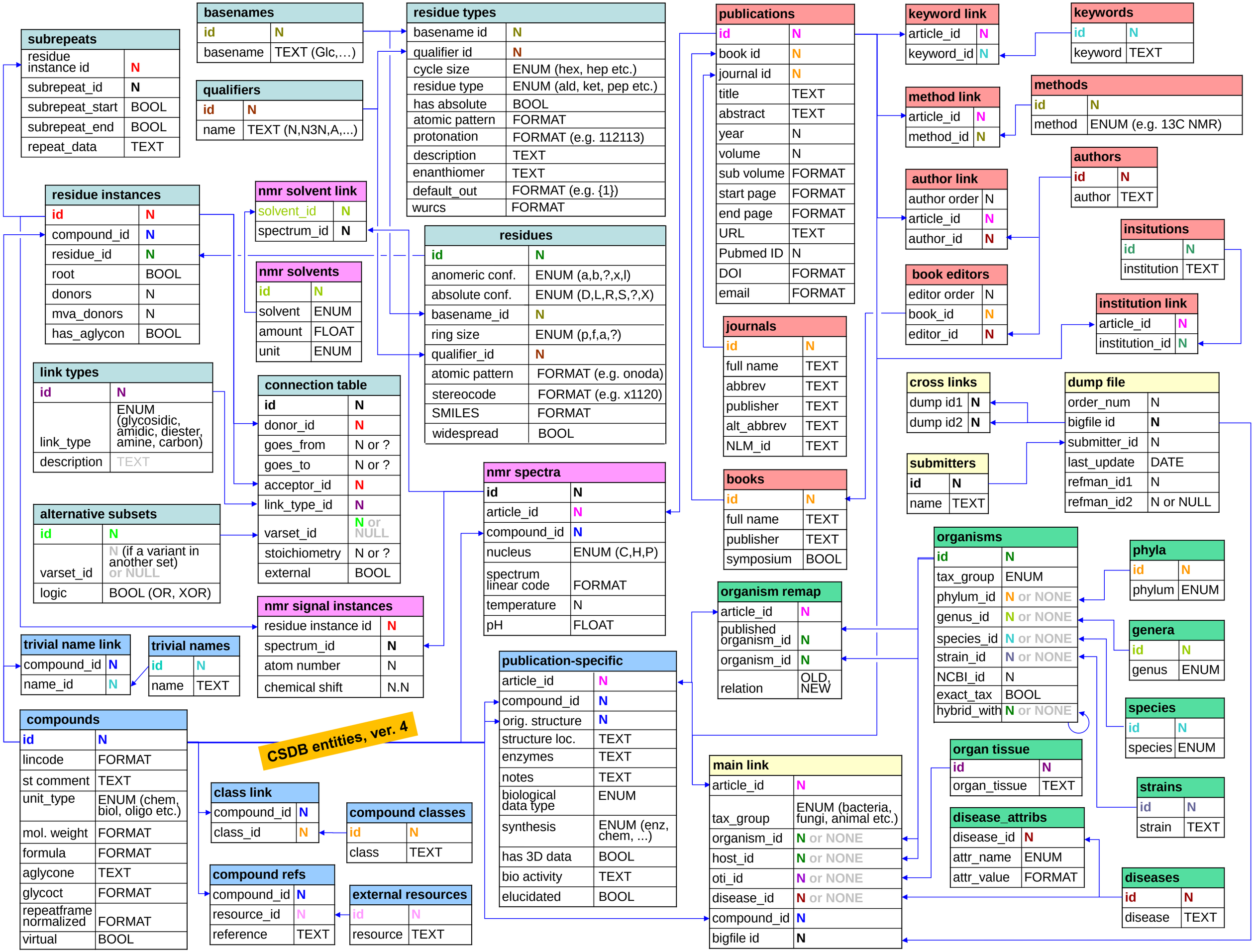
subrepeats
residue instance id N
subrepeat_id N
subrepeat_start BOOL
subrepeat_end BOOL
repeat_data TEXT
basenames
id N
basename TEXT (Glc,…)
qualifiers
id N
name TEXT (N,N3N,A,...)
residue types
basename id N
qualifier id N
cycle size ENUM (hex, hep etc.)
residue type ENUM (ald, ket, pep etc.)
has absolute BOOL
atomic pattern FORMAT
protonation FORMAT (e.g. 112113)
description TEXT
enanthiomer TEXT
default_out FORMAT (e.g. {1})
wurcs FORMAT
publications
id N
book id N
journal id N
title TEXT
abstract TEXT
year N
volume N
sub volume FORMAT
start page FORMAT
end page FORMAT
URL TEXT
Pubmed ID N
DOI FORMAT
email FORMAT
keyword link
article_id N
keyword_id N
keywords
id N
keyword TEXT
method link
article_id N
method_id N
methods
id N
method ENUM (e.g. 13C NMR)
author link
author order N
article_id N
author_id N
authors
id N
author TEXT
insitutions
id N
institution TEXT
book editors
editor order N
book_id N
editor_id N
institution link
article_id N
institution_id N
residue instances
id N
compound_id N
residue_id N
root BOOL
donors N
mva_donors N
has_aglycon BOOL
nmr solvent link
solvent_id N
spectrum_id N
nmr solvents
id N
solvent ENUM
amount FLOAT
unit ENUM
residues
id N
anomeric conf. ENUM (a,b,?,x,l)
absolute conf. ENUM (D,L,R,S,?,X)
basename_id N
ring size ENUM (p,f,a,?)
qualifier_id N
atomic pattern FORMAT (e.g. onoda)
stereocode FORMAT (e.g. x1120)
SMILES FORMAT
widespread BOOL
journals
id N
full name TEXT
abbrev TEXT
publisher TEXT
alt_abbrev TEXT
NLM_id TEXT
link types
id N
link_type ENUM (glycosidic, amidic, diester, amine, carbon)
description TEXT
connection table
id N
donor_id N
goes_from N or ?
goes_to N or ?
acceptor_id N
link_type_id N
varset_id N or NULL
stoichiometry N or ?
external BOOL
nmr spectra
id N
article_id N
compound_id N
nucleus ENUM (C,H,P)
spectrum linear code FORMAT
temperature N
pH FLOAT
books
id N
full name TEXT
publisher TEXT
symposium BOOL
cross links
dump id1 N
dump id2 N
dump file
order_num N
bigfile id N
submitter_id N
last_update DATE
refman_id1 N
refman_id2 N or NULL
submitters
id N
name TEXT
alternative subsets
id N
varset_id N (if a variant in another set) or NULL
logic BOOL (OR, XOR)
nmr signal instances
residue instance id N
spectrum_id N
atom number N
chemical shift N.N
organism remap
article_id N
published organism_id N
organism_id N
relation OLD, NEW
organisms
id N
tax_group ENUM
phylum_id N or NONE
genus_id N or NONE
species_id N or NONE
strain_id N or NONE
NCBI_id N
exact_tax BOOL
hybrid_with N or NONE
phyla
id N
phylum ENUM
genera
id N
genus ENUM
species
id N
species ENUM
trivial name link
compound_id N
name_id N
trivial names
id N
name TEXT
publication-specific
article_id N
compound_id N
orig. structure N
structure loc. TEXT
enzymes TEXT
notes TEXT
biological data type ENUM
synthesis ENUM (enz, chem, ...)
has 3D data BOOL
bio activity TEXT
elucidated BOOL
CSDB entities, ver. 4
compounds
id N
lincode FORMAT
st comment TEXT
unit_type ENUM (chem, biol, oligo etc.)
mol. weight FORMAT
formula FORMAT
aglycone TEXT
glycoct FORMAT
repeatframe normalized FORMAT
virtual BOOL
class link
compound_id N
class_id N
compound classes
id N
class TEXT
compound refs
compound_id N
resource_id N
reference TEXT
external resources
id N
resource TEXT
main link
article_id N
tax_group ENUM (bacteria, fungi, animal etc.)
organism_id N or NONE
host_id N or NONE
oti_id N or NONE
disease_id N or NONE
compound_id N
bigfile id N
organ tissue
id N
organ_tissue TEXT
disease_attribs
disease_id N
attr_name ENUM
attr_value FORMAT
strains
id N
strain TEXT
diseases
id N
disease TEXT