sb_ncbr_channel_layer_residue

Data items in the SB_NCBR_CHANNEL_LAYER_RESIDUE category record details about layer of residues in structure.

layer_id [PK] [FK] [code]

The value of _sb_ncbr_channel_layer_residue.layer_id must uniquely identify the layer of the residue in channel.

channel_id [PK] [FK] [code]

The value of _sb_ncbr_channel_layer_residue.channel_id must uniquely identify the channel.

order [PK] [int]

The value of _sb_ncbr_channel_layer_residue.order must uniquely identify the layer of the residue in channel.

residue_id [FK] [int]

The value of _sb_ncbr_channel_layer_residue.residue_id must uniquely identify the residue of the layer in channel.

layer_id → order

residue_id → order

channel_id → id

sb_ncbr_channel_layer

Data items in the SB_NCBR_CHANNEL_LAYER category record information about properties of individual layer of calculated channels and pores.

channel_id [PK] [FK] [code]

Item _sb_ncbr_channel_layer.channel_id must uniquely identify the channel.

order [PK] [int]

Order of the layer in a particular channel.

bottleneck [boolean]

Item refers to the narrowest part of a channel within a protein structure.

charge [int]

Charge is calculated as a sum of charged amino acid residues in layer (ARG, LYS, HIS = +1; ASP, GLU = -1).

end_distance [float] [angstroms]

Specifies the end point of the layer in the tunnel

hydropathy [float] [-4.5..4.5]

Hydropathy is calculated as an average of the hydropathy index assigned to residues according to the method of Kyte and Doolittle.

hydrophobicity [float] [-1.14..1.81]

Hydrophobicity is calculated as an average of normalised hydrophobicity scales of layer.

local_minimum [boolean]

Determines whether layer is in local minimum.

min_free_radius [float] [angstroms] [0.0..inf)

The minimal radius of a layer within the channel is limited by the three closest main chain atoms to allow sidechain flexibility

min_radius [float] [angstroms] [0.0..inf)

The minimal radius of a layer within the channel limited by the three closest atoms.

mutability [int] [0.0..inf)

Mutability is calculated as an average of the relative mutability index (Jones1992) of each layer. Relative mutability is based on empirical substitution matrices between similar protein sequences.

numNegatives [int] [0.0..inf)

Number of negatively charged amino acids in a particular layer.

numPositives [int] [0.0..inf)

Number of positively charged amino acids in a particular layer.

polarity [float] [0.0..52.0]

Polarity is calculated as an average of amino acid polarities of layer assigned according to the method of Zimmerman et al.

start_distance [float] [angstroms]

Specifies the start point of the layer in the tunnel.

sb_ncbr_channel_annotation

Data items in the SB_NCBR_CHANNEL_ANNOTATION category record details about the annotation of the channels from ChannelsDB. The SB_NCBR_CHANNEL_ANNOTATION records define the criteria used to identify these channels.

id [PK] [code]

Unique identifier of an annotation.

channel_id [FK] [code]

Identifier of a channel particular annotation belongs to.

description [text]

Description of the structure of the molecule or tunnel. It may contain information about its properties, location and function.

name [text]

Unique name assigned to a channel or a pore.

reference [code]

Identifier used to uniquely specify the bibliographic entry.

reference_type [code]

Type of the identifier used to uniquely specify bibliographic entry. For example 'DOI'.

sb_ncbr_channel_layer_weighted_props

Data items in the SB_NCBR_CHANNEL_LAYER_WEIGHTED_PROPS category record information about the properties of a channel calculated as the weighted average of the individual layer properties.

channel_id [PK] [FK] [code]

Item _sb_ncbr_channel_layer_weighted_props.channel_id must uniquely identify the channel.

hydropathy [float] [-4.5..4.5]

Hydropathy is calculated as an average of the hydropathy index in layer assigned to residues according to the method of Kyte and Doolittle.

hydrophobicity [float] [-1.14..1.81]

Hydrophobicity is calculated as an average of normalised hydrophobicity scales of layer.

logD [float] [-3.0..2.59]

Lipophilicity (logD-scale) is calculated as octanol/water distribution coefficients of Cβ side-chain fragments and mainchain (-0.86) at pH 7.4 of layer via www.chemicalize.org. The distribution coefficient takes into account the ionisation of compounds.

logP [float] [-1.03..2.59]

Lipophilicity (logP-scale) is calculated as octanol/water partition coefficients of Cβ fragments of side-chains and mainchain (-0.86) of layer via www.chemicalize.org.

logS [float] [-2.48..2.63]

Solubility (logS-scale) is calculated as water solubility of Cβ side-chain fragments and mainchain (0.81) at pH 7.4 of layer via www.chemicalize.org. Our estimated value is a unit stripped logarithm (base 10) of the solubility measured in mol/litre. It measures how well individual residues can interact with water molecules.

mutability [int] [0.0..inf)

Mutability is calculated as an average of the relative mutability index (Jones1992) of layer. Relative mutability is based on empirical substitution matrices between similar protein sequences.

polarity [float] [0.0..52.0]

Polarity is calculated as an average of amino acid polarities of layer assigned according to the method of Zimmerman et al.

sb_ncbr_channel_profile

Data items in the SB_NCBR_CHANNEL_PROFILE category record details about the calculated channels and pores.

channel_id [PK] [FK] [code]

Item _sb_ncbr_channel_profile.channel_id must uniquely identify the channel.

T [PK] [float] [0.0..1.0]

T is a normalized distance parameter ranging from 0 to 1, where 0 corresponds to the start point and 1 to the end point of the path.

charge [int]

Charge is calculated as a sum of charged amino acid residues (ARG, LYS, HIS = +1; ASP, GLU = -1)

distance [float] [angstroms] [0.0..inf)

The distance from starting point of trajectory

free_radius [float] [angstroms] [0.0..inf)

The radius of a sphere within the channel is limited by the three closest main chain atoms to allow sidechain flexibility.

radius [float] [angstroms] [0.0..inf)

The radius of a sphere within the channel limited by the three closest atoms.

x [float] [angstroms]

The item _sb_ncbr_channel_profile.x represents the position of x point in the Cartesian coordinate system.

y [float] [angstroms]

The item _sb_ncbr_channel_profile.y represents the position of y point in the Cartesian coordinate system.

z [float] [angstroms]

The item _sb_ncbr_channel_profile.z represents the position of z point in the Cartesian coordinate system.

sb_ncbr_channel_props

Data items in the SB_NCBR_CHANNEL_PROPS category record information about properties in calculated channels and pores.

channel_id [PK] [FK] [code]

Item _sb_ncbr_channel_props.channel_id must uniquely identify the channel.

bRadius [float]

Item represent Radius + RMSF calculated from B-factors of residues within individual layers

charge [int]

Charge is calculated as a sum of charged amino acid residues. Example ARG, LYS, HIS = +1; ASP, GLU = -1

hydropathy [float] [-4.5..4.5]

The hydropathy index is connected to hydrophilicity/hydrophobicity of amino acids. The most hydrophilic is ARG = -4.5; most hydrophobic ILE = 4.5.

hydrophobicity [float] [-1.14..1.81]

Hydrophobicity is calculated as an average of normalised hydrophobicity scales. According to the hydrophobicity value, the most hydrophilic amino acid is GLU (-1.140), and ILE (1.810) is the most hydrophobic.

ionizable [float]

Ionisable residues can also be viewed in the channel profile or directly as the selection on the visualised structure. Ionizable means that the substance can go into an ionic state, i.e. split into positively or negatively charged particles.

logD [float] [-3.0..2.59]

Lipophilicity (logD-scale) is calculated as octanol/water distribution coefficients of Cβ side-chain fragments and mainchain (-0.86) at pH 7.4 via www.chemicalize.org. The distribution coefficient takes into account the ionisation of compounds.

logP [float] [-1.03..2.59]

Lipophilicity (logP-scale) is calculated as octanol/water partition coefficients of Cβ fragments of side-chains and mainchain (-0.86) via www.chemicalize.org.

logS [float] [-2.48..2.63]

Solubility (logS-scale) is calculated as water solubility of Cβ side-chain fragments and mainchain (0.81) at pH 7.4 via www.chemicalize.org. Our estimated logS value is a unit stripped logarithm (base 10) of the solubility measured in mol/litre. It measures how well individual residues can interact with water molecules.

mutability [integer] [0.0..inf)

Mutability is calculated as an average of the relative mutability index. Relative mutability is based on empirical substitution matrices between similar protein sequences.

numNegatives [int] [0.0..inf)

Number of negatively charged amino acids

numPositives [int] [0.0..inf)

Number of positively charged amino acids

polarity [int] [0.0..52.0]

Polarity is calculated as an average of amino acid polarities assigned according to the method of Zimmerman et al. Polarity ranges from completely nonpolar amino acids (ALA, GLY = 0.00) through polar residues (e.g. SER = 1.67) towards charged residues (GLU = 49.90, ARG = 52.00).

sb_ncbr_channel_residue

Data items in the SB_NCBR_CHANNEL_RESIDUE category record details about residues in structure.

channel_id [PK] [FK] [code]

The value of _sb_ncbr_channel_residue.id must uniquely identify the residue in channel.

order [PK] [int]

The value of _sb_ncbr_channel_residue.order maintains the order of the residues along the channel.

backbone [boolean]

Specifies whether the residue is the part of the protein backbone.

chain_id [FK] [code]

Item _sb_ncbr_channel_residue.chain_id identify the chain of the residue in channel.

sequence_number [FK] [int]

Item _sb_ncbr_channel_residue.sequence_number provides a unique value assigned to the residue in sequence of the structure.

sb_ncbr_channel

Data items in the SB_NCBR_CHANNEL category record details about the method used to calculate the channels and pores.

id [PK] [code]

Unique identifier of a channel or a pore.

auto [boolean]

The item indicates whether the starting point for channel calculation was chosen automatically.

cavity [int]

The value of the item _sb_ncbr_channel.cavity provides information about the number of cavities occurring in the structure.

method [text]

Name of the method used for channel calculations. The options are CSATunnel, MOLEonline, etc.

software [text]

Software for channel calculations. The options might be MOLE, Caver, etc.

type [text]

Type of the channel. The options are Pore, Path, etc.

channel_id → id

channel_id → id

channel_id → id

channel_id → id

channel_id → id

sequence_number → auth_seq_id

chain_id → auth_asym_id

atom_site