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The Macromolecular Crystallographic Information File (mmCIF)

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Introduction

The Protein Data Bank (PDB) format provides a standard representation for macromolecular structure data derived from X-ray diffraction and NMR studies. This representation has served the community well since its inception in the 1970's (Bernstein *et al.*[1]) and a large amount of software that uses this representation has been written. However, it is widely recognized that the current PDB format cannot express adequately the large amount of data (content) associated with a single macromolecular structure and the experiment from which it was derived in a way (context) that is consistent and permits direct comparison with other structure entries. Structure comparison, for such purposes as better understanding biological function, assisting in the solution of new structures, drug design, and structure prediction, becomes increasingly valuable as the number of macromolecular structures continues to grow at a near exponential rate. It could be argued that the description of the required content of a structure submission could be met by additional PDB record types. However, this format does not permit the maintenance of the *automated* level of consistency, accuracy, and reproducibility required for such a large body of data.

A variety of approaches for improved scientific data representation is being explored (IEEE[2]). The approach described here, which has been developed under the auspices of the International Union of Crystallography (IUCr), is to extend the Crystallographic Information File (CIF) data representation used for describing small molecule structures and associated diffraction experiments. This extension is referred to as the macromolecular Crystallographic Information File (mmCIF) and is the subject of this paper. The paper briefly covers the history of mmCIF, similarities to and differences from the PDB format, contents of the mmCIF dictionary, and how to represent structures using mmCIF. The mmCIF home page (mmCIF[3]) contains a historic description of the development of the dictionary, current versions of the dictionary in text and HTML formats, software tools, archives of the mmCIF discussion list, and a detailed on-line tutorial (Bourne[4]).

Background

CIF was developed to describe small molecule organic structures and the crystallographic experiment by the International Union of Crystallography (IUCr) Working Party on Crystallographic Information at the behest of the IUCr Commission on Crystallographic Data and the IUCr Commission on Journals. The result of this effort was a core dictionary of data items[1] sufficient for archiving the small molecule crystallographic experiment and its results (Hall *et al.*[5], IUCr[6]). This core dictionary was adopted by the IUCr at its 1990 Congress in Bordeaux. The format of the small molecule CIF dictionary and the data files based upon that dictionary conform to a restricted version of the Self Defining Text Archive and Retrieval (STAR) representation developed by Hall (Cook and Hall[7], Hall and Spadaccini[8]). STAR permits a data organization that may be understood by analogy with a spoken language (Fig. 1).

[1]A data item refers to a data name and its associated value as will be discussed subsequently.

STAR defines a set of encoding rules similar to saying the English language is comprised of 26 letters. A Dictionary Definition Language (DDL) is defined which uses those rules and which provides a framework from which to define a dictionary of the terms needed by the discipline. Think of the DDL as a computer readable way of declaring that words are made up of arbitrary groups of letters and that words are organized into sentences and paragraphs. The DDL provides a convention for naming and defining data items within the dictionary, declaring specific attributes of those data items, for example, a range of values and the data type, and for declaring relationships between data items. In other words, the DDL defines the format of the dictionary and any new words that are added must conform to that format. Just as words are constantly being added to a language, data items will be added to the dictionaries as the discipline evolves. The STAR encoding rules and the DDL are being used to develop a variety of dictionaries and reference files, for example, the powder diffraction dictionary, the modulated structures dictionary, a file of ideal geometry for amino acids, and an NMR dictionary. This extensibility is attractive since the same basic reading and browsing software (context-based tools) can be used irrespective of the data content. Data files (this paper is an example in our language analogy) are composed of data items found in the dictionaries.

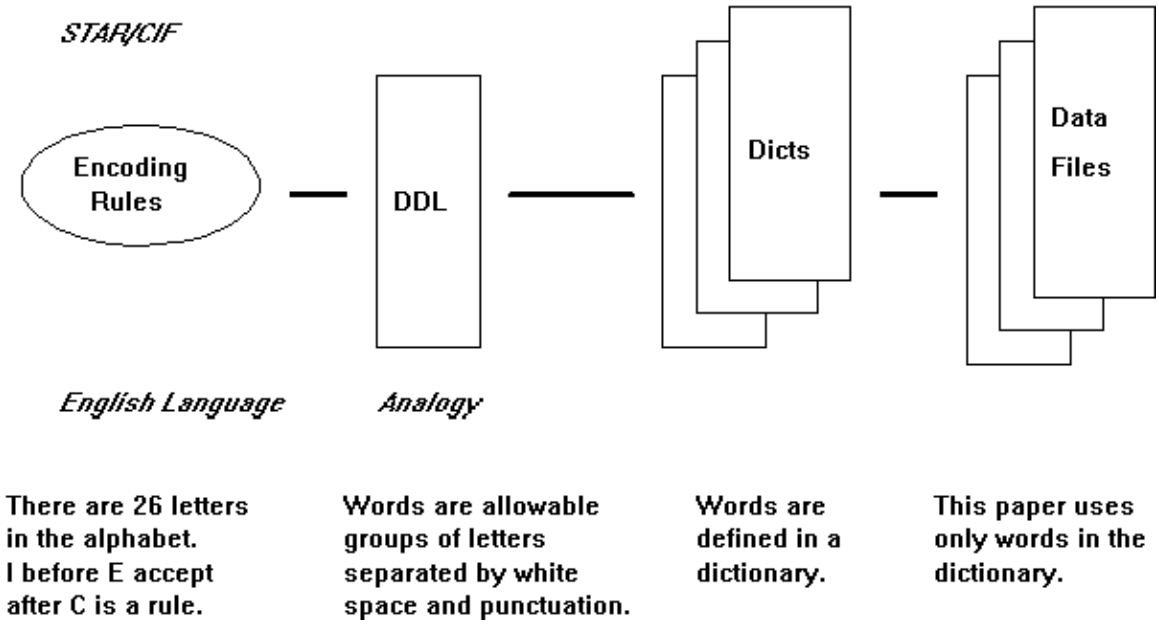


Figure 1 Components of the STAR/CIF data representation and their analogy to a natural language.

In 1990, the IUCr formed a working group to expand the core dictionary to include data items relevant to the macromolecular crystallographic experiment. Version 1.0 of the mmCIF dictionary (Fitzgerald *et al.*[9], mmCIF[3]), which encompasses many data items from the current core dictionary (IUCr[10]), is in the final stage of review by COMCIFs, the IUCr appointed committee overseeing CIF developments. This dictionary has been written using DDL v2.1.1

(Westbrook and Hall[11]), which is significantly enhanced, yet upwardly compatible with DDL v1.4 (IUCr[12]) currently used for the small molecule dictionary.

Considerations in the Development the mmCIF Dictionary

In developing version 1.0 of the mmCIF dictionary we made the following decisions.

- Every field of every PDB record type should be represented by a data item if that PDB field is important for describing the structure, the experiment that was conducted in determining the structure or the revision history of the entry. It is important to note that it is straightforward to convert a mmCIF data file to a PDB file without loss of information since all information is parsable. It is not possible, however, to automate completely the conversion of a PDB file to a mmCIF, since many mmCIF data items either are not present in the PDB file or are present in PDB REMARK records that in some instances cannot be parsed. The content of PDB REMARK records are maintained as separate data items within mmCIF so as to preserve all information, even if that information is not parsable.
- Data items should be defined such that all the information described in the materials and methods section of a structure paper could be referenced. This includes major features of the crystal, the diffraction experiment, phasing methodology, and refinement.
- Data items should be defined such that the biologically active molecule could be described as well as any structural sub-components deemed important by the crystallographer.
- Atomic coordinates should be representable as either orthogonal Ångstrom or fractional.
- Data items should be provided to describe final h,k,l's including those collected at different wavelengths.
- For the most part data items specific to an NMR experiment or modeling study would not be included in version 1.0. Exceptions are the data items that summarize the features of an ensemble of structures and permit the description of each member of the ensemble.
- Crystallographic and non-crystallographic symmetry should be defined.
- A comprehensive set of data items for providing a higher order structure description, for example, to cover supersecondary structure and functional classification, was considered beyond the scope of version 1.0.
- Data items should be present for describing the characteristics and geometry of canonical and non-canonical amino acids, nucleotides, and heterogen groups.
- Data items should be present that permit a detailed description of the chemistry of the component parts of the macromolecule, including the provision for 2-D projections.
- Data items should be present that provide specific pointers from elements of the structure (e.g., the sequence, bound inhibitors) to the appropriate entries in publicly available databases.
- Data items should be present that provide meaningful 3-D views of the structure so as to highlight functional and structural aspects of the macromolecule.

Based on the above, a mmCIF dictionary with approximately 1500 data items (including those data items taken from the small molecule dictionary) was developed. It is not expected that all relevant data items will be present in each mmCIF data file. What data items are mandatory to describe the structure and experiment adequately needs to be decided by community consensus.

Comparing a mmCIF Data File with a PDB File

The format of a mmCIF containing structural data can best be introduced through analogy with the existing PDB format. A PDB file consists of a series of records each identified by a keyword (e.g., HEADER, COMPND) of up to 6 characters. The format and content of fields within a record are dependent on the keyword. A mmCIF, on the other hand, always consists of a series of *name-value* pairs (a data item) defined by STAR, where the data name is preceded by a leading underscore (_) to distinguish it from the data value. Thus, every field in a PDB record is represented in mmCIF by a specific data name. The PDB HEADER record,

```
HEADER    PLANT SEED PROTEIN                      11-OCT-91   1CBN
```

becomes:

```
_struct.entry_id                    '1CBN'
_struct.title                       'PLANT SEED PROTEIN'

_struct_keywords.entry_id           '1CBN'
_struct_keywords.text               'plant seed protein'

_database_2.database_id             ‘PDB’
_database_2.database_code           ‘1CBN’

_database_PDB_rev.rev_num            1
_database_PDB_rev.date_original     ‘1991-10-11’
```

The *name-value* pairing represents a major departure from the PDB file format and has the advantage of providing an explicit reference to each item of data within the data file, rather than having the interpretation left to the software reading the file. The *name* matches an entry in the mmCIF dictionary where characteristics of that data item are explicitly defined. Where multiple values for the same data item exist, the name of the data item or items concerned is declared in a header and the associated values follow in strict rotation. This is a STAR rule referred to as a *loop_* construct. This *loop_* construct is illustrated in the representation of atomic coordinates.

```
 loop_
_atom_site.group_PDB
_atom_site.type_symbol
_atom_site.label_atom_id
_atom_site.label_comp_id
_atom_site.label_asym_id
```

```
      _atom_site.label_seq_id
      _atom_site.label_alt_id
      _atom_site.cartn_x
      _atom_site.cartn_y
      _atom_site.cartn_z
      _atom_site.occupancy
      _atom_site.B_iso_or_equiv
      _atom_site.footnote_id
      _atom_site.auth_seq_id
      _atom_site.id
  ATOM N  N   VAL  A  11 . 25.369  30.691  11.795  1.00  17.93 . 11 1
  ATOM C  CA  VAL  A  11 . 25.970  31.965  12.332  1.00  17.75 . 11 2
  ATOM C  C   VAL  A  11 . 25.569  32.010  13.881  1.00  17.83 . 11 3
#           [data omitted]
```

Note that the *name* construct is of the form *_category.extension*. The category explicitly defines a natural grouping of data items such that all data items of a single category are contained within a single *loop_*. There is no restriction on the length of *name*, beyond the record length limit of 80 characters mentioned below, and while there is no formal syntax within *name* beyond the category and extension separated by a period, by convention the category and extension are represented as an informal hierarchy of parts, with each part separated by an underscore (_). The *names* *_atom_site.label_atom_id* and *_atom_site.label_comp_id* are examples.

Questions that arise concerning the separation of data names and data values are solved with some additional syntax. For example, what if the data value contains white space, an underscore, or runs over several lines? Similarly, what if a value in a *loop_* is undefined or has no meaning in the context in which it is defined? The following syntax rules, which are a more restricted set of rules than permitted by STAR, complete the mmCIF description.

- Comments are preceded by a hash (#) and terminated by a new line.
- Data values on a single line may be delimited by pairs of single (') or double (") quotes.
- Data values that extend beyond a single line are enclosed within semicolons (;) as the first character of the line that begins the text block and the first character of the line following the last line of text.
- Data values which are unknown are represented by a question mark (?).
- Data values which are undefined are represented by a period (.).
- The length of a record in mmCIF is restricted to 80 characters.
- Only printable ASCII characters are permitted.
- Only a single level of *loop_* is permissible.

To complete the introductory picture of the appearance of a mmCIF data file consider the notion of scope. A PDB file has essentially one form of scope - the complete file. Thus, a single structure or an ensemble of structures is represented by a single file with each member of the ensemble separated by a PDB MODEL keyword record. There is no computer readable mechanism for associating components of say the REMARK records with a particular member

of the ensemble. The mmCIF representation deals with this issue by using the STAR data block concept. Data blocks begin with *data_* and have a scope that extends until the next *data_* or an end-of-file is reached. A *name* may appear only once in a data block, but data items may appear in any order. A consequence of these STAR rules is that the combination of data block name and data name is always unique.

Contents of the mmCIF Dictionary

Table I summarizes the category groups, their associated individual categories and their definitions as found in the mmCIF dictionary version 0.8.02 dated March 18, 1996. This comprehensive hierarchy of categories follows closely the progress of the experiment and the subsequent structure description.

Structure Representation Using mmCIF

The categories describing the crystallographic experiment are relatively self explanatory and will not be detailed here. We will, however, outline the data model used to describe the resulting structure and its description.

The structural data model can most simply be described as containing three interrelated groups of categories: *ATOM_SITE* categories, which give coordinates and related information for the structure; *ENTITY* categories, which describe the chemistry of the components of the structure, and *STRUCT* categories, which analyze and describe the structure.

The data items in the *ATOM_SITE* category record details about the atom sites including the coordinates, the thermal displacement parameters, the errors in the parameters and include a specification of the component of the asymmetric unit to which an atom belongs.

The *ENTITY* category categorizes the unique chemical components of the asymmetric unit as to whether they are polymer, non-polymer or water. The characteristics of a polymer are described by the *ENTITY_POLY* category and the sequence of the chemical components comprising the polymer by the *ENTITY_POLY_SEQ* category. The *CHEM_COMP* categories describe the standard geometries of the monomer units such as the amino acids and nucleotides as well as that of the ligands and solvent groups.

The *STRUCT_BIOL* category allows the author to describe the biologically relevant features of a structure and its component parts. The *STRUCT_BIOL_GEN* category provides the information about how to generate the biological unit from the components of the asymmetric unit which are in turn specified by the *STRUCT_ASYM* category. Various features of the structure such as intermolecular hydrogen bonds, special sites and secondary structure are specified in *STRUCT_CONN, STRUCT_SITE* and *STRUCT_CONF,* respectively. Figure 2 illustrates the interrelationships among these categories.

These and other major descriptive features of the mmCIF dictionary are best explored by example. A browsable dictionary can be found at the mmCIF WWW site (mmCIF[3]) as well as some complete examples. Complete examples for all nucleic acids can be found at the Nucleic Acid Database WWW site (NDB[13]). Partial mmCIFs for every structure in the PDB are available at two WWW sites (PDB[14], SDSC[15]) having been generated with the program *pdb2cif* (Bernstein *et al.*[16]).

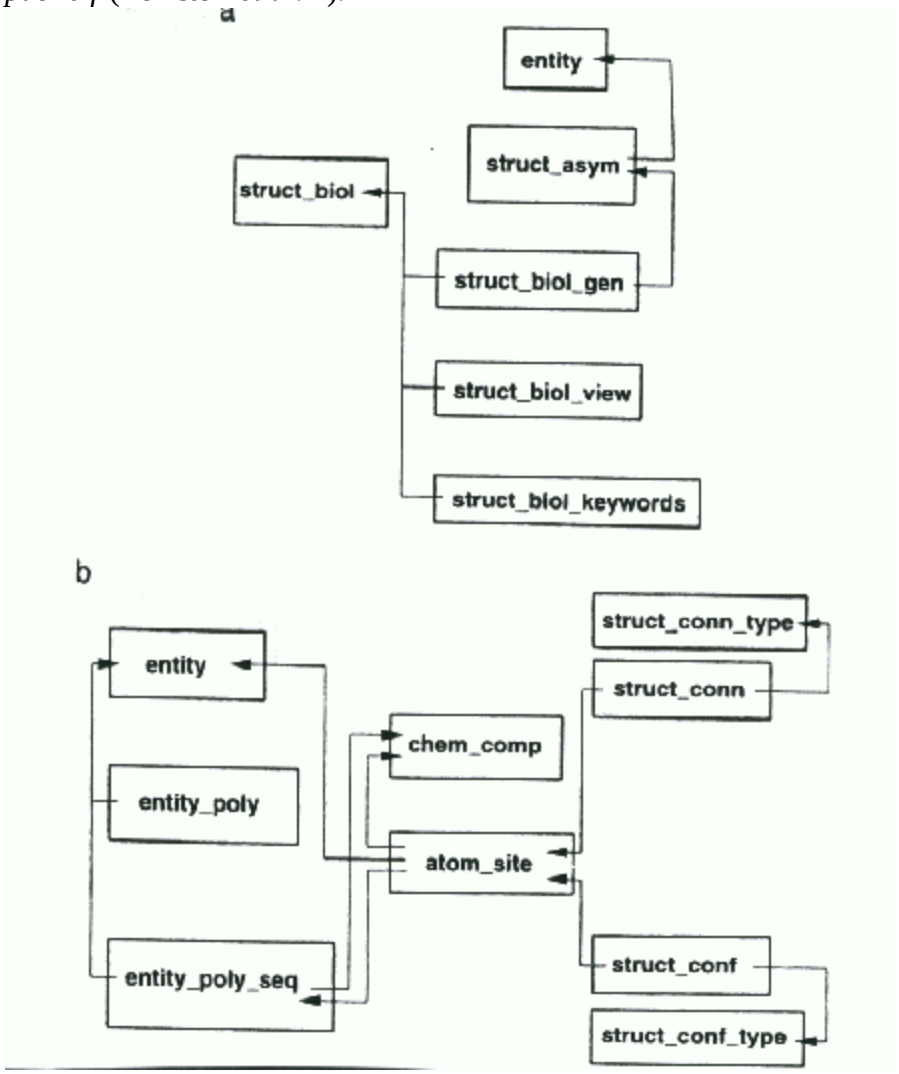


Figure 2 **a)** The relationships between categories which describe biologically relevant structure. **b)** The relationships between categories describing polymer structure, the atomic coordinates, and those categories which describe structural features such as hydrogen bonding and secondary structure.

Example One

Starting simply, consider the protein crambin which is a single polypeptide chain of 48 residues and in the low temperature form at 0.83 Å resolution (Teeter *et al.*[17]; PDB code 1CBN) has

nearly all the protein bound solvent resolved as well as an ethanol molecule co-crystallized. The protein shows recognizable sequence microheterogeneity at positions 22 (Pro/Ser) and 25 (Leu/Ile) and 24% of residues show discrete disorder. While microheterogeneity and disorder are described using data items in the mmCIF dictionary, they are not detailed here for the sake of simplicity.

Since the biological function of this molecule is unknown, no biologically relevant structural components are justified. A single identifier (*crambin_1*) is used to identify the unknown biological function of this molecule.

```
_struct_biol.id                    crambin_1
_struct_biol.details
;     The function of this protein is unknown and therefore the
      biological unit is assumed to be the single polypeptide
      chain without co-crystallization factors i.e. ethanol.
;
```

The single biological descriptor, *crambin_1*, is generated from the single polypeptide chain found in the asymmetric unit without any symmetry transformations applied. The polypeptide chain is designated *chain_a*.

```
_struct_biol_gen.biol_id           crambin_1
_struct_biol_gen.asym.id           chain_a
_struct_biol_gen.symmetry          1_555
```

The chemical components of the asymmetric unit are three entities: a single polypeptide chain characterized as a polymer, ethanol characterized as non-polymer, and water. Whether the source of the entity is a natural product, or it has been synthesized is also indicated.

```
 loop_
_entity.id
_entity.type
_entity.formula_weight
_entity.src_method
      A           polymer           4716        'NATURAL'
      ethanol     non-polymer       52          'SYNTHETIC'
      H20         water             18          .
```

It is then possible to expand upon this basic description of each entity using the *entity.id* as a reference. So for example the common and systematic names are specified as,

```
_entity_name_com.entity_id         A
_entity_name_com.name              crambin

_entity_name_sys.entity_id         A
_entity_name_sys.name              'Crambe Abyssinica'
```

Similarly, the natural and synthetic description can be given in more detail, so for the natural product we have,

```
_entity_src_nat.entity_id          A
_entity_src_nat.common_name        'Abyssinian cabbage seed'
_entity_src_nat.genus              Crambe
_entity_src_nat.species            Abyssinica
_entity_src_nat.details            ?
```

Using the entities as building blocks the contents of the asymmetric unit are specified. Crambin is straightforward since each entity appears only once in the asymmetric unit.

```
 loop_
_struct_asym.id
_struct_asym.entity_id
_struct_asym.details
      chain_a     A          'Single polypeptide chain'
      ethanol     ethanol    'Cocrystallized ethanol molecule'
      H20         H20        .
```

Entities classified as polymer, in this instance only that entity identified as *A*, is further described. First, the overall features of the polypeptide chain.

```
_entity_poly.entity_id        A
_entity_poly.type             polypeptide(L)
_entity_poly.nstd_chirality   no
_entity_poly.nstd_linkage     no
_entity_poly.nstd_monomers    no
_entity_poly.type_details     'Microheterogeneity at 22 and 25'
```

and then the component parts,

```
 loop_
_entity_poly_seq.entity_id
_entity_poly_seq.num
_entity_poly_seq.mon_id
      A     1     THR   A     2     THR
#     [data omitted]
      A     22    PRO   A     23    GLU
      A     24    ALA   A     25    LEU
#     [data omitted]
      A     47    ALA   A     48    ASN
```

The entity may also exist in other databases and these references may be cited and described. For the entity designated *A*, which is defined in Genbank but without sequence microheterogeneity we have,

```
 loop_
_struct_ref.id
_struct_ref.entity_id
```

```
      _struct_ref.biol_id
      _struct_ref.db_name
      _struct_ref.db_code
      _struct_ref.seq_align
      _struct_ref.seq_dif
      _struct_ref.details
      1     A     crambin_1   'Genbank'   '493916'    'entire'    'no' .
      2     A     crambin_1   'PDB'       '1CBN'      ‘entire’    ‘no’ .
```

Once each polymer entity is defined, the details of the secondary structure are defined using the STRUCT_CONF category.

```
       loop_
      _struct_conf.id
      _struct_conf.conf_type.id
      _struct_conf.beg_label_comp_id
      _struct_conf.beg_label_asym_id
      _struct_conf.beg_label_seq_id
      _struct_conf.end_label_comp_id
      _struct_conf.end_label_asym_id
      _struct_conf.end_label_seq_id
      _struct_conf.details
      H1  HELX_RH_AL_P ILE chain_a 7  PRO  chain_a  19 'HELX-RH3T 17-19'
      H2  HELX_RH_AL_P GLU chain_a 23 THR  chain_a  30 'Alpha-N start'
      S1  STRN_P       CYS chain_a 32 ILE  chain_a  35 .
      S2  STRN_P       THR chain_a  1 CYS  chain_a   4 .
      S3  STRN_P       ASN chain_a 46 ASN  chain_a  46 .
      S4  STRN_P       THR chain_a 39 PRO  chain_a  41 .
      T1  TURN-TY1_P   ARG chain_a 17 GLY  chain_a  20 .
      T2  TURN-TY1_P   PRO chain_a 41 TYR  chain_a  44 .
```

These assignments are further enumerated over those made in a PDB file for the record types HELIX, TURN and SHEET. Moreover, the STRUCT_CONF_TYPE category (Table I) specifies the method of assignment which could, for example, be deduced by the crystallographer from the electron density maps or defined algorithmically.

```
       loop_
      _struct_conf_type.id
      _struct_conf_type.criteria
      _struct_conf_type.reference
      HELX_RH_AL_P      'author judgement'      .
      STRN_P            'author judgement'      .
      TURN_TY1_P        'author judgement'      .
#     HELX_RH_P         'Kabsch and Sander' 'Biopolymers (1983) 22:2577'
```

The commented entry at the end is a hypothetical example for a calculated assignment. Data items also exist (Table I) for the description of beta sheets, but are not shown in this introductory example.

Interactions between various portions of the structure are described by the STRUCT_CONN and associated STRUCT_CONN_TYPE category.

```
       loop_
      _struct_conn.id
      _struct_conn.conn_type_id
      _struct_conn.ptnr1_label_comp_id
      _struct_conn.ptnr1_label_asym_id
      _struct_conn.ptnr1_label_seq_id
      _struct_conn.ptnr1_label_atom_id
      _struct_conn.ptnr1_role
      _struct_conn.ptnr1_symmetry
      _struct_conn.ptnr2_label_comp_id
      _struct_conn.ptnr2_label_asym_id
      _struct_conn.ptnr2_label_seq_id
      _struct_conn.ptnr2_label_atom_id
      _struct_conn.ptnr2_role
      _struct_conn.ptnr2_symmetry
      _struct_conn.details
      SS1 disulf CYS  chain_a  3  S  1_555  CYS  chain_a 40  S  1_555  .
      SS2 disulf CYS  chain_a  4  S  1_555  CYS  chain_a 32  S  1_555  .
#       [data omitted]
      HB1  hydrog  SER  chain_a  6  OG positive  1_555  .
                   LEU  chain_a  8  O  negative  1_556  .
      HB2  hydrog  ARG  chain_a 17  N  positive  1_555  .
                   ASP  chain_a 43  O  negative  1_554  .
#       [data omitted]
```

These intermolecular interactions are partially specified on PDB CONNECT records. However mmCIF provides an additional level of detail such that the criteria used to define an interaction may be given using the STRUCT_CONN_TYPE category. Here is a hypothetical example used to describe a salt bridge and a hydrogen bond.

```
       loop_
      _struct_conn_type.id
      _struct_conn_type.criteria
      _struct_conn_type.reference
      saltbr  'negative to positive distance > 2.5 \%A and < 3.2 \%A ' .
      hydrog  'N to O distance > 2.5 \%A, < 3.2 \%A, NOC angle < 120°' .
```

Example Two

Consider a mmCIF representation for a more complex structure. The gene regulatory protein 434 CRO complexed with a 20 base pair DNA segment containing operator (Mondragon and Harrison[18]; PDB code 3CRO).

```
       loop_
      _struct_biol.id
      _struct_biol.details
                  complex
;           The complex consists of 2 protein domains bound to a
            20 base pair DNA segment.
;
```

```
                protein
;           Each of the 2 protein domains is a single homologous
            polypeptide chain of 71 residues designated L and R.
;
                DNA
;           The two strands (A and B) are complementary given a one
            base offset.
;
```

The protein/DNA complex, the protein, and the DNA are considered as three separate biological components each generated from the contents of the asymmetric unit. No crystallographic symmetry need be applied to generate the biologically relevant components.

```
 loop_
_struct_biol_gen.biol_id
_struct_biol_gen.asym.id
_struct_biol_gen.symmetry
      complex     L     1_555
      complex     R     1_555
      complex     A     1_555
      complex     B     1_555
      protein     L     1_555
      protein     R     1_555
      DNA         A     1_555
      DNA         B     1_555

 loop_
_entity.id
_entity.type
      dimer       polymer
      DNA_A       polymer
      DNA_B       polymer
      water       water
```

Since each protein domain is chemically identical they constitute a single entity which has been designated *dimer*. The complementary DNA strands are not chemically identical and therefore constitute two separate entities:

```
 loop_
_struct_asym.id
_struct_asym.entity_id
_struct_asym.details
      L     dimer       '71 residue polypeptide chain'
      R     dimer       '71 residue polypeptide chain'
      A     DNA_A       '20 base strand'
      B     DNA_B       '20 base strand'
      H2O   water       'solvent'
```

Features of the CRO 434 secondary structure and intermolecular contacts can be described in the same way in which crambin was represented and are not repeated.

Conclusion

In preparing these examples of representing macromolecular structure using mmCIF it was necessary to return to the original papers since not all the relevant information could be retrieved from the PDB entry. This is evidence that mmCIF provides additional information which also has the advantage of being in a computer readable form. The consequence is that it places additional emphasis on the person preparing the mmCIF. It is anticipated that full use of the expressive power of mmCIF will only be made when existing structure solution and refinement programs are modified to maintain mmCIF data items and software tools exist to help prepare and use a mmCIF effectively. A variety of software tools have been developed for mmCIF (Bernstein, *et al*. [16]; Westbrook, *et al*. [19]). A description of a variety of other efforts can be found elsewhere (Bourne[20]). Code and documentation are available at the mmCIF WWW site (mmCIF[3]). A long term goal might be to maintain all aspects of the structure determination in an electronic laboratory notebook that uses mmCIF as its underlying data representation.

Acknowledgments

The development of the mmCIF dictionary has been a community effort. The Background and Introduction sections of the mmCIF WWW site describe the contributions of the many people who have participated in this project (mmCIF[3]).

References

1. F.C. Bernstein, T.F. Koetzle, G.J.B. Williams, E.F. Meyer,Jr., M.D. Brice, J.R.Rogers, O. Kennard, T. Shimanouchi, and M. Tasumi, *J. Mol. Biol.* **112**, 535 (1977).

2. IEEE Metadata. *http://www.llnl.gov/liv_comp/metadata/* (1996).

3. mmCIF. *http://ndbserver.rutgers.edu/mmcif/* (1996).

4. P.E. Bourne. *http://www.sdsc.edu/pb/cif/overview.html* (1996).

5. S.R. Hall, F.H. Allen, and I.D. Brown, *Acta Cryst.* **A47**, 655 (1991).

6. IUCr. *ftp://ftp.iucr.ac.uk/cifdics/cifdic.c91* (1996).

7. A. Cook and S.R. Hall, *J. Chem Inf. Comput. Sci.* **31**, 326 (1992).

8. S.R. Hall and N.Spadaccini, *J. Chem. Inf. Comput. Sci.* **34**, 505 (1994).

9. P.M.D. Fitzgerald, H.M. Berman, P.E. Bourne, B. McMahon, K. Watenpaugh, and J.D. Westbrook *Acta Cryst*. **A52 Sup**., C575 (1996).

10. IUCr. *ftp://ftp.iucr.ac.uk/cifdics/cifdic.c96* (1996).

11. J.D. Westbrook and S.R. Hall. *http://ndbserver.rutgers.edu/mmcif/ddl/* (1995).

12. IUCr. *ftp://ftp.iucr.ac.uk/cifdics/ddldic.c95* (1995).

13. NDB. *http://ndbserver.rutgers.edu/* (1996).

14. PDB. *http://www.pdb.bnl.gov/cgi-bin/pdbmain* (1996).

15. SDSC. *http://www.sdsc.edu/moose* (1996).

16. H.J. Bernstein, F.C. Bernstein, and P.E. Bourne. In preparation (1996).

17. M.M.Teeter, S.M. Roe, and N. Ho Heo, *J. Mol. Biol.* **230**, 292 (1993).

18. A.Mondragon and S.C.Harrison, *J Mol. Biol.* **219**, 321 (1991).

19. J.D. Westbrook, S.H. Hsieh, and P.M.D. Fitzgerald, *J. App. Cryst*. In press (1996).

20. P.E.Bourne (Ed.), *Proceedings of the first macromolecular CIF tools workshop.* Tarrytown NY (1993).

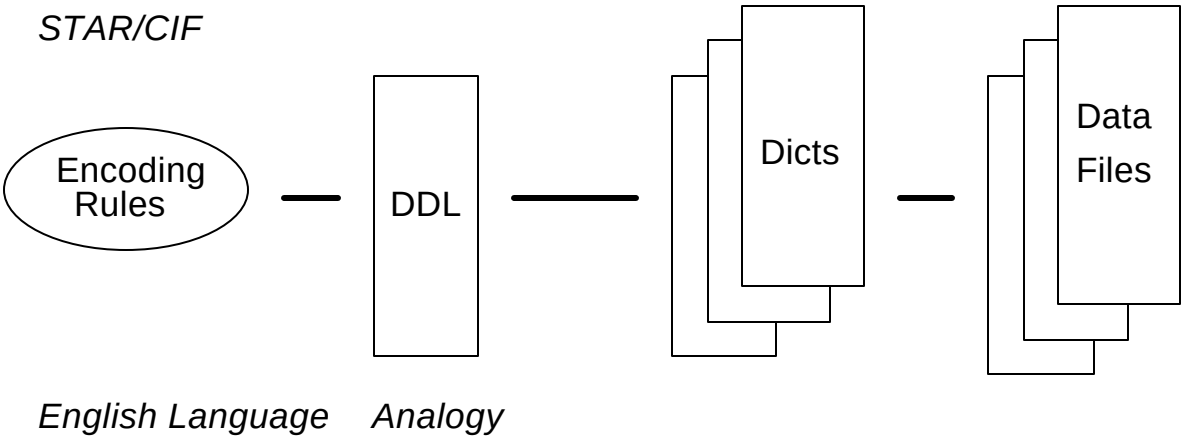
Table 1 The mmCIF category groups and associated categories taken from *http://ndbserver.rutgers.edu/mmcif/dictionary/dict-html/cifdic.m96/Index/*.

CATEGORY GROUPS AND MEMBERS	DEFINITION
INCLUSIVE GROUP	All category groups
ATOM GROUP	
ATOM_SITE	Details of each atomic position
ATOM_SITE_ANISOTROP	Anisotropic thermal displacement
ATOM_SITES	Details pertaining to all atom sites
ATOM_SITES_ALT	Details pertaining to alternative atoms sites as found in disorder etc.
ATOM_SITES_ALT_ENS	Details pertaining to alternative atoms sites as found in ensembles e.g. from NMR and modeling experiments
ATOM_SITES_ALT_GEN	Generation of ensembles from multiple conformations
ATOM_SITES_FOOTNOTE	Comments concerning one or more atom sites
ATOM_TYPE	Properties of an atom at a particular atom site
AUDIT GROUP	
AUDIT	Detail on the creation and updating of the mmCIF
AUDIT_AUTHOR	Author(s) of the mmCIF including address information
AUDIT_CONTACT_AUTHOR	Author(s) to be contacted
CELL GROUP	
CELL	Unit cell parameters
CELL_MEASUREMENT	How the cell parameters were measured
CELL_MEASUREMENT_REFLN	Details of the reflections used to determine the unit cell parameters
CHEM_COMP GROUP	
CHEM_COMP	Details of the chemical components
CHEM_COMP_ANGLE	Bond angles in a chemical component
CHEM_COMP_ATOM	Atoms defining a chemical component
CHEM_COMP_BOND	Characteristics of bonds in a chemical component
CHEM_COMP_CHIR	Details of the chiral centers in a chemical component
CHEM_COMP_CHIR_ATOM	Atoms comprising a chiral center in a chemical component
CHEM_COMP_LINK	Linkages between chemical groups
CHEM_COMP_PLANE	Planes found in a chemical component
CHEM_COMP_PLANE_ATOM	Atoms comprising a plane in a chemical component
CHEM_COMP_TOR	Details of the torsion angles in a chemical component
CHEM_COMP_TOR_VALUE	Target values for the torsion angles in a chemical component
CHEM_LINK GROUP	
CHEM_LINK	Details of the linkages between chemical components
CHEM_LINK_ANGLE	Details of the angles in the chemical component linkage
CHEM_LINK_BOND	Details of the bonds in the chemical component linkage
CHEM_LINK_CHIR	Chiral centers in a link between two chemical components
CHEM_LINK_CHIR_ATOM	Atoms bonded to a chiral atom in a linkage between two chemical components
CHEM_LINK_PLANE	Planes in a linkage between two chemical components

CHEM_LINK_PLANE_ATOM	Atoms in the plane forming a linkage between two chemical components
CHEM_LINK_TOR	Torsion angles in a linkage between two chemical components
CHEM_LINK_TOR_VALUE	Target values for torsion angles enumerated in a linkage between two chemical components
CHEMICAL GROUP	
CHEMICAL	Composition and chemical properties
CHEMICAL_CONN_ATOM	Atom position for 2-D chemical diagrams
CHEMICAL_CONN_BOND	Bond specifications for 2-D chemical diagrams
CHEMICAL_FORMULA	Chemical formula
CITATION GROUP	
CITATION	Literature cited in reference to the data block
CITATION_AUTHOR	Author(s) of the citations
CITATION_EDITOR	Editor(s) of citations where applicable
COMPUTING GROUP	
COMPUTING	Computer programs used in the structure analysis
SOFTWARE	More detailed description of the software used in the structure analysis
DATABASE GROUP	
DATABASE	Superseded by DATABASE_2
DATABASE_2	Codes assigned to mmCIFs by maintainers of recognized databases
DATABASE_PDB_CAVEAT	CAVEAT records originally found in the PDB version of the mmCIF data file
DATABASE_PDB_MATRIX	MATRIX records originally found in the PDB version of the mmCIF data file
DATABASE_PDB_REMARK	REMARK records originally found in the PDB version of the mmCIF data file
DATABASE_PDB_REV	Taken from the PDB REVDAT records
DATABASE_PDB_REV_RECORD	Taken from the PDB REVDAT records
DATABASE_PDB_TVECT	TVECT records originally found in the PDB version of the mmCIF data file
DIFFRN GROUP	
DIFFRN	Details of diffraction data and the diffraction experiment
DIFFRN_ATTENUATOR	Diffraction attenuator scales
DIFFRN_MEASUREMENT	Details on how the diffraction data were measured
DIFFRN_ORIENT_MATRIX	Orientation matrices used when measuring data
DIFFRN_ORIENT_REFLN	Reflections that define the orientation matrix
DIFFRN_RADIATION	Details on the radiation and detector used to collect data
DIFFRN_REFLN	Unprocessed reflection data
DIFFRN_REFLNS	Details pertaining to all reflection data
DIFFRN_SCALE_GROUP	Details of reflections used in scaling
DIFFRN_STANDARD_REFLN	Details of the standard reflections used during data collection
DIFFRN_STANDARDS	Details pertaining to all standard reflections
ENTITY GROUP	
ENTITY	Details pertaining to each unique chemical component of the structure
ENTITY_KEYWORDS	Keywords describing each entity
ENTITY_LINK	Details of the links between entities
ENTITY_NAME_COM	Common name for the entity
ENTITY_NAME_SYS	Systematic name for the entity
ENTITY_POLY	Characteristics of a polymer
ENTITY_POLY_SEQ	Sequence of monomers in a polymer
ENTITY_SRC_GEN	Source of the entity

ENTITY_SRC_NAT	Details of the natural source of the entity
ENTRY GROUP	
ENTRY	Identifier for the data block
EXPTL GROUP	
EXPTL	Experimental details relating to the physical properties of the material, particularly absorption
EXPTL_CRYSTAL	Physical properties of the crystal
EXPTL_CRYSTAL_FACE	Details pertaining to the crystal faces
EXPTL_CRYSTAL_GROW	Conditions and methods used to grow the crystals
EXPTL_CRYSTAL_GROW_COMP	Components of the solution from which the crystals were grown
GEOM GROUP	
GEOM	Derived geometry information
GEOM_ANGLE	Derived bond angles
GEOM_BOND	Derived bonds
GEOM_CONTACT	Derived intermolecular contacts
GEOM_TORSION	Derived torsion angles
JOURNAL GROUP	
JOURNAL	Used by journals and not the mmCIF preparer
PHASING GROUP	
PHASING	General phasing information
PHASING_AVERAGING	Phase averaging of multiple observations
PHASING_ISOMORPHOUS	Phasing information from an isomorphous model
PHASING_MAD	Phasing via multiwavelength anomolous dispersion (MAD)
PHASING_MAD_CLUST	Details of a cluster of MAD experiments
PHASING_MAD_EXPT	Overall features of the MAD experiment
PHASING_MAD_RATIO	Ratios between pairs of MAD datasets
PHASING_MAD_SET	Details of individual MAD datasets
PHASING_MIR	Phasing via single and multiple isomorphous replacement
PHASING_MIR_DER	Details of individual derivatives used in MIR
PHASING_MIR_DER_REFLN	Details of calculated structure factors
PHASING_MIR_DER_SHELL	As above but for shells of resolution
PHASING_MIR_DER_SITE	Details of heavy atom sites
PHASING_MIR_SHELL	Details of each shell used in MIR
PHASING_SET	Details of data sets used in phasing
PHASING_SET_REFLN	Values of structure factors used in phasing
PUBL GROUP	
PUBL	Used when submitting a publication as a mmCIF
PUBL_AUTHOR	Authors of the publication
PUBL_MANUSCRIPT_INCL	To include special data names in the processing of the manuscript
REFINE GROUP	
REFINE	Details of the structure refinement
REFINE_B_ISO	Details pertaining to the refinement of isotropic B values
REFINE_HIST	History of the refinement
REFINE_LS_RESTR	Details pertaining to the least squares restraints used in refinement
REFINE_LS_SHELL	Results of refinement broken down by resolution
REFINE_OCCUPANCY	Details pertaining to the refinement of occupancy factors
REFLN GROUP	
REFLN	Details pertaining to the reflections used to derive the atom sites
REFLNS	Details pertaining to all reflections
REFLNS_SCALE	Details pertaining to scaling factors used with respect to the structure factors

REFLNS_SHELL	As REFLNS, but by shells of resolution
STRUCT GROUP	
STRUCT	Details pertaining to a description of the structure
STRUCT_ASYM	Details pertaining to structure components within the asymmetric unit
STRUCT_BIOL	Details pertaining to components of the structure that have biological significance
STRUCT_BIOL_GEN	Details pertaining to generating biological components
STRUCT_BIOL_KEYWORDS	Keywords for describing biological components
STRUCT_BIOL_VIEW	Description of views of the structure with biological significance
STRUCT_CONF	Conformations of the backbone
STRUCT_CONF_TYPE	Details of each backbone conformation
STRUCT_CONN	Details pertaining to intermolecular contacts
STRUCT_CONN_TYPE	Details of each type of intermolecular contact
STRUCT_KEYWORDS	Description of the chemical structure
STRUCT_MON_DETAILS	Calculation summaries at the monomer level
STRUCT_MON_NUCL	Calculation summaries specific to nucleic acid monomers
STRUCT_MON_PROT	Calculation summaries specific to protein monomers
STRUCT_MON_PROT_CIS	Calculation summaries specific to cis peptides
STRUCT_NCS_DOM	Details of domains within an ensemble of domains
STRUCT_NCS_DOM_LIM	Beginning and end points within polypeptide chains forming a specific domain
STRUCT_NCS_ENS	Description of ensembles
STRUCT_NCS_ENS_GEN	Description of domains related by non-crystallographic symmetry
STRUCT_NCS_OPER	Operations required to superimpose individual members of an ensemble
STRUCT_REF	External database references to biological units within the structure
STRUCT_REF_SEQ	Describes the alignment of the external database sequence with that found in the structure
STRUCT_REF_SEQ_DIF	Describes differences in the external database sequence with that found in the structure
STRUCT_SHEET	Beta sheet description
STRUCT_SHEET_HBOND	Hydrogen bond description in beta sheets
STRUCT_SHEET_ORDER	Order of residue ranges in beta sheets
STRUCT_SHEET_RANGE	Residue ranges in beta sheets
STRUCT_SHEET_TOPOLOGY	Topology of residue ranges in beta sheets
STRUCT_SITE	Details pertaining to specific sites within the structure
STRUCT_SITE_GEN	Details pertaining to how the site is generated
STRUCT_SITE_KEYWORDS	Keywords describing the site
STRUCT_SITE_VIEW	Description of views of the specified site
SYMMETRY GROUP	
SYMMETRY	Details pertaining to space group symmetry
SYMMETRY_EQUIV	Equivalent positions for the specified space group



There are 26 letters in the alphabet. I before E accept after C is a rule.	Words are allowable groups of letters separated by white space and punctuation.	Words are defined in a dictionary.	This paper uses only words in the dictionary.