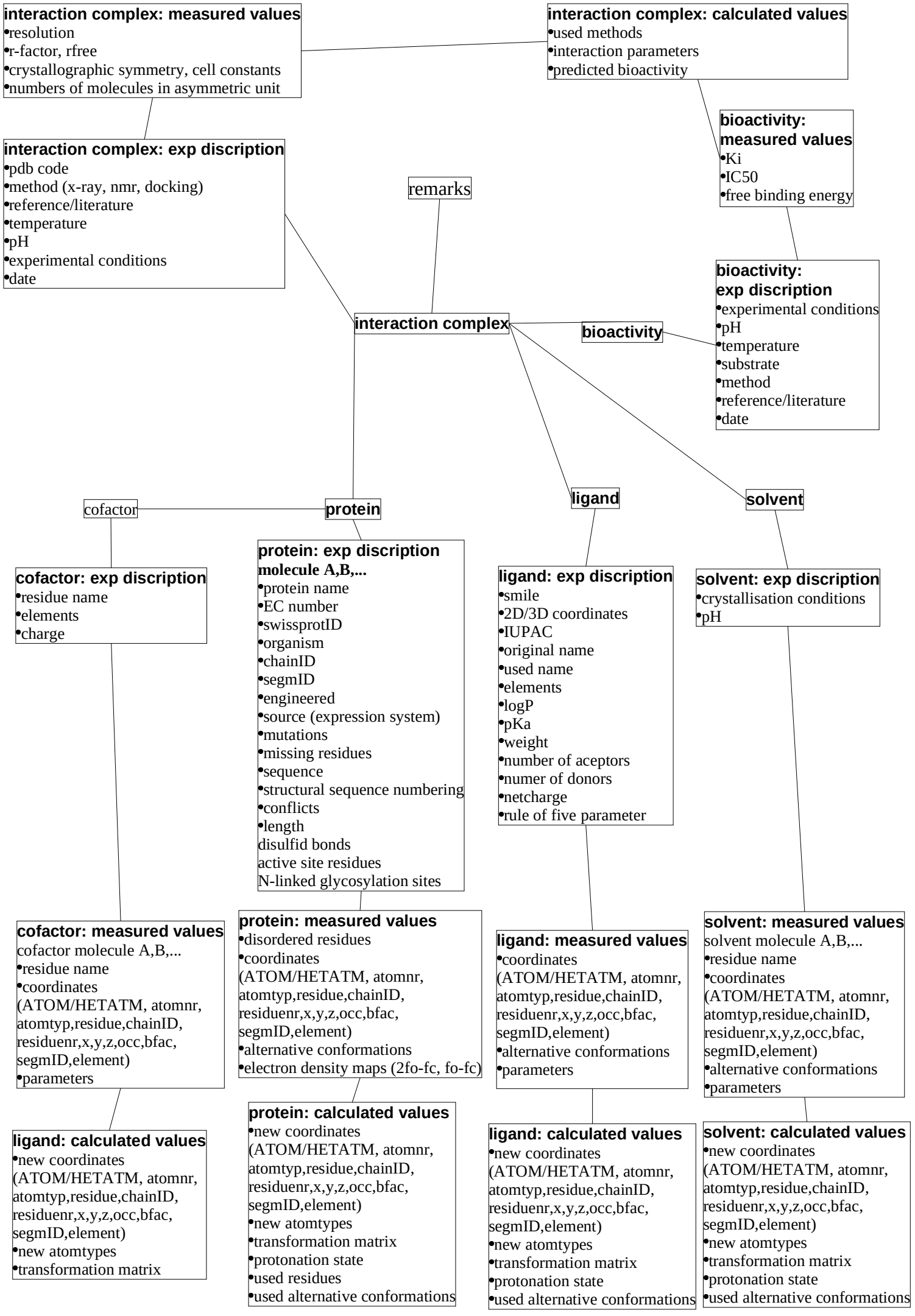
interaction complex: measured values
•resolution
•r-factor, rfree
•crystallographic symmetry, cell constants
•numbers of molecules in asymmetric unit
interaction complex: calculated values
•used methods
•interaction parameters
•predicted bioactivity
bioactivity: measured values
•Ki
•IC50
•free binding energy
interaction complex: exp discription
•pdb code
•method (x-ray, nmr, docking)
•reference/literature
•temperature
•pH
•experimental conditions
•date
remarks
bioactivity: exp discription
•experimental conditions
•pH
•temperature
•substrate
•method
•reference/literature
•date
interaction complex
bioactivity
cofactor
protein
ligand
solvent
cofactor: exp discription
•residue name
•elements
•charge
protein: exp discription
molecule A,B,...
•protein name
•EC number
•swissprotID
•organism
•chainID
•segmID
•engineered
•source (expression system)
•mutations
•missing residues
•sequence
•structural sequence numbering
•conflicts
•length
disulfid bonds
active site residues
N-linked glycosylation sites
ligand: exp discription
•smile
•2D/3D coordinates
•IUPAC
•original name
•used name
•elements
•logP
•pKa
•weight
•number of aceptors
•numer of donors
•netcharge
•rule of five parameter
solvent: exp discription
•crystallisation conditions
•pH
cofactor: measured values
cofactor molecule A,B,...
•residue name
•coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•parameters
protein: measured values
•disordered residues
•coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•alternative conformations
•electron density maps (2fo-fc, fo-fc)
ligand: measured values
•coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•alternative conformations
•parameters
solvent: measured values
solvent molecule A,B,...
•residue name
•coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•alternative conformations
•parameters
ligand: calculated values
•new coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•new atomtypes
•transformation matrix
protein: calculated values
•new coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•new atomtypes
•transformation matrix
•protonation state
•used residues
•used alternative conformations
ligand: calculated values
•new coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•new atomtypes
•transformation matrix
•protonation state
•used alternative conformations
solvent: calculated values
•new coordinates
(ATOM/HETATM, atomnr,
atomtyp,residue,chainID,
residuenr,x,y,z,occ,bfac,
segmID,element)
•new atomtypes
•transformation matrix
•protonation state
•used alternative conformations