**Table 1 The description of the selected DSSR property**

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| **Feature** | **Description** |
| **nt\_code** | (str), (e.g. ‘U’) |
| **alpha** | (float) base angle in degrees [-180, 180]. |
| **beta** | (float) base angle in degrees [-180, 180]. |
| **gamma** | (float) base angle in degrees [-180, 180]. |
| **delta** | (float) base angle in degrees [-180, 180]. |
| **epsilon** | (float) base angle in degrees [-180, 180]. |
| **zeta** | (float) base angle in degrees [-180, 180]. |
| **epsilon\_zeta** | (float) base angle in degrees [-180, 180]. |
| **chi** | (float) |
| **C5prime\_xyz** | 5’ Carbon xyz coordinates (e.g. `[-1.343, 8.453, 1.288]) |
| **P\_xyz** | Phosphate coordinates. |
| **ssZp** | (float) (e.g. 4.41) |
| **Dp** | (float) (e.g. 4.404) |
| **splay\_angle** | (float) (e.g. 21.6) |
| **splay\_distance** | (float) (e.g. 3.612) |
| **splay\_ratio** | (float) (e.g. 0.199) |
| **eta** | (float) (e.g. 169.652), |
| **theta** | (float) (e.g. -167.457), |
| **eta\_prime** | (float) (e.g. -176.189) |
| **theta\_prime** | (float) (e.g. -167.27) |
| **eta\_base** | (float) (e.g. -135.681) |
| **theta\_base** | (float) (e.g. -141.003) |
| **v0** | (float) (e.g 8.194) |
| **v1** | (float) (e.g. -28.393) |
| **v2** | (float) |
| **v3** | (float) |
| **v4** | (float) |
| **amplitude** | (float) |
| **phase\_angle** | (float) |
| **suiteness** | (float) (measure of conformer - match quality ( range 0 to 1) ) |
| **filter\_rmsd** | (float) |
| **puckering** | (str) (e.g. “C3’-endo”) |
| **sugar\_class** | (str) (e.g. “~C3’-endo”) |
| **bin** | (str) (e.g. ‘33t’) ( name of the 12 bins based on [ delta (i -1) , delta , gamma ], where delta (i -1) and delta can be either 3 ( for C3 ‘- endo sugar ) or 2 ( for C2 ‘- endo ) and gamma can be p/t/ m ( for gauche +/ trans / gauche - conformations , respectively ) (2 x2x3 =12 combinations : 33p , 33t , … 22m); ‘inc’ refers to incomplete cases (i .e., with missing torsions ) , and ‘trig’ to triages ( i.e., with torsion angle outliers ) |

**Table 2 The description of 20 edge types**

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| **Edge type** | **Description** |
| **CWW** | Cis-Watson-Crick/Watson-Crick:Refers to Watson-Crick pairs with a cis configuration, meaning both bases are on the same side. |
| **CWH** | Cis-Watson-Crick/Hoogsteen:Combination of Watson-Crick pairs with a cis configuration and Hoogsteen pairs. |
| **CWS** | Cis-Watson-Crick/Sugar:Combination of Watson-Crick pairs with a cis configuration and Sugar pairs. |
| **CHW** | Cis-Hoogsteen/Watson-Crick:Combination of Hoogsteen pairs with a cis configuration and Watson-Crick pairs. |
| **CWW** | Cis-Hoogsteen/Hoogsteen:Refers to Hoogsteen pairs with a cis configuration, meaning both bases are on the same side. |
| **CHS** | Cis-Hoogsteen/Sugar:Combination of Hoogsteen pairs with a cis configuration and Sugar pairs. |
| **CSW** | Cis-Sugar/Watson-Crick:Combination of Sugar pairs with a cis configuration and Watson-Crick pairs. |
| **CSH** | Cis-Sugar/Hoogsteen:Combination of Sugar pairs with a cis configuration and Hoogsteen pairs. |
| **CSS** | Cis-Sugar/Sugar:Refers to Sugar pairs with a cis configuration, meaning both bases are on the same side. |
| **TWW** | Trans-Watson-Crick/Watson-Crick:Refers to Watson-Crick pairs with a trans configuration, meaning bases are on opposite sides. |
| **TWH** | Trans-Watson-Crick/Hoogsteen：Combination of Watson-Crick pairs with a trans configuration and Hoogsteen pairs. |
| **TWS** | Trans-Watson-Crick/Sugar ：Combination of Watson-Crick pairs with a trans configuration and Sugar pairs. |
| **THW** | Trans-Hoogsteen/Watson-Crick：Combination of Hoogsteen pairs with a trans configuration and Watson-Crick pairs. |
| **THH** | Trans-Hoogsteen/Hoogsteen：Refers to Hoogsteen pairs with a trans configuration, meaning bases are on opposite sides. |
| **THS** | Trans-Hoogsteen/Sugar：Combination of Hoogsteen pairs with a trans configuration and Sugar pairs. |
| **TSW** | Trans-Sugar/Watson-Crick:Combination of Sugar pairs with a trans configuration and Watson-Crick pairs. |
| **TSH** | Trans-Sugar/Hoogsteen:Combination of Sugar pairs with a trans configuration and Hoogsteen pairs. |
| **TSS** | Trans-Sugar/Sugar:Refers to Sugar pairs with a trans configuration, meaning bases are on opposite sides. |
| **B53** | backbone |
| **B35** | backbone |