ing. However, in a comprehensive collection of structural data sets, such as in a public structural database, it might be possible to identify particular data items that could be used for weighting individual data sets when the database is being 'mined' for particular patterns or characteristic values. It will be interesting to see whether a consensus emerges on what items would be suitable. It is clear that reliance on a single indicator will not be appropriate for sophisticated studies. The old idea that a structure could be classed as 'good' or 'bad' on the basis of its final residual *R* factor alone has long been abandoned, but it may be possible to stipulate criteria for a set of interrelated data items and use these to filter specific information from a database.

5.7.2.7. Submission and review

When an author has previewed and checked the contents of the CIF and has made the changes suggested by a careful study of the preprint and the *checkcif* report, the article may finally be submitted to *Acta Cryst. C* or *E* by file upload over the web. Other files completing or supporting the submission are also transferred to the editorial office at this time. These include structure-factor or powder profile listings for each structure, figures and chemical diagrams, and sometimes other supplementary documents. Structure-factor listings are supplied in CIF format. Figures may be in one of a number of standard graphics file formats, and at the moment have to be uploaded as separate files. Future extensions to CIF, perhaps following the imgCIF approach, may allow all the items needed to submit an article, including figures, to be prepared as a single file.

When all the files have arrived at the editorial office, a review document is generated that can be sent to the referees. This document contains: the text and tables of the article that will appear in the final publication, but laid out in a more open style suitable for annotation by hand; tables of atomic positions and geometry (containing all the data in the CIF, not just the subset that has been selected for displaying in the published article); certain fields from the CIF that are not normally printed but which may contain details of the way in which the experiment was carried out (these fields might have been completed manually or by the software controlling the experiment); the figures and other supplementary documents; and a print-out of the report from a final *checkcif* cycle, including a displacement-ellipsoid plot of the molecule in a minimal-overlap least-squares plane view. This composite document provides the information that a referee will typically want to consider in a compact and convenient form. Because the CIF is so highly structured, producing this review document is in most cases entirely automatic. The complete CIF as submitted by the author and the experimental data are also made available to the reviewer.

If revisions are requested, authors may upload modified files. The generation of revised versions of an article is also largely automatic.

5.7.2.8. Publication

When the final version of a CIF for *Acta Cryst. C* or *E* is approved, the article is ready for publication. Once more, the data fields required for the published article are extracted from the CIF and sorted. If the author has asked for additional items to be printed by using `_publ_manuscript_incl_extra_item`, these also are extracted. The result is transformed to a file suitable for processing by typesetting software. For *Acta Cryst. C* this was originally a TEX file; now a further transformation generates an SGML file that conforms to the document type definition (DTD) common to all IUCr journals. This allows not only typesetting and printing, but also the generation of the HTML for the navigable online version of the article, and the extraction of metadata for building online tables of contents and for supplying to bibliographic databases.

The conventional published article then appears in a monthly issue. Each article is still similar in style to the type of structure report published in journals for decades, although tables of atomic positions and geometric data are not usually displayed now, since these data are so readily available from the online article.

The online version of the journal, however, presents a much more information-rich version of the article. Each article is generally available in the form of a PDF file, suitable for downloading and offline printing. There is also an HTML version of the same text, and this version has rich internal links that make it easy to scroll back and forth through the article, jump to specific sections and see figures in low-resolution thumbnail or high-resolution views. The reference list contains links to the articles that are cited. There may also be links to related records in chemical or crystal structure databases. The reader may also download the experimental data and any supplementary documents associated with the article. As mentioned above, for *Acta Cryst. E* a summary of the check report is also available.

Finally, the structural data may be downloaded directly in CIF format. The CIF is presented in two ways. If a reader follows one link in a web browser, the file is interpreted simply as a text file and appears as a simple listing in the browser window, from which it may be printed or saved to disk. However, if the reader follows the other link, the CIF is transmitted to the browser with a header declaring its MIME type (Freed & Borenstein, 1996) as 'chemical/x-cif'. This is one of several MIME types registered for particular presentations of chemistry-related content by Rzepa & Murray-Rust (1998). The reader may then configure a web browser to respond in a specific way to content tagged with this MIME type; typically a helper application such as a molecular visualizer [*e.g. Mercury* (Bruno *et al.*, 2002)] will be launched that allows three-dimensional visualization and manipulation of the molecular or crystal structure.

When an article has been published in *Acta Cryst. C* or *E*, the CIF is transferred to the relevant public structural databases. Thus, the transcription errors that used to cause so many problems for data harvesters are completely avoided and one of the initial goals of the CIF project is achieved: uncorrupted data transfer from diffractometer, through publication, to a final repository.

Because *Acta Cryst. C* and *E* handle almost exclusively the publication of structure reports, the editorial workflow based on CIF lends itself to a very high level of automation and the journals are produced efficiently and on short timescales. Routine refereeing of structures is made very easy by the provision of checking reports, and the universal use of e-mail and web file transfer means that production times can be very fast.

5.7.3. CIF and other journals

Not every journal will be able to benefit to the same extent from the handling of CIFs. For many journals, structure reports will be secondary to the main purpose of most articles, and CIF data will more usually be deposited as supplementary or supporting documents, while only a summary (if anything) of the structure will be reported in the article body.

Nevertheless, the ability to extract data from CIFs automatically and the ability of much crystallographic software to read CIFs mean that even journals that do not specialize in crystallography can provide a production stream that includes careful checking of crystal structure data. The IUCr continues to develop *checkcif* as