```
##############################################################################
#                                                                            #
#                       CIF CORE DICTIONARY                                  #
#                                                                            #
##############################################################################

data_CIF_CORE

    _dictionary.title            CIF_CORE
    _dictionary.class            Instance
    _dictionary.version          1.4.02
    _dictionary.date             2012-12-18
    _dictionary.uri              www.iucr.org/cif/dic/cif_core.dic
    _dictionary.ddl_conformance  3.11.01
    _dictionary.namespace        CifCore
    _description.text
;
     Dictionary shell for the definitions of COMCIFS-approved CORE data
     used within the Crystallographic Information Framework.
;

save_CIF_CORE
    _definition.id               CIF_CORE
    _definition.scope            Category
    _definition.class            Head
    _definition.update           2012-12-18
    _description.text
;
     The DICTIONARY group encompassing all CORE data items defined and
     used with in the Crystallographic Information Framework (CIF).
;
    _name.category_id           CIF_DIC
    _name.object_id             CIF_CORE

   _import.get
        [{"save":'EXPERIMENTAL', "file":'core_exptl.dic', "mode":'full' },
         {"save":'DIFFRACTION',  "file":'core_diffr.dic', "mode":'full' },
         {"save":'STRUCTURE',    "file":'core_struc.dic', "mode":'full' },
#        {"save":'MODEL',        "file":'core_model.dic', "mode":'full' },


save_MODEL
    _definition.id               MODEL
    _definition.scope            Category
    _definition.class            Head
    _definition.update           2012-11-22
    _description.text
;
    Items in the MODEL Category specify data for the crystal structure
    postulated and modelled from the atomic coordinates derived and
    refined from the diffraction information. The structural model is
    described principally in terms of the geometry of the 'connected'
    atom sites and the crystal symmetry in which they reside.
;
    _name.category_id            CIF_CORE
    _name.object_id              MODEL

#============================================================================

save_GEOM
    _definition.id               GEOM
    _definition.scope            Category
    _definition.class            Set
    _definition.update           2012-11-22
    _description.text
;
     The CATEGORY of data items used to specify the geometry
     of the structural model as derived from the atomic sites.
     The geometry is expressed in terms of the interatomic
     angles (GEOM_ANGLE data), covalent bond distances
     (GEOM_BOND data), contact distances (GEOM_CONTACT data),
     hydrogen bonds (GEOM_HBOND data) and torsion geometry
     (GEOM_TORSION data).
     Geometry data are usually redundant, in that they can be
     calculated from other more fundamental quantities in the data
     block. However, they serve the dual purposes of providing a
     check on the correctness of both sets of data and of enabling
     the most important geometric data to be identified for
     publication by setting the appropriate publication flag.
;
    _name.category_id            MODEL
    _name.object_id              GEOM


save_geom.bond_distance_incr
    _definition.id              '_geom.bond_distance_incr'
    _definition.update           2012-11-22
    _description.text
;
     Increment added to the bond radii for the atomic species to
     specify the maximum permitted "bonded" distance between two
     atom sites.
;
    _name.category_id            geom
    _name.object_id              bond_distance_incr
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Real
    _enumeration.default         0.2
    _units.code                  angstroms
     save_


save_geom.bond_distance_min
    _definition.id              '_geom.bond_distance_min'
    _definition.update           2012-11-22
    _description.text
;
     Minimum permitted "bonded" distance between two atom sites.
;
    _name.category_id            geom
    _name.object_id              bond_distance_min
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Real
    _enumeration.default         0.2
    _units.code                  angstroms
     save_


save_geom.contact_distance_incr
    _definition.id              '_geom.contact_distance_incr'
    _definition.update           2012-11-22
    _description.text
;
     Increment added to the bond radii for the atomic species to
```

```
     specify the maximum permitted "contact" distance between two
     "non-bonded" atom sites.
;
    _name.category_id            geom
    _name.object_id              contact_distance_incr
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Real
    _enumeration.default         0.2
    _units.code                  angstroms
     save_


save_geom.contact_distance_min
    _definition.id             '_geom.contact_distance_min'
    _definition.update           2012-11-22
    _description.text
;
     Minimum permitted "contact" distance between two "non-bonded" atom sites.
;
    _name.category_id            geom
    _name.object_id              contact_distance_min
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Real
    _enumeration.default         0.2
    _units.code                  angstroms
     save_


save_geom.special_details
    _definition.id             '_geom.special_details'
     loop_
    _alias.definition_id       '_geom_special_details'
                               '_geom.details'
    _definition.update           2012-11-22
    _description.text
;
     Description of geometry information not covered by the existing data
     names in the geometry categories, such as least-squares planes.
;
    _name.category_id            geom
    _name.object_id              special_details
    _type.purpose                Describe
    _type.source                 Recorded
    _type.container              Single
    _type.contents               Text
     save_

#-------------------------------------------------------------------------------

save_GEOM_ANGLE
    _definition.id               GEOM_ANGLE
    _definition.scope            Category
    _definition.class            Loop
    _definition.update           2012-11-22
    _description.text
;
     The CATEGORY of data items used to specify the geometry angles in the
     structural model as derived from the atomic sites.
;
    _name.category_id            GEOM
    _name.object_id              ANGLE
    _category.key_id           '_geom_angle.key'
    loop_
    _method.purpose
    _method.expression
     Evaluation
;
     dmin =  _geom.bond_distance_min

     Loop  m1  as  model_site  :i  {   # loop vertex model site

        rad1  =   m1.radius_bond + _geom.bond_distance_incr

        Loop  m2  as  model_site  :j  {  # loop first target site

           If (i==j or m1.mole_index != m2.mole_index) Next
           v1 =  m2.Cartn_xyz - m1.Cartn_xyz
           d1 =  Norm (v1)

           If (d1<dmin or d1>(rad1+m2.radius_bond))  Next

           rad2  =   m2.radius_bond + _geom.bond_distance_incr

           Loop  m3  as  model_site  :k>j  {  # loop second target site

              If (i==k or m1.mole_index != m3.mole_index) Next
              v2 =  m3.Cartn_xyz - m1.Cartn_xyz
              d2 =  Norm (v2)

              If (d2<dmin or d2>(rad2+m3.radius_bond)) Next

              angle =  Acosd ( v1*v2 / (d1*d2) )

              geom_angle( .id        =  List ( m2.id, m1.id, m3.id ),
                          .distances =  List ( d1, d2 ),
                          .value     =  angle )
     }   }   }
;


save_geom_angle.key
    _definition.id             '_geom_angle.key'
    _definition.update           2012-11-22
    _description.text
;
     Value is a unique key to a set of GEOM_ANGLE items
     in a looped list.
;
    _name.category_id            angle
    _name.object_id              key
    _type.purpose                Key
    _type.source                 Related
    _type.container              Single
    _type.contents               Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;              _type.contents = Type_Contents(geom_angle.id)
;
     Evaluation
;              _geom_angle.key = _geom_angle.id
;
     save_
```

```
save_geom_angle.atom_site_label_1
    _definition.id              '_geom_angle.atom_site_label_1'
     loop_
    _alias.definition_id        '_geom_angle_atom_site_label_1'
                                '_geom_angle.atom_site_id_1'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             angle
    _name.object_id               atom_site_label_1
     save_


save_geom_angle.atom_site_label_2
    _definition.id              '_geom_angle.atom_site_label_2'
     loop_
    _alias.definition_id        '_geom_angle_atom_site_label_2'
                                '_geom_angle.atom_site_id_2'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             angle
    _name.object_id               atom_site_label_2
     save_


save_geom_angle.atom_site_label_3
    _definition.id              '_geom_angle.atom_site_label_3'
     loop_
    _alias.definition_id        '_geom_angle_atom_site_label_3'
                                '_geom_angle.atom_site_id_3'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             angle
    _name.object_id               atom_site_label_3
     save_


save_geom_angle.distances
    _definition.id              '_geom_angle.distances'
    _definition.update            2012-11-22
    _description.text
;
     The pair of distances between sites 1 - 2 and 2 - 3.
;
    _name.category_id             angle
    _name.object_id               distances
    _type.purpose                 Measurand
    _type.source                  Derived
    _type.container               List
    _type.contents                Real
    _type.dimension               [2]
    _units.code                   angstroms
     save_


save_geom_angle.id
    _definition.id              '_geom_angle.id'
    _definition.update            2012-11-22
    _description.text
;
     Atom site labels and symmetry operators as pairs for each of the
     three atom sites which identify the angle. The second label-symop
     pair in the list identifies the site at the apex of the angle.
;
    _name.category_id             angle
    _name.object_id               id
    _type.purpose                 Composite
    _type.source                  Derived
    _type.container               List
    _type.contents                List(Code,Symop)
    _type.dimension               [3]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With  a  as  geom_angle

         _geom_angle.id =  [[ a.atom_site_label_1, a.site_symmetry_1 ],
                           [ a.atom_site_label_2, a.site_symmetry_2 ],
                           [ a.atom_site_label_3, a.site_symmetry_3 ]]
;
     save_


save_geom_angle.publ_flag
    _definition.id              '_geom_angle.publ_flag'
     loop_
    _alias.definition_id        '_geom_angle_publ_flag'
    _definition.update            2012-11-22
    _description.text
;
     Code signals if the angle is referred to in a publication or
     should be placed in a table of significant angles.
;
    _name.category_id             angle
    _name.object_id               publ_flag
    _type.purpose                 State
    _type.source                  Assigned
    _type.container               Single
    _type.contents                Code
  loop_
    _enumeration_set.state
    _enumeration_set.detail
                                  no  'do not include angle in special list'
                                  n   'abbreviation for "no"'
                                  yes 'do include angle in special list'
                                  y   'abbreviation for "yes"'
    _enumeration.default          no
     save_


save_geom_angle.site_symmetry_1
    _definition.id              '_geom_angle.site_symmetry_1'
     loop_
    _alias.definition_id        '_geom_angle_site_symmetry_1'
    _import.get           [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id             angle
    _name.object_id               site_symmetry_1
     save_


save_geom_angle.site_symmetry_2
    _definition.id              '_geom_angle.site_symmetry_2'
     loop_
    _alias.definition_id        '_geom_angle_site_symmetry_2'
    _import.get           [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id             angle
    _name.object_id               site_symmetry_2
     save_
```

```
save_geom_angle.site_symmetry_3
    _definition.id              '_geom_angle.site_symmetry_3'
     loop_
    _alias.definition_id        '_geom_angle_site_symmetry_3'
    _import.get           [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id             angle
    _name.object_id               site_symmetry_3
     save_


save_geom_angle.value
    _definition.id              '_geom_angle.value'
    loop_
    _alias.definition_id        '_geom_angle'
    _definition.update            2012-12-14
    _description.text
;
     Angle defined by the sites identified by _geom_angle.id
;
    _name.category_id             angle
    _name.object_id               value
    _type.purpose                 Measurand
    _type.source                  Derived
    _type.container               Single
    _type.contents                Real
    _enumeration.range            -180.:180.
    _units.code                   degrees
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With a as geom_angle

     xc = List()

     For [label,symop] in  a.id   {

         xf   =   SymEquiv(symop,  _atom_site[label].fract_xyz)

         xc ++=  _atom_sites_Cartn_transform.matrix * xf
      }
         v1,v2  =  xc[0]-xc[1], xc[2]-xc[1]

      _geom_angle.value =  Acosd ( v1 * v2 / ( Norm (v1) * Norm (v2) ) )
;
     save_

     save_    #----------- close of GEOM_ANGLE category

#-------------------------------------------------------------------------------


save_GEOM_BOND
    _definition.id                GEOM_BOND
    _definition.scope             Category
    _definition.class             Loop
    _definition.update            2012-11-22
    _description.text
;
     The CATEGORY of data items used to specify the geometry bonds in the
     structural model as derived from the atomic sites.
;
    _name.category_id             GEOM
    _name.object_id               BOND
    _category.key_id            '_geom_bond.key'
    loop_
    _method.purpose
    _method.expression
     Evaluation
;
     dmin =  _geom.bond_distance_min

     Loop  m1  as  model_site  :i  {

        rad   =   m1.radius_bond + _geom.bond_distance_incr

        Loop  m2  as  model_site  :j  {

           If (i==j or m1.mole_index != m2.mole_index) Next

           d =  Norm (m1.Cartn_xyz - m2.Cartn_xyz)

           If (d<dmin or d>(rad+m2.radius_bond)) Next

           geom_bond( .id        =  List ( m1.id, m2.id ),
                      .distance  =  d  )
      }   }
;


save_geom_bond.key
    _definition.id              '_geom_bond.key'
    _definition.update            2012-11-22
    _description.text
;
     Value is a unique key to a set of GEOM_BOND items
     in a looped list.
;
    _name.category_id             bond
    _name.object_id               key
    _type.purpose                 Key
    _type.source                  Related
    _type.container               Single
    _type.contents                Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;               _type.contents = Type_Contents(geom_bond.id)
;
     Evaluation
;               _geom_bond.key = _geom_bond.id
;
     save_


save_geom_bond.atom_site_label_1
    _definition.id              '_geom_bond.atom_site_label_1'
     loop_
    _alias.definition_id        '_geom_bond_atom_site_label_1'
                                '_geom_bond.atom_site_id_1'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             bond
    _name.object_id               atom_site_label_1
     save_
```

```
save_geom_bond.atom_site_label_2
    _definition.id              '_geom_bond.atom_site_label_2'
     loop_
    _alias.definition_id        '_geom_bond_atom_site_label_2'
                                '_geom_bond.atom_site_id_2'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             bond
    _name.object_id               atom_site_label_2
     save_


save_geom_bond.distance
    _definition.id              '_geom_bond.distance'
     loop_
    _alias.definition_id        '_geom_bond_distance'
                                '_geom_bond.dist'
    _definition.update            2012-12-14
    _description.text
;
     Intramolecular bond distance between the sites identified
     by _geom_bond.id
;
    _name.category_id             bond
    _name.object_id               distance
    _type.purpose                 Measurand
    _type.source                  Derived
    _type.container               Single
    _type.contents                Real
    _enumeration.range            0.:
    _units.code                   angstroms
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With b as geom_bond

     xc = List()

     For [label,symop] in  b.id   {

         xf   =   SymEquiv(symop, _atom_site[label].fract_xyz)

         xc ++=  _atom_sites_Cartn_transform.matrix * xf
      }
      _geom_bond.distance =  Norm ( xc[0] - xc[1] )
;
     save_


save_geom_bond.valence
    _definition.id              '_geom_bond.valence'
     loop_
    _alias.definition_id        '_geom_bond_valence'
    _definition.update            2012-12-11
    _description.text
;
     Bond valence calculated from the bond distance.
;
    _name.category_id             bond
    _name.object_id               valence
    _type.purpose                 Measurand
    _type.source                  Derived
    _type.container               Single
    _type.contents                Real
    _enumeration.range            0.:
    _units.code                   electrons
     save_


save_geom_bond.id
    _definition.id              '_geom_bond.id'
    _definition.update            2012-11-22
    _description.text
;
     Identity of bond distance in terms of the atom site labels and
     symmetry operators as pairs for each of the two "bonded" atom sites.
;
    _name.category_id             bond
    _name.object_id               id
    _type.purpose                 Composite
    _type.source                  Derived
    _type.container               List
    _type.contents                List(Code,Symop)
    _type.dimension               [2]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With  a  as  geom_bond

           _geom_bond.id =  [[ a.atom_site_label_1, a.site_symmetry_1 ],
                            [ a.atom_site_label_2, a.site_symmetry_2 ]]
;
     save_


save_geom_bond.publ_flag
    _definition.id              '_geom_bond.publ_flag'
     loop_
    _alias.definition_id        '_geom_bond_publ_flag'
    _definition.update            2012-11-22
    _description.text
;
     This code signals whether the angle is referred to in a
     publication or should be placed in a table of significant angles.
;
    _name.category_id             bond
    _name.object_id               publ_flag
    _type.purpose                 State
    _type.source                  Assigned
    _type.container               Single
    _type.contents                Code
  loop_
    _enumeration_set.state
    _enumeration_set.detail
                                  no  'do not include bond in special list'
                                  n   'abbreviation for "no"'
                                  yes 'do include bond in special list'
                                  y   'abbreviation for "yes"'
    _enumeration.default          no
     save_


save_geom_bond.multiplicity
```

```
    _definition.id             '_geom_bond.multiplicity'
     loop_
    _alias.definition_id       '_geom_bond_multiplicity'
    _definition.update           2013-01-22
    _description.text
;
     The number of times the given bond appears in the environment
     of the atoms labelled _geom_bond.atom_site_label_1. In cases
     where the full list of bonds is given, one of the series of
     equivalent bonds may be assigned the appropriate multiplicity
     while the others are assigned a value of 0.
;
    _name.category_id            bond
    _name.object_id              multiplicity
    _type.purpose                Number
    _type.source                 Derived
    _type.container              Single
    _type.contents               Count
    _enumeration.range           1:
     save_


save_geom_bond.site_symmetry_1
    _definition.id             '_geom_bond.site_symmetry_1'
     loop_
    _alias.definition_id       '_geom_bond_site_symmetry_1'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            bond
    _name.object_id              site_symmetry_1
     save_


save_geom_bond.site_symmetry_2
    _definition.id             '_geom_bond.site_symmetry_2'
     loop_
    _alias.definition_id       '_geom_bond_site_symmetry_2'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            bond
    _name.object_id              site_symmetry_2
     save_

     save_    #----------- close of GEOM_BOND category

#-------------------------------------------------------------------------------


save_GEOM_CONTACT
    _definition.id               GEOM_CONTACT
    _definition.scope            Category
    _definition.class            Loop
    _definition.update           2012-11-22
    _description.text
;
     The CATEGORY of data items used to specify the interatomic
     contact distances in the structural model.
;
    _name.category_id            GEOM
    _name.object_id              CONTACT
    _category.key_id           '_geom_contact.key'
    loop_
    _method.purpose
    _method.expression
     Evaluation
;
```

```
      Loop  m1  as  model_site  {

         rb  =   m1.radius_bond    + _geom.bond_distance_incr
         rc  =   m1.radius_contact + _geom.contact_distance_incr

         Loop  m2  as  model_site  {

            If (m2.id[1] != '1_555')  Next
            radb  =   rb + m2.radius_bond
            radc  =   rc + m2.radius_contact
            label =   m2.id[0]

            Loop  s  as  symmetry_equiv  :ns   {

               axyz      =   s.R * m2.fract_xyz + s.T

               Do i = -2,2 { Do j = -2,2 { Do k = -2,2 { # cell translations

                  tran  =   List ([i,j,k])
                  bxyz  =   axyz + tran
                  cxyz  =  _atom_sites_Cartn_transform.matrix * bxyz
                  d     =   Norm (cxyz - m1.Cartn_xyz)

                  If (d < radb or d > radc) Next

                  id        =  List( m1.id, List( label, Symop(ns+1,tran) ) )

                  geom_contact( .id        =  id,
                                .distance  =  d  )
      }  }  }  }  }  }
;


save_geom_contact.key
    _definition.id             '_geom_contact.key'
    _definition.update           2012-11-22
    _description.text
;
     Value is a unique key to a set of GEOM_CONTACT items
     in a looped list.
;
    _name.category_id            contact
    _name.object_id              key
    _type.purpose                Key
    _type.source                 Related
    _type.container              Single
    _type.contents               Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;              _type.contents = Type_Contents(geom_contact.id)
;
     Evaluation
;              _geom_contact.key = _geom_contact.id
;
     save_


save_geom_contact.atom_site_label_1
    _definition.id             '_geom_contact.atom_site_label_1'
     loop_
    _alias.definition_id       '_geom_contact_atom_site_label_1'
                               '_geom_contact.atom_site_id_1'
```

```
    _import.get          [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             contact
    _name.object_id               atom_site_label_1
     save_


save_geom_contact.atom_site_label_2
    _definition.id             '_geom_contact.atom_site_label_2'
     loop_
    _alias.definition_id       '_geom_contact_atom_site_label_2'
                               '_geom_contact.atom_site_id_2'
    _import.get          [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             contact
    _name.object_id               atom_site_label_2
     save_


save_geom_contact.distance
    _definition.id             '_geom_contact.distance'
     loop_
    _alias.definition_id       '_geom_contact_distance'
                               '_geom_contact.dist'
    _definition.update            2012-12-14
    _description.text
;
     Intermolecular distance between the atomic sites identifyed
     by _geom_contact.id
;
    _name.category_id             contact
    _name.object_id               distance
    _type.purpose                 Measurand
    _type.source                  Derived
    _type.container               Single
    _type.contents                Real
    _enumeration.range            0.:
    _units.code                   angstroms
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With c as geom_contact

     xc = List()

     For [label,symop] in  c.id   {

         xf   =   SymEquiv(symop, _atom_site[label].fract_xyz)

         xc +=  _atom_sites_Cartn_transform.matrix * xf
     }
     _geom_contact.distance =  Norm ( xc[0] - xc[1] )
;
     save_


save_geom_contact.id
    _definition.id             '_geom_contact.id'
    _definition.update            2012-11-22
    _description.text
;
     Atom site labels and symmetry operators as pairs for each of the
     two atom sites which define the contact bond.
;
    _name.category_id             contact
    _name.object_id               id
    _type.purpose                 Composite
    _type.source                  Derived
    _type.container               List
    _type.contents                List(Code,Symop)
    _type.dimension               [2]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With  a  as  geom_contact

          _geom_contact.id =  [[ a.atom_site_label_1, a.site_symmetry_1 ],
                              [ a.atom_site_label_2, a.site_symmetry_2 ]]
;
     save_


save_geom_contact.publ_flag
    _definition.id             '_geom_contact.publ_flag'
     loop_
    _alias.definition_id       '_geom_contact_publ_flag'
    _definition.update            2012-11-22
    _description.text
;
     This code signals whether the contact distance is referred to
     in a publication or should be placed in a list of significant
     contact distances.
;
    _name.category_id             contact
    _name.object_id               publ_flag
    _type.purpose                 State
    _type.source                  Assigned
    _type.container               Single
    _type.contents                Code
  loop_
    _enumeration_set.state
    _enumeration_set.detail
                                  no  'do not include distance in special list'
                                  n   'abbreviation for "no"'
                                  yes 'do include distance in special list'
                                  y   'abbreviation for "yes"'
    _enumeration.default          no
     save_


save_geom_contact.site_symmetry_1
    _definition.id             '_geom_contact.site_symmetry_1'
     loop_
    _alias.definition_id       '_geom_contact_site_symmetry_1'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id             contact
    _name.object_id               site_symmetry_1
     save_


save_geom_contact.site_symmetry_2
    _definition.id             '_geom_contact.site_symmetry_2'
     loop_
    _alias.definition_id       '_geom_contact_site_symmetry_2'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id             contact
```

```
    _name.object_id              site_symmetry_2
     save_

     save_    #----------- close of GEOM_CONTACT category

#------------------------------------------------------------------------------


save_GEOM_HBOND
    _definition.id               GEOM_HBOND
    _definition.scope            Category
    _definition.class            Loop
    _definition.update           2012-11-22
    _description.text
;
     The CATEGORY of data items used to specify the hydrogen bond
     distances in the structural model as derived from atomic sites.
;
    _name.category_id            GEOM
    _name.object_id              HBOND
    _category.key_id           '_geom_hbond.key'


save_geom_hbond.key
    _definition.id             '_geom_hbond.key'
    _definition.update           2012-11-22
    _description.text
;
     Value is a unique key to a set of GEOM_HBOND items
     in a looped list.
;
    _name.category_id            hbond
    _name.object_id              key
    _type.purpose                Key
    _type.source                 Related
    _type.container              Single
    _type.contents               Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;              _type.contents = Type_Contents(geom_hbond.id)
;
     Evaluation
;              _geom_hbond.key = _geom_hbond.id
;
     save_


save_geom_hbond.angle_DHA
    _definition.id             '_geom_hbond.angle_DHA'
     loop_
    _alias.definition_id       '_geom_hbond_angle_DHA'
    _definition.update           2012-12-14
    _description.text
;
     Angle subtended by the sites identifyed in _geom_hbond.id.
     The hydrogen at site H is at the apex of the angle.
;
    _name.category_id            hbond
    _name.object_id              angle_DHA
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           -180.:180.
    _units.code                  degrees
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With h as geom_hbond

     xc = List()

     For [label,symop] in  h.id   {

         xf   =   SymEquiv(symop, _atom_site[label].fract_xyz)

         xc ++=  _atom_sites_Cartn_transform.matrix * xf
      }
         v1,v2  =  xc[0]-xc[1], xc[2]-xc[1]

     _geom_hbond.angle_DHA  =  Acosd ( v1 * v2 / ( Norm (v1) * Norm (v2) ) )
;
    save_


save_geom_hbond.atom_site_label_A
    _definition.id             '_geom_hbond.atom_site_label_A'
     loop_
    _alias.definition_id       '_geom_hbond_atom_site_label_A'
                               '_geom_hbond.atom_site_id_A'
    _import.get          [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id            hbond
    _name.object_id              atom_site_label_A
     save_


save_geom_hbond.atom_site_label_D
    _definition.id             '_geom_hbond.atom_site_label_D'
     loop_
    _alias.definition_id       '_geom_hbond_atom_site_label_D'
                               '_geom_hbond.atom_site_id_D'
    _import.get          [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id            hbond
    _name.object_id              atom_site_label_D
     save_


save_geom_hbond.atom_site_label_H
    _definition.id             '_geom_hbond.atom_site_label_H'
     loop_
    _alias.definition_id       '_geom_hbond_atom_site_label_H'
                               '_geom_hbond.atom_site_id_H'
    _import.get          [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id            hbond
    _name.object_id              atom_site_label_H
     save_


save_geom_hbond.distance_DH
    _definition.id             '_geom_hbond.distance_DH'
     loop_
    _alias.definition_id       '_geom_hbond_distance_DH'
                               '_geom_hbond.dist_DH'
    _definition.update           2012-12-14
```

```
    _description.text
;
     The set of data items which specify the distance between the
     three atom sites identified by _geom_hbond.id.
;
    _name.category_id            hbond
    _name.object_id              distance_DH
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           0.0:
    _units.code                  angstroms
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     xc = List()

     Do i=0,1  {
         l,s  =   _geom_hbond.id [i]
         xf   =   SymEquiv(s, _atom_site[l].fract_xyz)
         xc +=  _atom_sites_Cartn_transform.matrix * xf
     }
      _geom_hbond.distance_DH =  Norm ( xc[0] - xc[1] )
;
     save_


save_geom_hbond.distance_HA
    _definition.id             '_geom_hbond.distance_HA'
     loop_
    _alias.definition_id       '_geom_hbond_distance_HA'
                               '_geom_hbond.dist_HA'
    _definition.update           2012-12-14
    _description.text
;
     The set of data items which specify the distance between the
     three atom sites identified by _geom_hbond.id.
;
    _name.category_id            hbond
    _name.object_id              distance_HA
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           0.0:
    _units.code                  angstroms
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     xc = List()

     Do i=1,2  {
         l,s  =   _geom_hbond.id [i]
         xf   =   SymEquiv(s, _atom_site[l].fract_xyz)
         xc +=  _atom_sites_Cartn_transform.matrix * xf
     }
      _geom_hbond.distance_HA =  Norm ( xc[0] - xc[1] )
;
     save_


save_geom_hbond.distance_DA
    _definition.id             '_geom_hbond.distance_DA'
     loop_
    _alias.definition_id       '_geom_hbond_distance_DA'
                               '_geom_hbond.dist_DA'
    _definition.update           2012-12-14
    _description.text
;
     The set of data items which specify the distance between the
     three atom sites identified by _geom_hbond.id.
;
    _name.category_id            hbond
    _name.object_id              distance_DA
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           0.0:
    _units.code                  angstroms
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     xc = List()

     Do i=0,2,2  {
         l,s  =   _geom_hbond.id [i]
         xf   =   SymEquiv(s, _atom_site[l].fract_xyz)
         xc +=  _atom_sites_Cartn_transform.matrix * xf
      }
       _geom_hbond.distance_DA =  Norm ( xc[0] - xc[1] )
;
     save_


save_geom_hbond.id
    _definition.id             '_geom_hbond.id'
    _definition.update           2012-11-22
    _description.text
;
     Atom site labels and symmetry operators as pairs for each of the
     three atom sites which define the hydrogen angle and distances.
     Site H is at the apex of the angle.
;
    _name.category_id            hbond
    _name.object_id              id
    _type.purpose                Composite
    _type.source                 Derived
    _type.container              List
    _type.contents               List(Code,Symop)
    _type.dimension              [3]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With  a  as  geom_hbond

         _geom_hbond.id =  [[ a.atom_site_label_D, a.site_symmetry_D ],
                           [ a.atom_site_label_H, a.site_symmetry_H ],
                           [ a.atom_site_label_A, a.site_symmetry_A ]]
```

```
;
     save_


save_geom_hbond.publ_flag
    _definition.id             '_geom_hbond.publ_flag'
     loop_
    _alias.definition_id       '_geom_hbond_publ_flag'
    _definition.update          2012-11-22
    _description.text
;
     This code signals whether the hydrogen-bond information
     is referred to in a publication or should be placed in a
     table of significant hydrogen-bond geometry.
;
    _name.category_id            hbond
    _name.object_id              publ_flag
    _type.purpose                State
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Code
  loop_
    _enumeration_set.state
    _enumeration_set.detail
                                 no  'do not include bond in special list'
                                 n   'abbreviation for "no"'
                                 yes 'do include bond in special list'
                                 y   'abbreviation for "yes"'
    _enumeration.default         no
     save_


save_geom_hbond.site_symmetry_A
    _definition.id             '_geom_hbond.site_symmetry_A'
     loop_
    _alias.definition_id       '_geom_hbond_site_symmetry_A'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            hbond
    _name.object_id              site_symmetry_A
     save_


save_geom_hbond.site_symmetry_D
    _definition.id             '_geom_hbond.site_symmetry_D'
     loop_
    _alias.definition_id       '_geom_hbond_site_symmetry_D'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            hbond
    _name.object_id              site_symmetry_D
     save_


save_geom_hbond.site_symmetry_H
    _definition.id             '_geom_hbond.site_symmetry_H'
     loop_
    _alias.definition_id       '_geom_hbond_site_symmetry_H'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            hbond
    _name.object_id              site_symmetry_H
     save_

     save_    #---------- close of GEOM_HBOND category

#------------------------------------------------------------------------------
```

```
save_GEOM_TORSION
    _definition.id               GEOM_TORSION
    _definition.scope            Category
    _definition.class            Loop
    _definition.update           2013-03-14
    _description.text
;
     The CATEGORY of data items used to specify the torsion angles in the
     structural model as derived from the atomic sites.
;
    _name.category_id            GEOM
    _name.object_id              TORSION
    _category.key_id           '_geom_torsion.key'
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     dmin =  _geom.bond_distance_min

     Loop  m1  as  model_site  :i  {

        rad1  =   m1.radius_bond + _geom.bond_distance_incr

        Loop  m2  as  model_site  :j  {

           If (i==j or m2.mole_index!=m1.mole_index) Next
           v21 =  m1.Cartn_xyz - m2.Cartn_xyz
           d21 =  Norm (v21)

           If (d21 < dmin or d21 > (rad1+m2.radius_bond)) Next
           rad2  =   m2.radius_bond + _geom.bond_distance_incr

           Loop  m3  as  model_site  :k  {

              If (k==i or k==j or m3.mole_index!=m2.mole_index) Next
              v23 =  m3.Cartn_xyz - m2.Cartn_xyz
              d23 =  Norm (v23)

              If (d23 < dmin or d23 > (rad2+m3.radius_bond)) Next
              rad3  =   m3.radius_bond + _geom.bond_distance_incr

              Loop  m4  as  model_site  :l  {

                 If (l==k or l==j or l==i or m4.mole_index!=m3.mole_index) Next
                 v34 =  m4.Cartn_xyz - m3.Cartn_xyz
                 d34 =  Norm (v34)

                 If (d34 < dmin or d34 > (rad3+m4.radius_bond)) Next

                 u1    =   v21 ^ v23
                 u2    =   v34 ^ v23

                 angle =  Acosd ( u1 * u2 / ( Norm(u1) * Norm(u2) ) )
                 If ( (u1^u2)*v23 < 0 ) angle = -angle
###############  If ( (u1^u2)*v23 > 0 ) angle = -angle

                 geom_torsion( .id        =  List ( m1.id,m2.id,m3.id,m4.id ),
                               .distances =  List ( d21,d23,d34 ),
                               .angle     =  angle )
     }   }   }    }
;
```

```
save_geom_torsion.key
    _definition.id              '_geom_torsion.key'
    _definition.update            2012-11-22
    _description.text
;
     Value is a unique key to a set of GEOM_TORSION items
     in a looped list.
;
    _name.category_id             torsion
    _name.object_id               key
    _type.purpose                 Key
    _type.source                  Related
    _type.container               Single
    _type.contents                Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;               _type.contents = Type_Contents(geom_torsion.id)
;
     Evaluation
;              _geom_torsion.key = _geom_torsion.id
;
     save_


save_geom_torsion.atom_site_label_1
    _definition.id              '_geom_torsion.atom_site_label_1'
     loop_
    _alias.definition_id        '_geom_torsion_atom_site_label_1'
                                '_geom_torsion.atom_site_id_1'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             torsion
    _name.object_id               atom_site_label_1
     save_


save_geom_torsion.atom_site_label_2
    _definition.id              '_geom_torsion.atom_site_label_2'
     loop_
    _alias.definition_id        '_geom_torsion_atom_site_label_2'
                                '_geom_torsion.atom_site_id_2'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             torsion
    _name.object_id               atom_site_label_2
     save_


save_geom_torsion.atom_site_label_3
    _definition.id              '_geom_torsion.atom_site_label_3'
     loop_
    _alias.definition_id        '_geom_torsion_atom_site_label_3'
                                '_geom_torsion.atom_site_id_3'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             torsion
    _name.object_id               atom_site_label_3
     save_


save_geom_torsion.atom_site_label_4
    _definition.id              '_geom_torsion.atom_site_label_4'
     loop_
    _alias.definition_id        '_geom_torsion_atom_site_label_4'
                                '_geom_torsion.atom_site_id_4'
    _import.get           [{"file":'templ_attr.cif',"save":'atom_site_label'}]
    _name.category_id             torsion
    _name.object_id               atom_site_label_4
     save_


save_geom_torsion.distances
    _definition.id              '_geom_torsion.distances'
    _definition.update            2012-11-22
    _description.text
;
     Distances between sites 1 - 2, 2 - 3 and 3 - 4.
;
    _name.category_id             torsion
    _name.object_id               distances
    _type.purpose                 Measurand
    _type.source                  Derived
    _type.container               List
    _type.contents                Real
    _type.dimension               [3]
    _units.code                   angstroms
     save_


save_geom_torsion.id
    _definition.id              '_geom_torsion.id'
    _definition.update            2012-11-22
    _description.text
;
     Atom site labels and symmetry operators as pairs for each of the
     four atom sites which define the torsion angle.
;
    _name.category_id             torsion
    _name.object_id               id
    _type.purpose                 Composite
    _type.source                  Derived
    _type.container               List
    _type.contents                List(Code,Symop)
    _type.dimension               [4]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With  a  as  geom_torsion

         _geom_torsion.id =  [[ a.atom_site_label_1, a.site_symmetry_1 ],
                              [ a.atom_site_label_2, a.site_symmetry_2 ],
                              [ a.atom_site_label_3, a.site_symmetry_3 ],
                              [ a.atom_site_label_4, a.site_symmetry_4 ]]
;
     save_


save_geom_torsion.publ_flag
    _definition.id              '_geom_torsion.publ_flag'
     loop_
    _alias.definition_id        '_geom_torsion_publ_flag'
    _definition.update            2012-11-22
    _description.text
;
     Code signals if the torsion angle is required for publication.
```

```
;
    _name.category_id            torsion
    _name.object_id              publ_flag
    _type.purpose                State
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Code
     loop_
    _enumeration_set.state
    _enumeration_set.detail
                                 Yes  'Publish'
                                 No   'Do not publish'
    _enumeration.default         No
     save_


save_geom_torsion.angle
    _definition.id             '_geom_torsion.angle'
     loop_
    _alias.definition_id       '_geom_torsion'
                               '_geom_torsion.value'
    _definition.update           2012-11-22
    _description.text
;
     Angle defined by the sites identifyed in _geom_torsion.id.
     The torsion-angle definition should be that of Klyne and Prelog.
     The vector direction *_label_2 to *_label_3 is the viewing
     direction, and the torsion angle is the angle of twist required
     to superimpose the projection of the vector between site 2 and
     site 1 onto the projection of the vector between site 3 and
     site 4. Clockwise torsions are positive, anticlockwise torsions
     are negative.
     Ref: Klyne, W. & Prelog, V. (1960). Experientia, 16, 521-523.
;
    _name.category_id            torsion
    _name.object_id              angle
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           -180.:180.
    _units.code                  degrees
     save_


save_geom_torsion.site_symmetry_1
    _definition.id             '_geom_torsion.site_symmetry_1'
     loop_
    _alias.definition_id       '_geom_torsion_site_symmetry_1'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            torsion
    _name.object_id              site_symmetry_1
     save_


save_geom_torsion.site_symmetry_2
    _definition.id             '_geom_torsion.site_symmetry_2'
     loop_
    _alias.definition_id       '_geom_torsion_site_symmetry_2'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            torsion
    _name.object_id              site_symmetry_2
     save_


save_geom_torsion.site_symmetry_3
    _definition.id             '_geom_torsion.site_symmetry_3'
     loop_
    _alias.definition_id       '_geom_torsion_site_symmetry_3'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            torsion
    _name.object_id              site_symmetry_3
     save_


save_geom_torsion.site_symmetry_4
    _definition.id             '_geom_torsion.site_symmetry_4'
     loop_
    _alias.definition_id       '_geom_torsion_site_symmetry_4'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            torsion
    _name.object_id              site_symmetry_4
     save_

     save_    #----------- close of GEOM_TORSION category

     save_    #----------- close of GEOM category


#===============================================================================

save_VALENCE
    _definition.id               VALENCE
    _definition.scope            Category
    _definition.class            Set
    _definition.update           2012-12-13
    _description.text
;
     The CATEGORY of items used to specify bond valence parameters
     used to calculate bond valences from bond lengths.
;
    _name.category_id            MODEL
    _name.object_id              VALENCE


#-------------------------------------------------------------------------------

save_VALENCE_PARAM
    _definition.id               VALENCE_PARAM
    _definition.scope            Category
    _definition.class            Loop
    _definition.update           2012-12-13
    _description.text
;
     The CATEGORY of items for listing bond valences.
;
    _name.category_id            VALENCE
    _name.object_id              PARAM
    _category.key_id           '_valence_param.key'


save_valence_param.key
    _definition.id             '_valence_param.key'
    _definition.update           2012-12-13
    _description.text
;
     Unique key to looped list of VALENCE_PARAM items.
;
```

```
    _name.category_id            param
    _name.object_id              key
    _type.purpose                Key
    _type.source                 Related
    _type.container              Single
    _type.contents               Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;              _type.contents = Type_Contents(valence_param.id)
;
     Evaluation
;              _valence_param.key = _valence_param.id
;
     save_


save_valence_param.id
    _definition.id             '_valence_param.id'
     loop_
    _alias.definition_id       '_valence_param_id'
    _definition.update           2012-12-13
    _description.text
;
     Unique index loop number of the valence parameter loop.
;
    _name.category_id            param
    _name.object_id              id
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Index
    _enumeration.range           1:
     save_


save_valence_param.ref_id
    _definition.id             '_valence_param.ref_id'
     loop_
    _alias.definition_id       '_valence_param_ref_id'
    _definition.update           2012-12-13
    _description.text
;
     Code linking parameters to the key valence_ref.id key
     in the reference list in category VALENCE_REF.
;
    _name.category_id            param
    _name.object_id              ref_id
    _name.linked_item_id       '_valence_ref.id'
    _type.purpose                Encode
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Code
     save_


save_valence_param.atom_1
    _definition.id             '_valence_param.atom_1'
     loop_
    _alias.definition_id       '_valence_param_atom_1'
    _definition.update           2012-12-13
    _description.text
;
     Atom type symbol for atom 1 forming a bond whose
     valence parameters are given in this category.
;
    _name.category_id            param
    _name.object_id              atom_1
    _name.linked_item_id       '_atom_type.symbol'
    _type.purpose                Encode
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Code
     save_


save_valence_param.atom_2
    _definition.id             '_valence_param.atom_2'
     loop_
    _alias.definition_id       '_valence_param_atom_2'
    _definition.update           2012-12-13
    _description.text
;
     Atom type symbol for atom 2 forming a bond whose
     valence parameters are given in this category.
;
    _name.category_id            param
    _name.object_id              atom_2
    _name.linked_item_id       '_atom_type.symbol'
    _type.purpose                Encode
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Code
     save_


save_valence_param.atom_1_valence
    _definition.id             '_valence_param.atom_1_valence'
     loop_
    _alias.definition_id       '_valence_param_atom_1_valence'
    _definition.update           2012-12-13
    _description.text
;
     The valence (formal charge) of the atom 1 whose bond
     valence parameters are given in this category.
;
    _name.category_id            param
    _name.object_id              atom_1_valence
    _type.purpose                Number
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           0.:
    _units.code                  coulomb
     save_


save_valence_param.atom_2_valence
    _definition.id             '_valence_param.atom_2_valence'
     loop_
    _alias.definition_id       '_valence_param_atom_2_valence'
    _definition.update           2012-12-13
    _description.text
;
     The valence (formal charge) of the atom 2 whose bond
     valence parameters are given in this category.
;
```

```
    _name.category_id            param
    _name.object_id              atom_2_valence
    _type.purpose                Number
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           0.:
    _units.code                  coulomb
     save_


save_valence_param.B
    _definition.id             '_valence_param.B'
     loop_
    _alias.definition_id       '_valence_param_B'
    _definition.update           2012-12-13
    _description.text
;
     The bond valence parameter B used in the expression
     s = exp[(Ro - R)/B] where s is the valence of bond length R.
;
    _name.category_id            param
    _name.object_id              B
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Real
    _enumeration.range           0.1:
    _units.code                  Angstroms
     save_


save_valence_param.Ro
    _definition.id             '_valence_param.Ro'
     loop_
    _alias.definition_id       '_valence_param_Ro'
    _definition.update           2012-12-13
    _description.text
;
     The bond valence parameter Ro used in the expression
     s = exp[(Ro - R)/B] where s is the valence of bond length R.
;
    _name.category_id            param
    _name.object_id              Ro
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Real
    _enumeration.range           1.:
    _units.code                  Angstroms
     save_


save_valence_param.details
    _definition.id             '_valence_param.details'
     loop_
    _alias.definition_id       '_valence_param_details'
    _definition.update           2012-12-13
    _description.text
;
     Details of valence parameters of stated bond.
;
    _name.category_id            param
    _name.object_id              details
    _type.purpose                Describe
    _type.source                 Recorded
    _type.container              Single
    _type.contents               Text
     save_

     save_    #----------- close of VALENCE_PARAM category


#-------------------------------------------------------------------------------

save_VALENCE_REF
    _definition.id               VALENCE_REF
    _definition.scope            Category
    _definition.class            Loop
    _definition.update           2012-12-13
    _description.text
;
     The CATEGORY of items for listing valence references.
;
    _name.category_id            VALENCE
    _name.object_id              REF
    _category.key_id           '_valence_ref.key'


save_valence_ref.key
    _definition.id             '_valence_ref.key'
    _definition.update           2012-12-13
    _description.text
;
     Unique key to looped list of VALENCE_REF items.
;
    _name.category_id            ref
    _name.object_id              key
    _type.purpose                Key
    _type.source                 Related
    _type.container              Single
    _type.contents               Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;              _type.contents = Type_Contents(valence_ref.id)
;
     Evaluation
;              _valence_ref.key = _valence_ref.id
;
     save_


save_valence_ref.id
    _definition.id             '_valence_ref.id'
     loop_
    _alias.definition_id       '_valence_ref_id'
    _definition.update           2012-12-13
    _description.text
;
     Unique loop code of the valence references.
;
    _name.category_id            ref
    _name.object_id              id
    _type.purpose                Encode
    _type.source                 Assigned
    _type.container              Single
```

```
    _type.contents                Code
     save_


save_valence_ref.reference
    _definition.id              '_valence_ref.reference'
     loop_
    _alias.definition_id        '_valence_ref_reference'
    _definition.update            2012-12-13
    _description.text
;
     Literature reference from which the valence parameters
     identified by _valence_param.id were taken
;
    _name.category_id             ref
    _name.object_id               reference
    _type.purpose                 Describe
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Text
     save_

     save_    #----------- close of VALENCE_REF category

     save_    #----------- close of VALENCE category


#============================================================================

save_MODEL_SITE
    _definition.id                MODEL_SITE
    _definition.scope             Category
    _definition.class             Loop
    _definition.update            2012-11-22
    _description.text
;
     The CATEGORY of data items used to describe atomic sites and
     connections in the proposed atomic model.
;
    _name.category_id             MODEL
    _name.object_id               SITE
    _category.key_id            '_model_site.key'
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
# Store unique sites as a local list

     atomlist  = List()
     Loop  a  as  atom_site  {
        axyz       =    a.fract_xyz
        cxyz       =   _atom_sites_Cartn_transform.matrix * axyz
        radb       =   _atom_type[a.type_symbol].radius_bond
        radc       =   _atom_type[a.type_symbol].radius_contact
        ls         =   List ( a.label, "1_555" )
        atomlist +=:   [ls, axyz, cxyz, radb, radc, 0]
     }

# Store closest connected sites as a list

     molelist  = List()
     dmin      =  _geom.bond_distance_min
     m         =  0
     n         =  0

     For [ls1,a1,c1,rb1,rc1,m1] in atomlist  {
         If (m1 != 0) Next
         m         +=  1
         n         +=  1
         molelist +:=  [ls1,a1,c1,rb1,rc1,n,m]
         atomlist -:=  [ls1,a1,c1,rb1,rc1,m]

         Repeat  {
             connect =  "no"

             For [ls2,a2,c2,rb2,rc2,n2,m2] in molelist  {
                 If (m2 != m) Next

                 For [ls3,a3,c3,rb3,rc3,m3] in atomlist  {
                     dmax  =  rb2 + rb3 + _geom.bond_distance_incr

                     Loop  s  as  symmetry_equiv  :ns   {

                         axyz      =   s.R * a3 + s.T
                         bxyz,tran =   Closest (axyz, a2)
                         cxyz      =  _atom_sites_Cartn_transform.matrix *bxyz
                         d         =   Norm (cxyz - c2)

                        If (d > dmin and d < dmax)          {
                            ls  =   List ( ls3[0], Symop(ns+1, tran) )

                            If (ls not in Strip(molelist,0))    {
                                n         +=  1
                                molelist +:=  [ls,bxyz,cxyz,rb3,rc3,n,m]
                                atomlist -:=  [ls3,a3,c3,rb3,rc3,m]
                                connect    =  "yes"
     }   }   }   }   }
         If (connect == "no") Break
     }  }

# Store connected molecular sites as MODEL_SITE list

     For [ls,ax,cx,rb,rc,n,m] in molelist  {

        model_site( .id              =  ls,
                    .fract_xyz       =  ax,
                    .Cartn_xyz       =  cx,
                    .radius_bond     =  rb,
                    .radius_contact  =  rc,
                    .index           =  n,
                    .mole_index      =  m  )
      }
;


save_model_site.key
    _definition.id              '_model_site.key'
    _definition.update            2012-11-22
    _description.text
;
     Value is a unique key to a set of MODEL_SITE items
     in a looped list.
;
    _name.category_id             site
    _name.object_id               key
    _type.purpose                 Key
    _type.source                  Related
```

```
    _type.container              Single
    _type.contents               Implied
     loop_
    _method.purpose
    _method.expression
     Definition
;              _type.contents = Type_Contents(model_site.id)
;
     Evaluation
;              _model_site.key = _model_site.id
;
     save_


save_model_site.display_colour
    _definition.id             '_model_site.display_colour'
    _definition.update           2013-01-23
    _description.text
;
     Display colour code assigned to this atom site. Note that the
     possible colours are enumerated in the colour_RBG list, and
     the default code is enumerated in the colour_hue list.
;
    _name.category_id            site
    _name.object_id              display_colour
    _type.purpose                State
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Code
    _import.get          [{"file":'templ_enum.cif',"save":'colour_RGB'},
                          {"file":'templ_enum.cif',"save":'colour_hue'}]
    _enumeration.def_index_id  '_model_site.type_symbol'
     save_


save_model_site.radius_bond
    _definition.id             '_model_site.radius_bond'
    _definition.update           2012-11-22
    _description.text
;
     Atomic radius of atom located at this site.
;
    _name.category_id            site
    _name.object_id              radius_bond
    _type.purpose                Number
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           0.1:
    _units.code                  angstroms
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
    With  m  as  model_site

    _model_site.radius_bond =  _atom_type[m.type_symbol].radius_bond
;
     save_


save_model_site.adp_matrix_beta
    _definition.id             '_model_site.adp_matrix_beta'
    _definition.update           2013-03-08
    _description.text
;
     Matrix of dimensionless anisotropic atomic displacement parameters.
;
    _name.category_id            site
    _name.object_id              adp_matrix_beta
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Matrix
    _type.contents               Real
    _type.dimension              [3,3]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     [label,symop] =   _model_site.id

     a = atom_site[label]
     s = symmetry_equiv[SymKey(symop)]

     _model_site.adp_matrix_beta =  s.R * a.tensor_beta * s.RT
;
     save_


save_model_site.adp_eigen_system
    _definition.id             '_model_site.adp_eigen_system'
    _definition.update           2012-11-22
    _description.text
;
     The set of three adp eigenvales and associated eigenvectors
     in the form of 4 element List. Each list has the form

                  (val, vecX, vecY, vecZ)

     where the vector elements are direction cosines to the orthogonal
     axes X,Y,Z. The lists are sorted in descending magnitude of val.
     That is, the list with the largest val is first, and the smallest
     val is last.
;
    _name.category_id            site
    _name.object_id              adp_eigen_system
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              List
    _type.contents               List(Real,Real,Real,Real)
    _type.dimension              [3]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
      A    =  _cell.orthogonal_matrix
      U    =  A * _model_site.adp_matrix_beta * Transpose(A) /(2*Pi**2)

      _model_site.adp_eigen_system  =  Eigen( U )

;
     save_


save_model_site.radius_contact
```

```
    _definition.id             '_model_site.radius_contact'
    _definition.update           2012-11-22
    _description.text
;
     Atomic contact radius of atom specie located at this site.
;
    _name.category_id            site
    _name.object_id              radius_contact
    _type.purpose                Number
    _type.source                 Derived
    _type.container              Single
    _type.contents               Real
    _enumeration.range           1.:
    _units.code                  angstroms
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With  m  as  model_site

    _model_site.radius_contact =  _atom_type[m.type_symbol].radius_contact
;
     save_


save_model_site.Cartn_xyz
    _definition.id             '_model_site.Cartn_xyz'
    _definition.update           2012-11-22
    _description.text
;
     Vector of Cartesian (orthogonal angstrom) atom site coordinates.
;
    _name.category_id            site
    _name.object_id              Cartn_xyz
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Matrix
    _type.contents               Real
    _type.dimension              [3]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With  m  as  model_site

    _model_site.Cartn_xyz =  _atom_sites_Cartn_transform.matrix * m.fract_xyz
;
     save_


save_model_site.fract_xyz
    _definition.id             '_model_site.fract_xyz'
    _definition.update           2012-12-14
    _description.text
;
     Vector of fractional atom site coordinates.
;
    _name.category_id            site
    _name.object_id              fract_xyz
    _type.purpose                Measurand
    _type.source                 Derived
    _type.container              Matrix
    _type.contents               Real
    _type.dimension              [3]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
        With  m  as  model_site

                       xyz =  _atom_site[m.label].fract_xyz

    _model_site.fract_xyz =  SymEquiv(m.symop, xyz)
;
     save_


save_model_site.id
    _definition.id             '_model_site.id'
    _definition.update           2012-11-22
    _description.text
;
     Identifier of model site in terms of the atom site label and
     symmetry operator.
;
    _name.category_id            site
    _name.object_id              id
    _type.purpose                Composite
    _type.source                 Derived
    _type.container              List
    _type.contents               Code,Symop
    _type.dimension              [1]
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
     With m as model_site

      _model_site.id =   List ( m.label, m.symop )
;
     save_


save_model_site.index
    _definition.id             '_model_site.index'
    _definition.update           2012-11-22
    _description.text
;
     Index number of an atomic site in the connected molecule.
;
    _name.category_id            site
    _name.object_id              index
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Index
    _enumeration.range           1:
     save_


save_model_site.label
    _definition.id             '_model_site.label'
    _definition.update           2012-11-22
    _description.text
```

```
;
     Code identifies a site in the atom_site category of data.
;
    _name.category_id            site
    _name.object_id              label
    _name.linked_item_id       '_atom_site.label'
    _type.purpose                Link
    _type.source                 Related
    _type.container              Single
    _type.contents               Code
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
      _model_site.label =   _model_site.id [0]
;
     save_


save_model_site.mole_index
    _definition.id             '_model_site.mole_index'
    _definition.update           2013-03-09
    _description.text
;
     Index number of a distinct molecules in the cell, not related by
     symmetry.
;
    _name.category_id            site
    _name.object_id              mole_index
    _type.purpose                Number
    _type.source                 Assigned
    _type.container              Single
    _type.contents               Index
    _enumeration.default         1
     save_


save_model_site.symop
    _definition.id             '_model_site.symop'
    _import.get          [{"file":'templ_attr.cif',"save":'site_symmetry'}]
    _name.category_id            site
    _name.object_id              symop
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
      _model_site.symop =   _model_site.id [1]
;
     save_


save_model_site.type_symbol
    _definition.id             '_model_site.type_symbol'
    _definition.update           2012-11-22
    _description.text
;
     Code to identify the atom specie(s) occupying this site.
;
    _name.category_id            site
    _name.object_id              type_symbol
    _name.linked_item_id       '_atom_type.symbol'
    _type.purpose                Link
    _type.source                 Related
    _type.container              Single
    _type.contents               Code
     loop_
    _method.purpose
    _method.expression
     Evaluation
;
    _model_site.type_symbol  =   AtomType ( _model_site.label )
;
     save_

     save_    #----------- close of MODEL_SITE category

     save_    #----------- close of MODEL category

         {"save":'PUBLICATION',  "file":'core_publn.dic', "mode":'full' },
         {"save":'FUNCTION',     "file":'core_funct.dic', "mode":'full' }]


    save_   #---------- close of CIF_CORE category

#===============================================================================
#  The dictionary's creation history.
#===============================================================================

     loop_
    _dictionary_audit.version
    _dictionary_audit.date
    _dictionary_audit.revision

      1.0.0   2005-12-12
;
   Initial version created from the CORE_3 version 3.5.02.
;
      1.0.01   2006-02-06
;
   Place all _import_dictionary.id components into a tuple.
;
      1.1.01   2006-02-08
;
   Remove save frame from dictionary definition attributes.
   Add definition id to the import dictionary tuple.
;
      1.1.02   2006-02-12
;
   Add attribute _dictionary.parent_id
;
      1.1.03   2006-02-12
;
   Change loop_ of _import_dictionary.id to a tuple.
;
      1.2.01   2006-02-21
;
   Basic change in dictionary structure where the dictionary data block now
   contains a saveframe defining the category of the DICTIONRY to which
   contained data categories are linked. It differs from other CATEGORY
   definitions in that its name is NOT part of the child data tags.
   This change allows imported dictionaries to be inserted without their
   data block header or non-savedframed attributes.
;
      1.2.02   2006-02-30
;
   Apply the DDL 3.6.05 attribute changes.
```

```
;
      1.2.03   2006-11-13
;
   Apply the DDL 3.6.10 attribute changes.
;
      1.2.04   2008-02-12
;
   Updated the IMPORT values as per ddl.dic 3.07.09
;
      1.2.05   2008-05-18
;
   Changed looped list of imports to _import_list.id syntax.
;
     1.3.01   2011-06-07
;
   Place all import lists into [[......]]
;
     1.4.01   2012-01-25
;
   For import.get change the key "fram" to "save".
;
     1.4.02   2012-12-18
;
   Add import for FUNCTION category containing all function definitions.
;
```