A. CONF17 Benchmark

A.1. Data Generation

The ISO17 dataset (Schütt et al., 2017a) was processed in the following way. First, conformations in which could not be parsed by the tool XYZ2MOL (Jensen, 2019) were discarded. Second, the molecular graphs were augmented by adding auxiliary edges for reasons described in the main text. This can lead to an over-specification of the system's geometry, however, this did not pose a problem in our experiments.

A.2. Input Features

Below we list the node and edge features in the CONF17 benchmark.

Table 3. Node features.

Feature	Data Type	Dimension
atomic number	one-hot (H, He, ... F)	9
chiral tag	one-hot (R, S, and None)	3

Table 4. Edge features.

Feature	Data Type	Dimension
kind	one-hot (E_{bond}, E_{angle}, or E_{dihedral})	3
stereo chemistry	one-hot (E, Z, Any, None)	4
type	one-hot (single, double, triple, aromatic or None)	5
is aromatic	binary	1
is conjugated	binary	1
is in ring of size	one-hot (3, 4, . . . , 9) or None	7

B. Model Architecture

The source code of the model (including pre-processing scripts) is available online https://github.com/gncs/graphdg. In Table 5, the model architecture are summarized. After each hidden layer, a ReLU non-linearity is used. In Table 6, all hyperparameters are listed.

Table 5. Model architecture for generative model.

Network	Output Layers
$F_{\text{enc},v}$	$50, 50, 10$
$F_{\text{enc},e}$	$50, 50, 10$
$\text{MP}_{\text{enc}}^{(t)}$	$50, 50, 10$
$\text{MP}_{\text{dec}}^{(t)}$	$50, 50, 10$
$R_{\text{dec},v}$	$50, 50, 1$
$R_{\text{dec},e}$	$50, 50, 1$

Table 6. Hyperparameters used throughout this work.

Hyperparameter	Value
Minibatch size	32
Learning rate	0.001
Number of convolutions T	3

C. Computational Details

C.1. Quantum-Chemical Calculations

All quantum-chemical calculations were carried out with the PySCF program package (version 1.5) (Sun et al., 2018) employing the exchange-correlation density functional PBE (Perdew et al., 1996), and the def2-SVP (Weigend & Ahlrichs, 2005; Weigend, 2006) basis set.

Conformations generated by DL4CHEM did not succeed as some atoms were too close to each other. Self-consistent field algorithms in quantum-chemical software such as PySCF do not converge for such molecular structures.

With quantum-chemical methods, we calculate several properties that concern the states of the electrons in the conformation. These are the total electronic energy E_{elec}, the energy of the electron in the highest occupied molecular orbital (HOMO in eV) ϵ_{HOMO}, the energy of the lowest unoccupied molecular orbital (LUMO in eV) ϵ_{LUMO}, and the norm of the dipole moment μ (in debye).

C.2. Euclidean Distance Geometry

We refer the reader to Havel (2002) for theory on EDG, algorithms, and chemical applications. In summary, the EDG procedure consists of the following three steps:

1. Bound smoothing: extrapolating a complete set of lower and upper limits on all the distances from the sparse set of lower and upper bounds.

2. Embedding: choosing a random distance matrix from within these limits, and computing coordinates that are a certain best-fit to the distances.

3. Optimization: optimizing these coordinates versus an

error function which measures the total violation of the distance (and chirality) constraints.

We use the EDG implementation found in RDKIT (Riniker & Landrum, 2015) with default settings.

D. Generation of Conformations

Fig. 7 shows an overlay of 50 conformations from the ground-truth, RDKIT, DL4CHEM, and GRAPHDG based on two random molecular graphs from a test set.

E. Distributions over Distances

We show the marginal distributions $p(d_k|G)$ and $p(d_i, d_j|G)$ of ground-truth and predicted distances (in Å) for additional molecules from a test set.
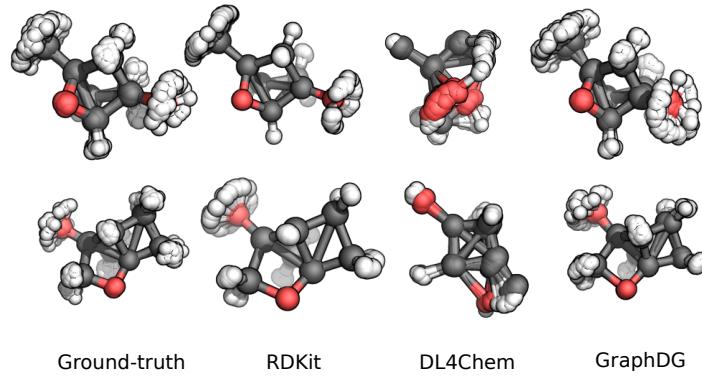
Figure 7. Overlay of 50 conformations from the ground-truth, RDKIT, DL4CHEM, and GRAPHDG based on two random molecular graphs from a test set. C, O, and H atoms are colored gray, red, and white, respectively.
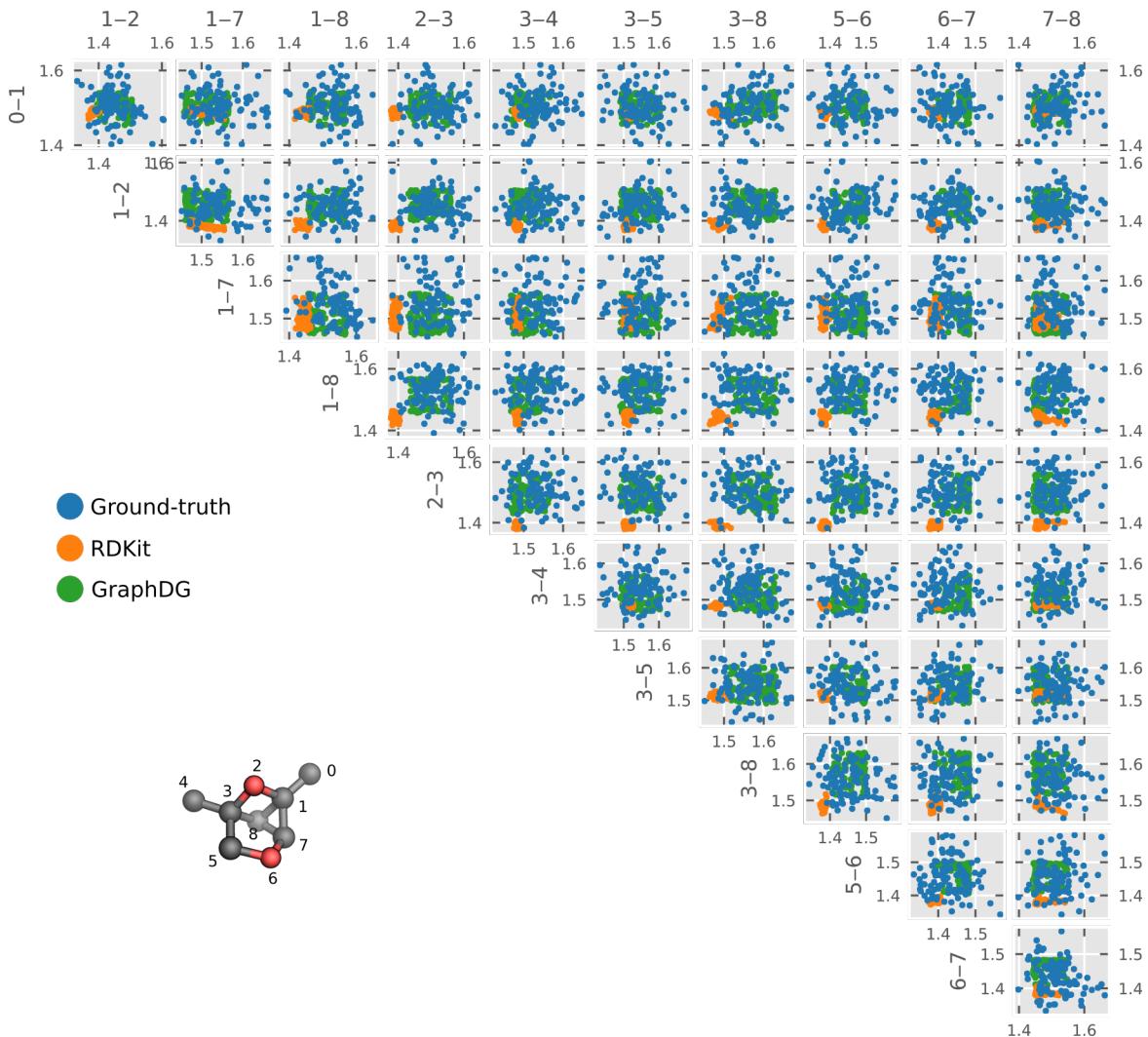

Figure 8. Marginal distributions $p(d_i, d_j|G)$ of ground-truth and predicted distances for a molecular graph from a test set (in Å). Here, d_i and d_j are restricted to edges representing bonds between C and O atoms. In the 3D structure of the molecule, carbon and oxygen atoms are colored gray and red, respectively. H atoms are omitted for clarity.
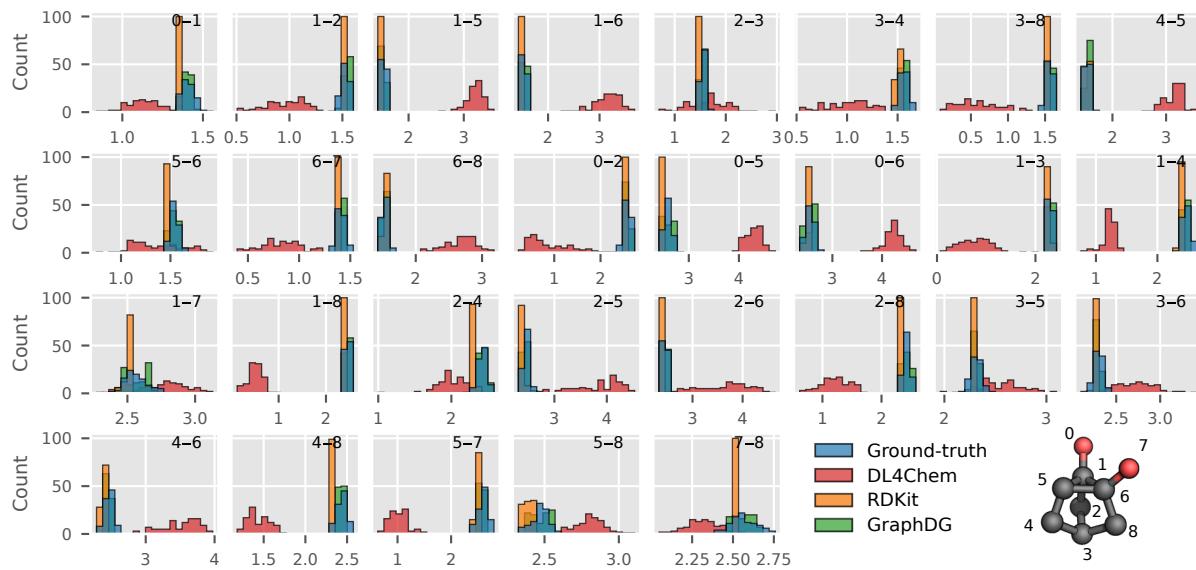
Figure 9. See caption of Fig. 5
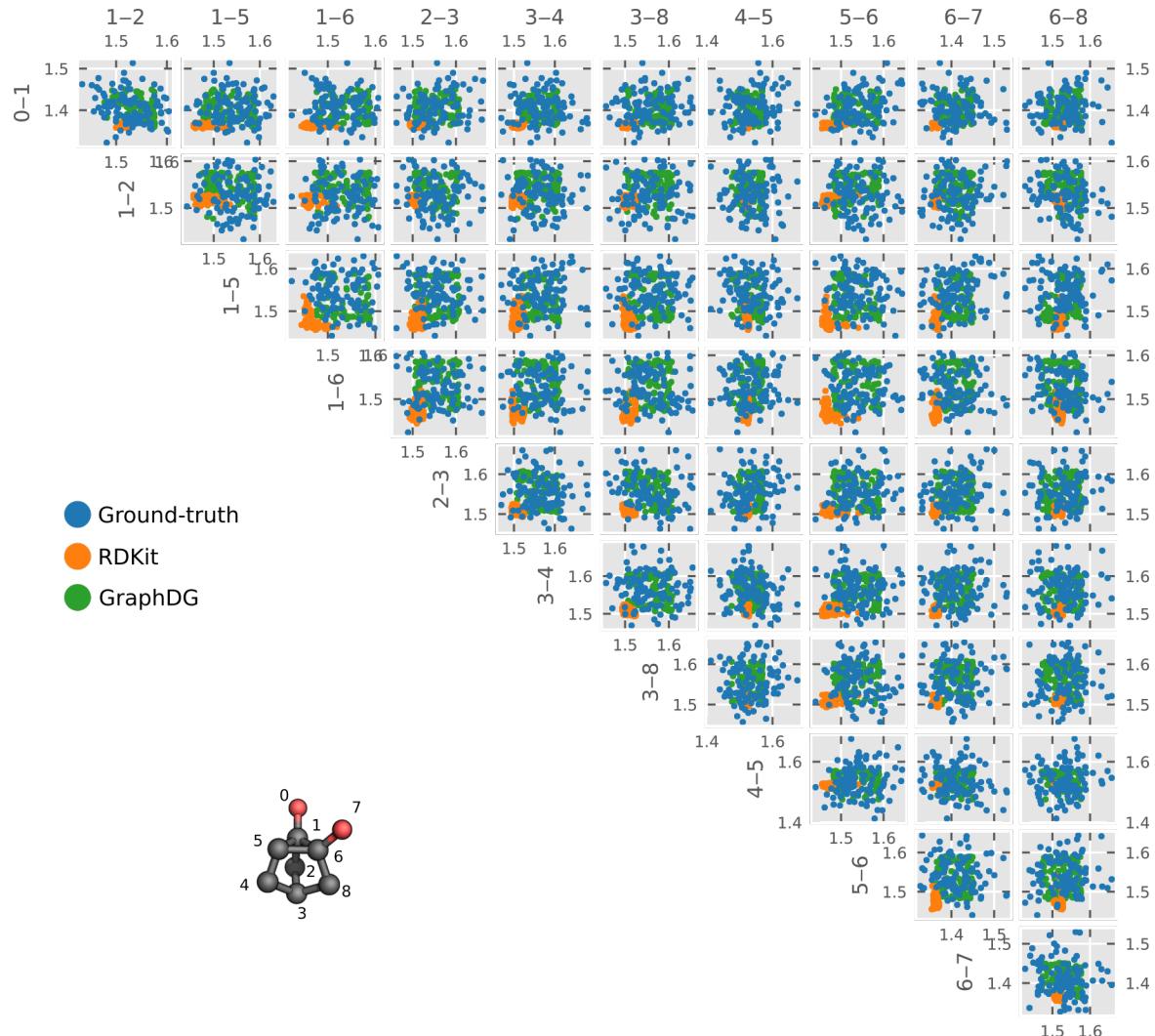
Figure 10. See caption of Fig. 8
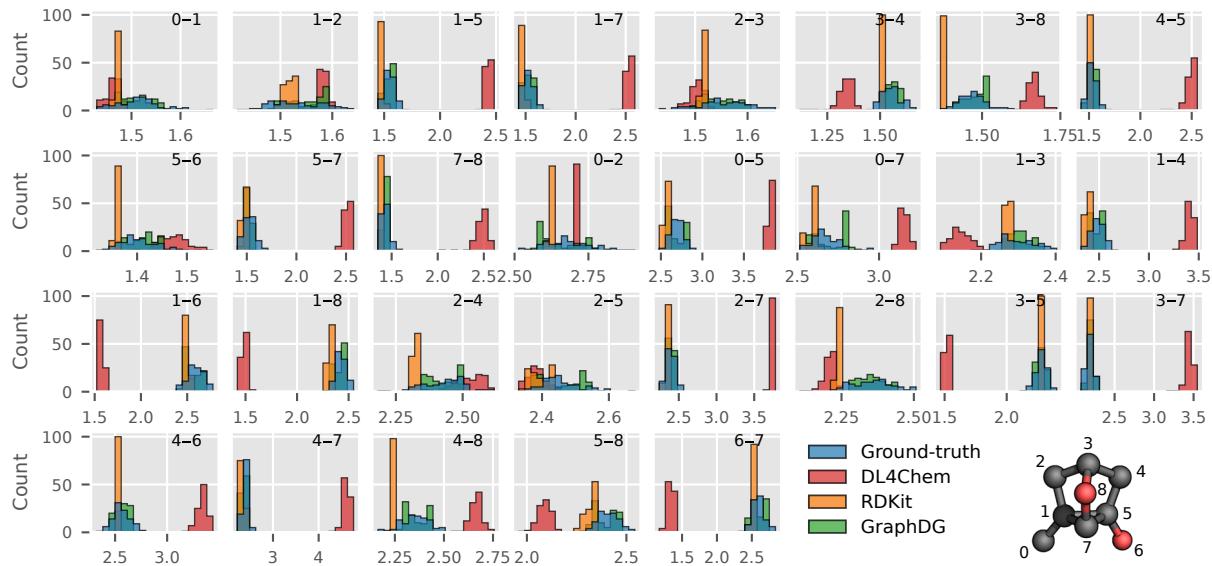
*Figure 11.* See caption of Fig. 5
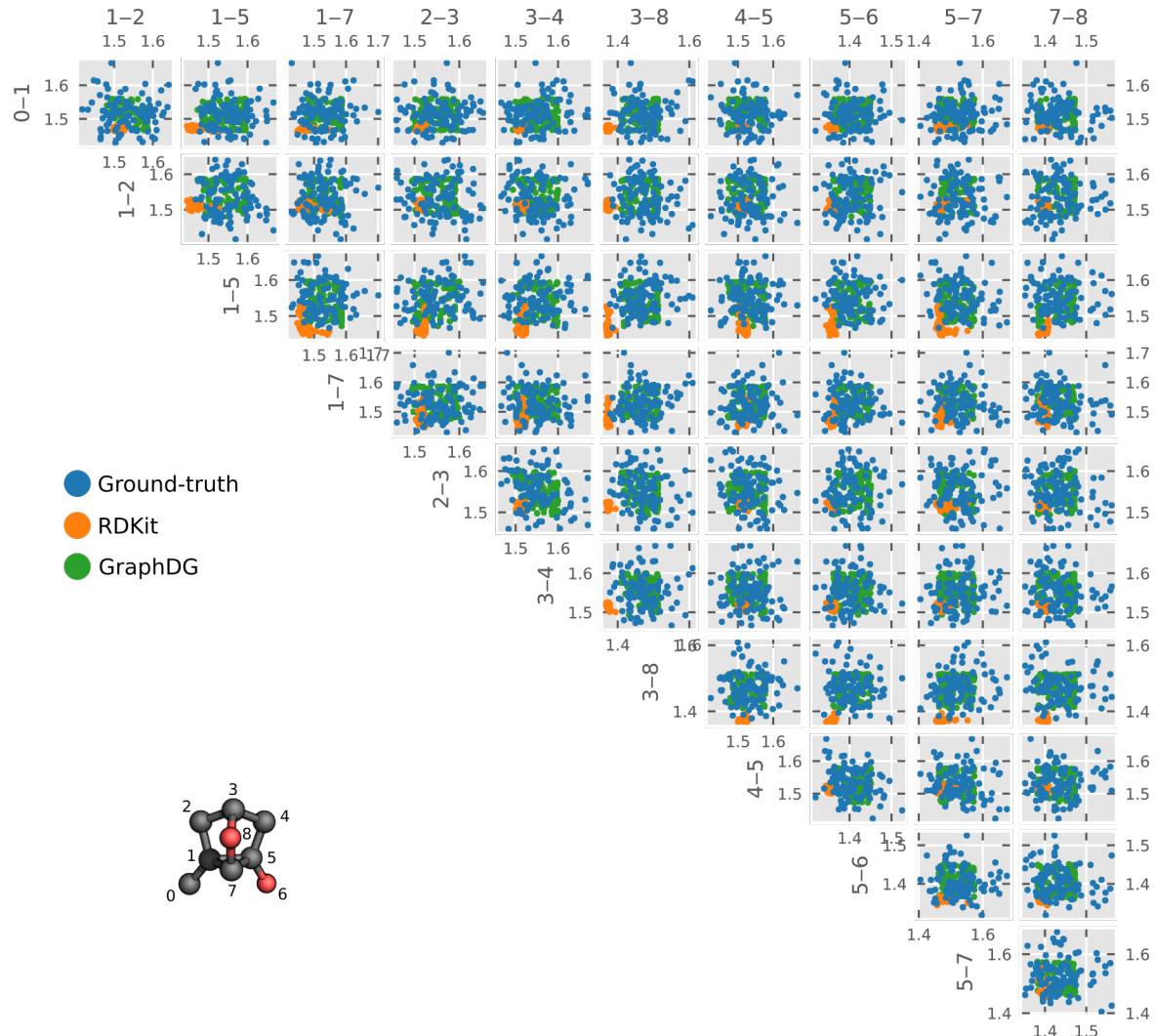
Figure 12. See caption of Fig. 8
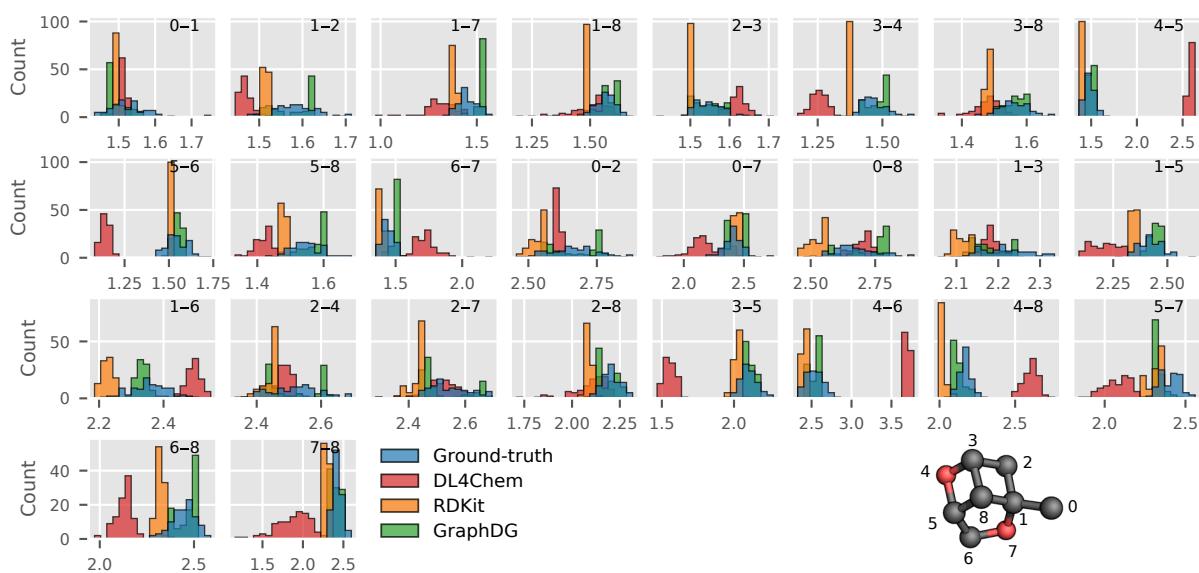
Figure 13. See caption of Fig. 5
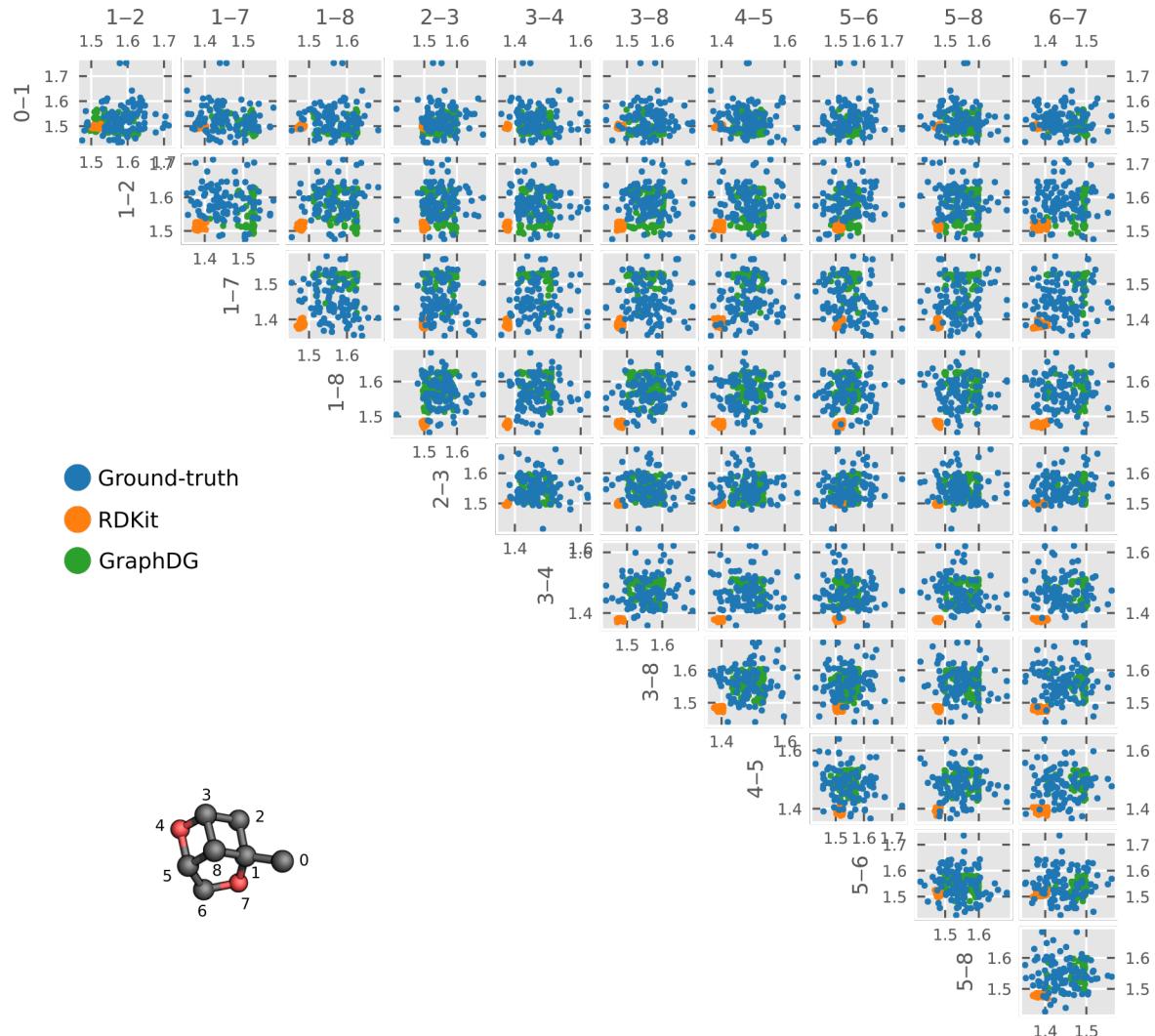
Figure 14. See caption of Fig. 8