

ACA 2007, Salt Lake City UT

Workshop WK.02

Room 259, Salt Palace Conference Center



**Validation of Macromolecular Structures:
Updating Standards for Publication of NMR Structures
in an IUCr Journal**

Howard Einspahr

Editor, *Acta Crystallographica* Section F

hmeinspahr@yahoo.com



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Workshop WK.02: Organizers



J. Mitchell Guss

Manfred Weiss, Luciano Mueller

Gaetano Montelione, John Markley



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Workshop WK.02: Schedule



09:00 AM	Introduction: The Purpose of Publication Standards.	H. Einspahr
09:30 AM	The NMR Task Force of the Worldwide PDB.	R. Kaptein
10:00 AM	BioMagResBank (BMRB) Data Deposition and Entry Annotation Requirements.	E. Ulrich
10:30 AM	Coffee Break	
11:00 AM	Standards for Crystallographic Publishing.	M. Weiss
11:30 AM	Evaluating Protein Structures Determined by Structural Genomics Consortia.	J. Aramini
12:00 PM	Discussions & Breakout Assignments	H. Einspahr
12:15 PM	Lunch	
01:00 PM	Breakouts: Discussions & Drafting Recommendations	
02:30 PM	Break	
03:00 PM	Presentations of Draft Recommendations & Discussions	
04:30 PM	Adjourn	



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Workshop WK.02: Origin



Lytle *et al.* (2006), “Solution structure of *Arabidopsis thaliana* protein At5g39720.1, a member of the AIG2-like protein family.”
Acta Crystallogr. **F62**, 490-493.

Standards: Markely *et al.* (1998) IUPAC Recommendations.

Referees used current standards: 1998 IUPAC Recommendations needed update.

The NMR Task Force of the wwPDB

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Why have standards?

To facilitate judgments of veracity of results.

To assure archival access to results.



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Judging Results: Four Cornerstones

Assurance of peers

Reproducibility

Consistency with experimental data

Consistency with existing knowledge



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Workshop WK.02: Assurance of peers



Assurance takes many forms:

Quality of refereeing and editing

Citations metrics

Prestige, selectivity

Popularity, subscriptions

Journal focus

Other factors

Not within our scope today:

***Acta Cryst.* are journals of record for our science.**



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Workshop WK.02: Reproducibility



A result may be discounted if:

repeating the experiment fails to reproduce the result.

Journals must therefore assure that:

papers they publish provide sufficient detail to support repetition of experiments to test results.

Universal requirement applying to all scientific journals.



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Consistency with experimental data

Consistency with existing knowledge



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Workshop WK.02: Archives



Assuring archival access to results:

**Publication in journals should assure access
in perpetuity.**

**Publication in journals should facilitate deposition
of complete record in the database.**



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Workshop WK.02: Standards



Standards evolve:

Tag remnants

Synchrotron data at 100°K

Standard errors of lattice constants



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Workshop WK.02: Actabiostandards



Updating crystallographic standards for Acta Cryst. D & F

[“journals.iucr.org/f/services/structuralcommunications/requirements”](http://journals.iucr.org/f/services/structuralcommunications/requirements)

E-mail discussions of matters arising

Focus and drafting of updates by leadership

Standards and updates established by consensus



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IUCr and its Journals Editors take the matter of standards seriously

IUCr Recommendations for the Presentation of Crystal Structures of Biological Macromolecules



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Workshop WK.02: Objectives



For publication in IUCr journals:
standards for NMR structure papers as stringent as
standards maintained for crystal structure papers.

Journals of record

Reproducible

Results consistent with experiments

Results consistent with current knowledge

Proper deposition



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Workshop WK.02: Charge(s)



Relative to 1998 IUPAC standards -

Reproducibility: Additional sample and data collection specifications.

Ex: protein concentration, buffer composition, [TFE], temperature

Data quality: Improvements in best practices, measures of quality

Experiment: Improved correlations of results and experimental data

Ex: analyses of assignments, constraint violations, RPF

Validation: Improved comparisons to accepted structural principles

Ex: Z-scores, 2006 NESG requirements

Deposition: NMR data that should be deposited

Ex: local analyses of precision along sequence, clashes

Differentiating good, average and poor structures



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Rob Kaptein

**The NMR Task Force of the
Worldwide PDB**



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