Capture what is inside. (lig dic. Map.) CC, rsr as property of atoms, not residues. It is important that ligand interacts with the sidechain. How to get the correct ligand lib?

- Idealized dic is better way? Standardize proct. for validation. Geometry vs density, remarks in pdb, what was the ligands in the pocket? Provide map around ligand and the environment.
- Mandatory annotation field for ligands
 - Fit to density
 - Plausibility of conformation
 - Tautomerism
- Show ligand hydrogens
- His/Asn/Gln-flip tool for ligands

- Deposit dictionary for ligand
- PDB provides "Grade"-like server
- Add refinement restraints to component dictionary entry
- Look at Buster Report for inspiration of visualized validation
- Did Mogul pick correct reference structures for Z calculations?
- Not only show outliers, also suggest how to fix them
- Offer QM optimizations

- Clearly separated from crystal structure, link value-added models ("computationally enhanced")
- Build Wiki on top of PDB archive (would even address question 5.)
- Introduce versioning

- Q4:
- Disordered ligand, density?, occupancy?
 Pseudo-symmetry? (50% split?), missing part of ligand. (NMR over crystal)

• Q4; (batch deposition), provide map (2Fo-Fc, Fo-Fc, omit),

More mandatory annotation of ligand

Information about how samples were prepared

Ligand definition (dictionary used in refinement)

Additional refinement restraints

Ligand quality

Fit quality

Irregular conformation

Intermolecular interaction

Provide example and control vocabularies in deposition system such as

Ligand exists but not seen in density

Ligand exists but only seen partially in density

Ligand exists and seen clearly in density

Better way to deliver annotation data (other than REMARK)

Make user aware of missing data

Make user aware if interpretation of structural data conflicts with biological view

Work with graphical software developers to better display data

Include all hydrogens if possible (include zero occupancy hydrogen)

Help refinement

Help to identify tautomer and chirality

Validation report should

Include density map

For journal review to see map

Atom level RSR

Provide possible solution to fix problem(s)