Package 'compas'

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Type Package

Title Conformational Manipulations of Protein Atomic Structures

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Author Samuel W.K. Wong, Dylan Shi, Megan Hazlett, Jasmine Cheng

Maintainer Samuel W.K. Wong <samuel.wong@uwaterloo.ca>

Description Manipulate and analyze 3-D structural geometry of Protein Data Bank (PDB) files.

License GPL-3

Imports Rcpp (>= 0.12.18), bio3d

LinkingTo Rcpp, RcppEigen

RoxygenNote 6.1.1

LazyData true

Depends R (>= 3.2.0)

NeedsCompilation yes

Repository CRAN

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Contents

atomdeps *Atom parameters and definitions for side chains*

Description

List of the atom dependencies and typical bond parameters in protein structures for side chains of the 20 standard amino acid types.

Usage

```
atomdeps
```

Format

A list for the 20 amino acid types, each having the attributes

- "tangle": Dihedral angle defined by atoms A-B-C-D as described below. NA's represent the free side chain dihedral angles *chi* for that amino acid.
- "names": The component atoms of the amino acid side chain. Represents atom D in the dihedral.
- "matx": The names of atoms A,B,C in the dihedral, with rows corresponding to the atoms in "names".
- "bangle": Planar bond angle formed between B-C-D
- "blength": Bond length between C-D

References

Engh, Richard A., and Robert Huber. "Accurate bond and angle parameters for X-ray protein structure refinement." *Acta Crystallographica* Section A 47.4 (1991): 392-400.

atomtype *Atom Type Table*

Description

Table listing the 167 standard atom types in protein structures (amino acid type and atom identifier pairs). Hydrogen atoms are not considered.

Usage

```
atomtype
```

Format

A two-column data frame, with "resid" providing the 3-letter amino acid abbreviation and "atomid" providing the component atoms of each amino acid.

Source

PDB ATOM entry: http://www.wwpdb.org/documentation/file-format-content/format33/sect9.html#ATOM

`calCo` *Calculate Cartesian coordinates for 1-4 bonded atoms*

Description

Consider atoms A-B-C-D forming a dihedral. Given coordinates for atoms A,B,C of the dihedral, the dihedral angle, bond angle, and bond length, calculate the Cartesian coordinates of atom D in the dihedral.

Usage

```
calCo(prev_atoms, length, bAngle, tAngle)
```

Arguments

`prev_atoms`	a 3x3 matrix of coordinates for atoms A-B-C in dihedral, listed by row
`length`	bond length between atoms C-D in dihedral
`bAngle`	planar bond angle between atoms B-C-D (in degrees)
`tAngle`	dihedral angle formed by atoms A-B-C-D (in degrees)

Value

Returns the vector of coordinates for the fourth atom in the dihedral

Examples

```
prevAtoms <- matrix(c(50.051, 37.144, -4.723,
 50.044, 36.248, -3.559,
 51.296, 35.369, -3.476), nrow=3, ncol=3, byrow=TRUE)
calCo(prevAtoms, length=1.33, bAngle=116.8, tAngle=-25.3)
```

calscco *Calculate Cartesian coordinates of side chains*

Description

Rotates the free side chain dihedral angles of an amino acid to the specified values. Calculates the updated Cartesian coordinates of all the atoms of that amino acid side chain.

Usage

```
calscco(pdb, resno, chi)
```

Arguments

pdb	A PDB object
resno	The residue number of the amino acid side chain to rotate
chi	A vector of dihedral angles (in degrees), with length matching the number of free side chain dihedral angles for that amino acid type. See atomdeps for definitions.

Details

Calls calCo successively for each atom in the amino acid side chain, using the bond parameters defined in atomdeps.

Value

Returns a PDB object with updated coordinates of side chain atoms in "resno".

Examples

```
## Position 10 of nat879 is ASP with 2 side chain dihedrals chi1 and chi2
nat879$atom[nat879$atom$resno==10,]
pdbn <- calscco(nat879,10,c(60.0,-80.0))
pdbn$atom[pdbn$atom$resno==10,]
```

dfireE *DFIRE Energy Evaluation for Protein Conformations*

Description

Calculates the energy of a protein conformation using the DFIRE potential.

Usage

```
dfireE(pdb)
```

Arguments

pdb	A PDB object, read using read.pdb.

Value

Returns the DFIRE energy.

References

Zhou, Hongyi, and Yaoqi Zhou. "Distance-scaled, finite ideal-gas reference state improves structure-derived potentials of mean force for structure selection and stability prediction." *Protein science* 11.11 (2002): 2714-2726.

Examples

```
dfireE(nat879)
```

---

nat879 *Sample Protein Conformation 1*

Description

A sample protein conformation in PDB format. Excerpted from the native structure of CASP12 target 879, residues 5-24

Usage

```
nat879
```

Format

A PDB object, read using read.pdb

Source

CASP12 data archive on Prediction Center: http://predictioncenter.org/download_area/CASP12/targets/casp12.targets_T0.releaseDec022016.tgz

pdbrmsd *Root Mean Squared Deviation (RMSD) of Two Protein Conformations*

Description

RMSD calculation between the atoms of two PDB objects.

Usage

```
pdbrmsd(pdb1, pdb2, start, end, type='all', optimal=FALSE)
```

Arguments

pdb1	PDB object containing reference coordinates of atoms in protein conformation.
pdb2	PDB object containing coordinates of atoms in protein conformation to compare with pdb1.
start	The starting residue position for the RMSD calculation. If not supplied, defaults to first residue of chain.
end	The ending residue position for the RMSD calculation. If not supplied, defaults to final residue of chain.
type	Specifies atoms to be included in the calculation. Can be 'all', 'CA' (CA atoms only), or 'backbone' (CA, N, C, O).
optimal	Apply optimal rotation and superposition? As described in https://cnx.org/contents/HV-RsdwL@23/Molecular-Distance-Measures

Details

Similar to rmsd, but with implementation in C++.

Value

Returns a list with calculated RMSD value and the optimal rotation matrix.

Examples

```
pdbrmsd(nat879, pred879, start=10, end=20, 'all', optimal=TRUE)
```

pred879 *Sample Protein Conformation 2*

Description

A sample protein conformation in PDB format. Excerpted from a structure prediction of CASP12 target 879, residues 5-24

Usage

```
pred879
```

Format

A PDB object, read using read.pdb

Source

CASP12 data archive on Prediction Center: http://predictioncenter.org/download_area/CASP12/targets/casp12.targets_TR.releaseDec022016.tgz

torsion *Calculate dihedral angle formed by four atoms*

Description

For Cartesian coordinates of atoms A-B-C-D, calculate the dihedral angle formed by viewing down the B-C axis.

Usage

```
torsion(a, b, c, d)
```

Arguments

a	length 3 vector of coordinates of atom A
b	length 3 vector of coordinates of atom B
c	length 3 vector of coordinates of atom C
d	length 3 vector of coordinates of atom D

Details

Similar to torsion.xyz, but with implementation in C++.

Value

Returns the dihedral angle (in degrees between -180 and 180).

Examples

```
torsion(c(50.051, 37.144, -4.723), c(50.044, 36.248, -3.559),
        c(51.296, 35.369, -3.476), c(51.930,35.119,-4.618))
```

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