Red lettering = no response received

Purple highlighting = response, not sure if satisfactory

Black lettering = My problem and I have found the solution

Blue lettering = comment not yet submitted

Green lettering = response received - fixed

Yellow highlighting = need to check out the comment further before submitting

Comments - 8/22/2014

1. There seems to be a whole missing page at the beginning where people

upload the constraints files. They were to be asked for a sequence file,

if they used AMBER. Has this been changed?

Not problem - Found how it works -

2. After starting a deposition and getting in and filling out a lot of

information, when I clicked on the 'Re-upload files' button, I am now in

an X-ray deposition and cannot proceed without providing a structure

factor file. This might be some kind of timing problem. I had actually clicked on ‘Re-upload files’ but it was taking a long time to refresh so I clicked on ‘Upload summary’. That also was taking sometime so I again clicked on ‘Re-upload files’ and waited and when the system refreshed I was in the X-ray UI. After starting a new deposition completely, I can now click on these two items and I am staying in the NMR UI.

3. Even after logging out and reentering the DepUI using my ID and

password, I end up in an X-ray deposition.

Comments before getting kicked into the X-ray UI:

4. In NMR samples section, 'concentration value' was not mandatory and

'Concentration value uncertainty' possibly should be mandatory. The

IUPAC definitions on how to report isotopic labeling should be used in

the example.

A list is there, but text definitions are at the top. The IUPAC format should be used and more examples can be provided, if you would like.

5. In NMR samples section, if a drop down list is not provided with

common names for compounds this field will become very disorganized.

Also useful to link to the molecule names in the Macromolecule section

so that consistent names for molecules are entered through out the

deposition - a list from BMRB was provided.

6. In NMR data collection, by auto-filling 'Sample Label' will likely

get many mismatches that may not make sense (i.e., 15N sample used for

HNCO experiment).

7. In NMR data collection, very useful to have a drop down list of

common NMR experiment names - a list from BMRB was provided.

Not problem - I need to remember how the interface works

8. In NMR software, author information can be linked to software

packages and be automatically filled in - BMRB can provide a list

9. In the chemical shift references section, the option to have all the

fields filled in with IUPAC values is at the bottom of the table. I

would suggest putting this option at the top of the table as being at

the bottom many users might not see the option and be frustrated

spending the time filling in all of the fields. I believe 'Referencing

method, Referencing Type, and Indirect ratio should be mandatory.

10. Chemical Shift connection does not seem to be working.

11. In NMR software, Is Software name field supposed to be a drop down list?

12. Mac/Safari - drop down lists do not seem to appear on first try always (need to do more testing)

13. In the chemical shift references section, for Atom type would be useful to have most common ones at the top. Also type for deuterium is really H and the isotope number is 2. This consistent with using N with 15 and N with 14, etc. Also, people do use tritium NMR so having H with 3 would be useful.

14. In several of the pull down list where BMRB supplied the enumerations, the ‘$’ have not been replaced with a comma.

15. In NMR refinement, looks like all of the NMR conformer statistics fields need to be made mandatory. The example for Representative conformer needs to be made ‘1’. (check when starting new deposition)

16. In NMR refinement, Conformer selection criterium and Representative conformer selection criterium should have open enumerations. These enumerations exist and were agreed on with the PDB. The current text examples do not provide a controlled vocabulary.

17. In natural source, seems like ‘heart’ could be either an organ or a tissue. Is there a better example?

18. Does not appear that anything is mandatory in sample conditions. Check with new deposition

19. BMRB needs to begin receiving test pdbx files from the NMR DepUI as soon as possible so we can develop the software required to complete an NMR-STAR file and go back to the depositors for further information. The files BMRB receives from the wwPDB DepUI will differ in many significant ways in information content from what is generated from ADIT-NMR, including the description of the molecular assembly studied, labels for samples, sample conditions, and most other save frames.

9/4/2014 test results:

Just running a brief test of the system and these are the results:   
  
1. Using Safari Version 7.0.6 (9537.78.2) on a Mac running OSX v10.9.4   
2. D\_8000200263   
  
Issues:   
General:   
1. I thought harvesting data from an NMR-STAR file was in the specs. No information was harvested from the NMR-STAR file uploaded in this case.   
2. System did not recognize a full NMR-STAR file - gave a warning message that 'file does not look right'   
3. I was able to delete the chemical shift file and the system still presented the 'Continue deposition' button, did not warn that there was not a chemical shift file present, and when I clicked on the 'Continue deposition' button the system seems to have now hung with the gear image showing and the words "Still processing Upload type processed".   
4. Under Admin, Grant information has a green check mark even though no information was provided. Is this intended to have 'N' checked by default so depositors will not fill it out?   
  
Citation information:   
1. Example for Title is X-ray specific   
  
NMR Samples:   
1. Enumerations for 'Molecule common name' in samples do not appear   
2. Enumerations for Isotopic labeling still contain text versions that are not IUPAC consistent along with the IUPAC examples   
3. Mouse over examples for isotopic labeling are not IUPAC consistent   
4. Enumerations for Concentration value units are not present   
5. Mouse over example for Concentration value units is not a commonly used value   
6. Not clear why examples for Sample label includes an underscore. Is this required for some reason?   
  
NMR data collection:   
1. Sample label field appears malformed and clicking on the pulldown does not provide a list of the sample labels. Will not accept typing in a '1' or other value.   
2. Sample Conditions has same problem as Sample Label   
3. Picky but some field names are fully capitalized and others are not throughout the system (i.e. Field strength versus Sample State)

**10/23/2014 test results:**

Tested using a Mac running Yosemite and Safari

Files: 1LKN-2.pdb, 5357\_cs\_loop\_only\_31.str, 5357\_cs\_loop\_missing\_tag\_31.str

1. Grant information seems to default to 'no' and therefore the section is marked with a green check and most users will not correctly fill in this section.

2. In Release status - Related entries, the Database ID field seemed to be populated with an unknown value. None of the other related fields were populated.

3. Entry author names extracted from PDB file were all presented as lower case, 'northeast Structural Genomics ...', while citation author names were presented in all upper case.

4. The NMR sample view was malformed with the left hand frame overlapping the data entry frame.

5. In NMR sample view, 'Concentration value error' tag is missing?

6. In NMR sample view - sample conditions, the pH units drop down list should include 'pH\*'. This the correct units for the condition when a pH electrode filled with H2O is used to measure a sample that is in D2O.

7. Software name is not linked to authors for automatic fill in. I think this was a feature requested earlier.

8. Because the interface at times has a drop down list and other times has auto fill-in it is difficult to tell what is working and what is not. But, software tasks does not seem to have the short list of enumerations.

9. In Chemical shift referencing, if IUPAC referencing is selected the reference method default should be 'internal' for all nuclei defined.

10. Pop ups are generally annoying. When they appear, they often seem to obscure the field that needs to be filled in and only disappear at times when the cursor is moved outside the browser window. For the Chemical shift referencing section, clicking on IUPAC referencing seemed to bring up all of the pop ups (mouse overs) and the page became a transparent dark. This went away when the mouse was moved outside of the browser window.

11. In Constraints section, the 'Software file format' field did not seem to have a drop down or be enumerated.