(*a*) Material common to the article as a whole:
- (i) title and authors;
- (ii) synopsis and/or abstract;
- (iii) comment section;
- (iv) acknowledgements;
- (v) references.

(*b*) Material relevant to each structure:
- (i) description of the experimental apparatus;
- (ii) description of the settings and environmental conditions for the experiment;
- (iii) experimental data, typically a list of measured and calculated structure factors for a single-crystal X-ray structure determination, or powder diffraction data with measured and calculated powder diffraction profiles;
- (iv) information about the compound, including source, preparation and formula;
- (v) summary of structure solution and refinement;
- (vi) coordinates of atomic sites, their elemental composition, occupancy, anisotropic displacement parameters, whether they are in part of the structure affected by positional disorder, and information about their refinement restraints;
- (vii) selected geometrical data.

(*c*) Graphical illustrations:
- (i) chemical structural diagrams;
- (ii) chemical diagrams of reaction pathways, tautomerism, bond properties *etc.*;
- (iii) crystallographic displacement-ellipsoid diagrams;
- (iv) crystallographic packing diagrams;
- (v) other graphs, plots or images.

Different journals will have different requirements for the arrangement of these items. For example, at the time of publication (2005), *Acta Crystallographica* requires that diffraction data (structure factors or Rietveld refinement profiles) are provided as supplementary information in separate files from that containing the body of the paper. This policy originated in the early days of network file transfer where relatively large files of experimental data could be transferred only with difficulty. This is less of a practical constraint now, and a case could be made for including the experimental results as an integral part of a single submission file, especially since there is still no formal mechanism in the core CIF dictionary to enforce an unambiguous connection between separate data blocks containing related data.

There is also not at present a standard way to include graphics within a CIF. The mechanisms of the imgCIF dictionary (Chapter 3.7) offer a possible approach to this problem. It is also possible to envisage the automated generation of views of the structure directly from the numerical data in the CIF. Three-dimensional ellipsoid plots are routinely generated from CIFs submitted to *Acta Crystallographica* for use in the review process and incomplete categories of data names exist in the core dictionary for the representation of two-dimensional diagrams of chemical connectivity. At present, however, neither of these is sufficiently well developed to generate publication-quality graphics in different orientations and styles as preferred by an author.

A journal may provide a *request list* of the data items that it considers recommended or mandatory. The request list for *Acta Cryst. C* and *E* is given in Appendix 5.7.1. An author can test a file intended for publication against a request list with a general-purpose CIF parsing tool such as *cif2cif* (Bernstein, 1998) or *QUASAR* (Hall & Sievers, 1993) (Chapter 5.3). Different request lists may be provided for different kinds of experiments, such as for powder diffraction experiments or for single-crystal studies using area detectors.

Note that an author always has the freedom to include additional data items in a CIF; the journal will exercise its own policy for the handling of data items not specified in its public request lists. The PUBL_MANUSCRIPT_INCL category available in the CIF core dictionary provides a mechanism for requesting the publication of data items that are not normally published by the journal (see Sections 5.7.2.3 and 3.2.5.5).

5.7.2.2. Reporting multiple structures and using templates

In CIF format, a data name cannot be repeated within a data block. Therefore, each structure reported in a CIF must occupy a separate data block. A journal might request a separate file for each structure; in the case of *Acta Cryst. C*, however, a single file for the entire submission is required. This file therefore contains several data blocks if the article reports several structures. The data-block codes (*i.e.* the changeable *label* part of a data-block header `data_label`) have no particular significance and are usually chosen by the authors as meaningful identifiers within their own collection of structures. However, each block code may be used *once only* in any individual file.

If an article reports only one structure, the author can include the general text of the article in the same data block that records the structure or in a separate data block. If the file already contains several data blocks (because it reports multiple structures), using a distinct data block for the text of the article is the most natural way of organizing the contents of the file. Fig. 5.7.2.1 shows the structure of a CIF that describes several structures.

Authors often have one or more local template data blocks that already include standard information about their contact details and details of the experiment. These templates may then be added or merged into the data blocks reporting the structures. Several standard crystallographic software packages include programs for merging CIF templates; one of the best known and most widespread is *SHELX97* (Sheldrick, 1997).

Some authors also use programmable macro facilities within commercial word-processing packages to achieve the same purpose. The IUCr application *printCIF for Word* (Westrip, 2004) extends this approach by creating a custom editing and formatting environment within Microsoft *Word*. These are very helpful utilities for authors who are not CIF experts. However, they are restricted to particular operating systems or software environments and are thus not universally available.

The program *enCIFer* (Allen *et al.*, 2004) provides facilities for importing templates and external files, and for adding and maintaining standard information about the authors of a CIF. It provides alternative representations of a CIF as a text file and as a collection of containers and object fields, and provides a great deal of support for authors who are not familiar with the technical details of the CIF format. *enCIFer* and other useful text-editing programs are described in Chapter 5.3.

5.7.2.3. Adding extra information to an article

An article for publication in *Acta Cryst. C* or *E* is built from a standard request list of CIF data items. Among the items included in this list are ones that describe molecular geometry: bond and contact distances, bond angles and torsion angles. In most cases, unexceptional values of these are not worth displaying (particularly as *Acta Cryst. C* and *E* make the original CIF data available as supplementary material). Authors can choose which values are to be displayed using a 'publication flag'. For example, the category