Fig. S1. QULLUF optimized asymmetric unit calculated using wrong atom types.
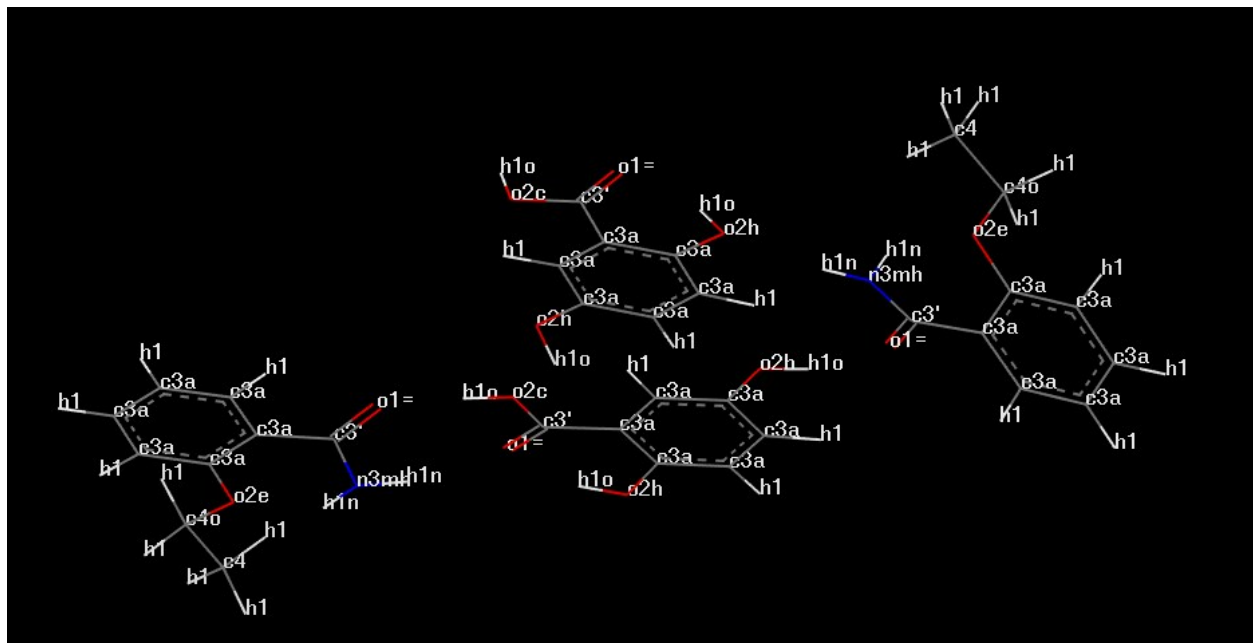
Fig. S2. QULLUF optimized asymmetric unit calculated using correct atom types.
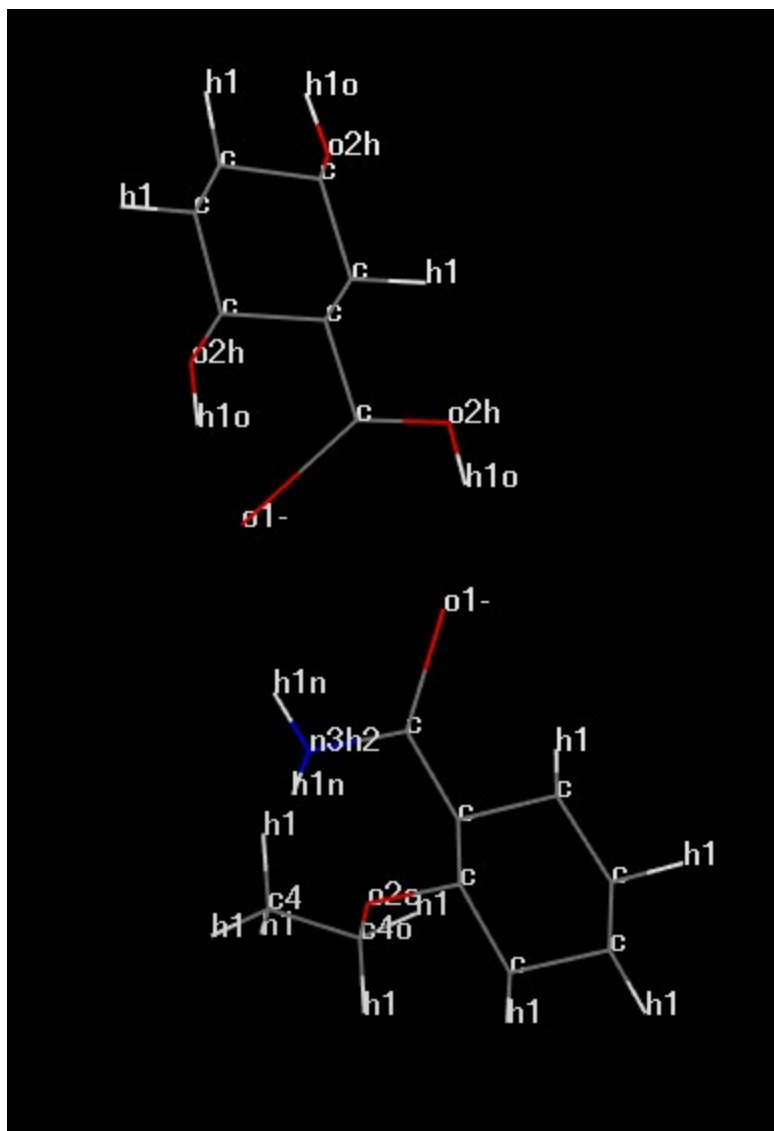
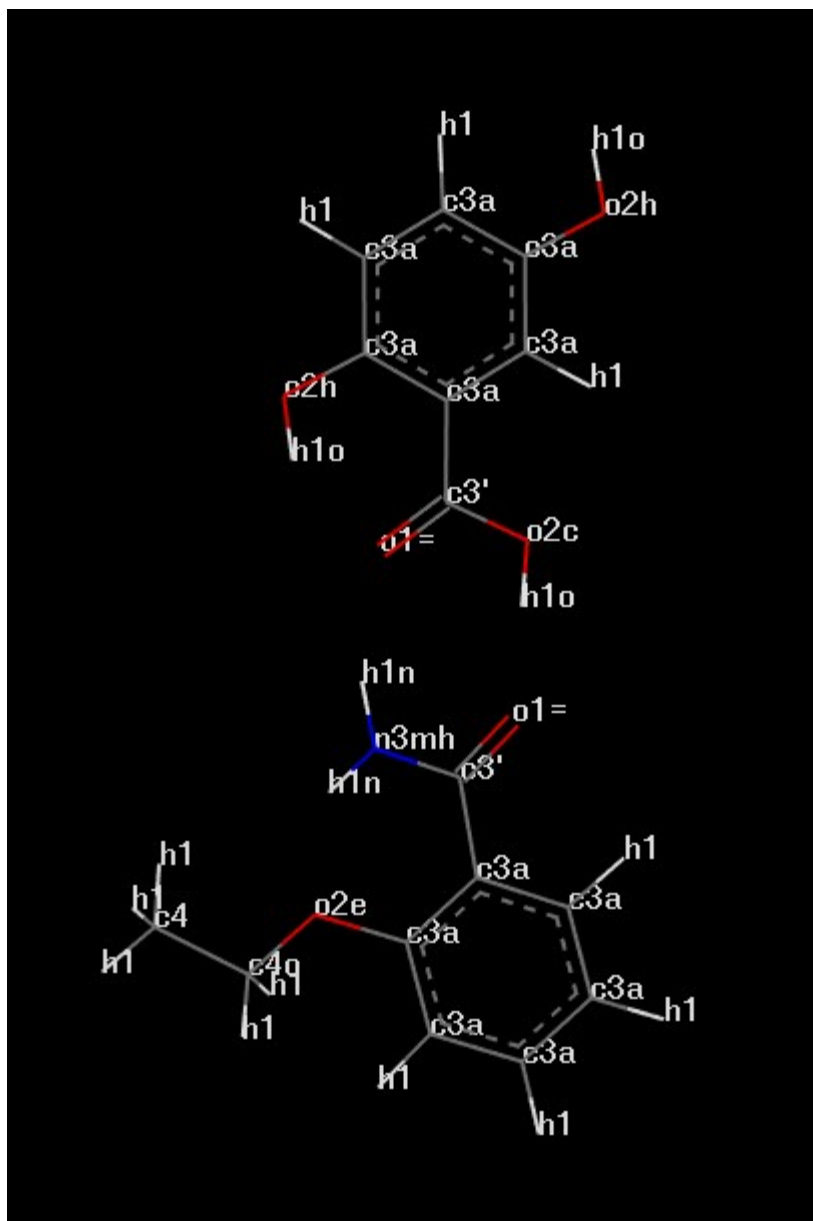Fig. S3. QULLUF01 optimized asymmetric unit calculated using wrong atom types.

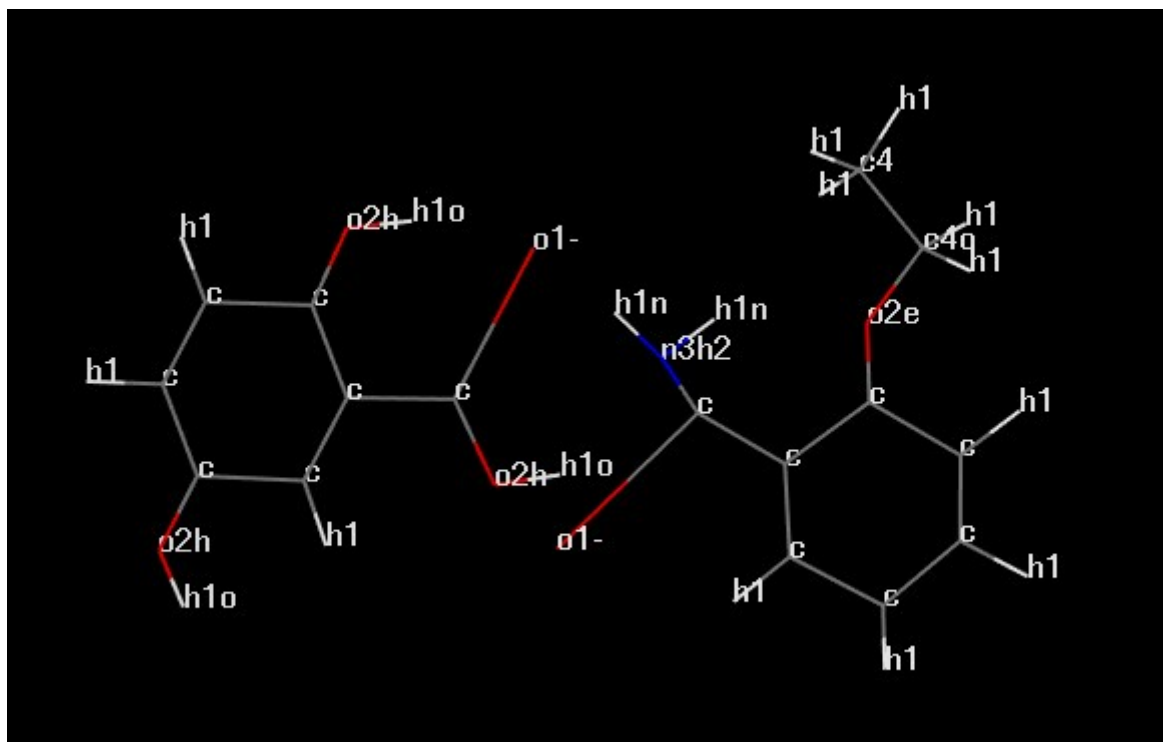Fig. S4. QULLUF01 optimized asymmetric unit calculated using correct atom types.

Fig. S5. QULLUF02 optimized asymmetric unit calculated using wrong atom types.
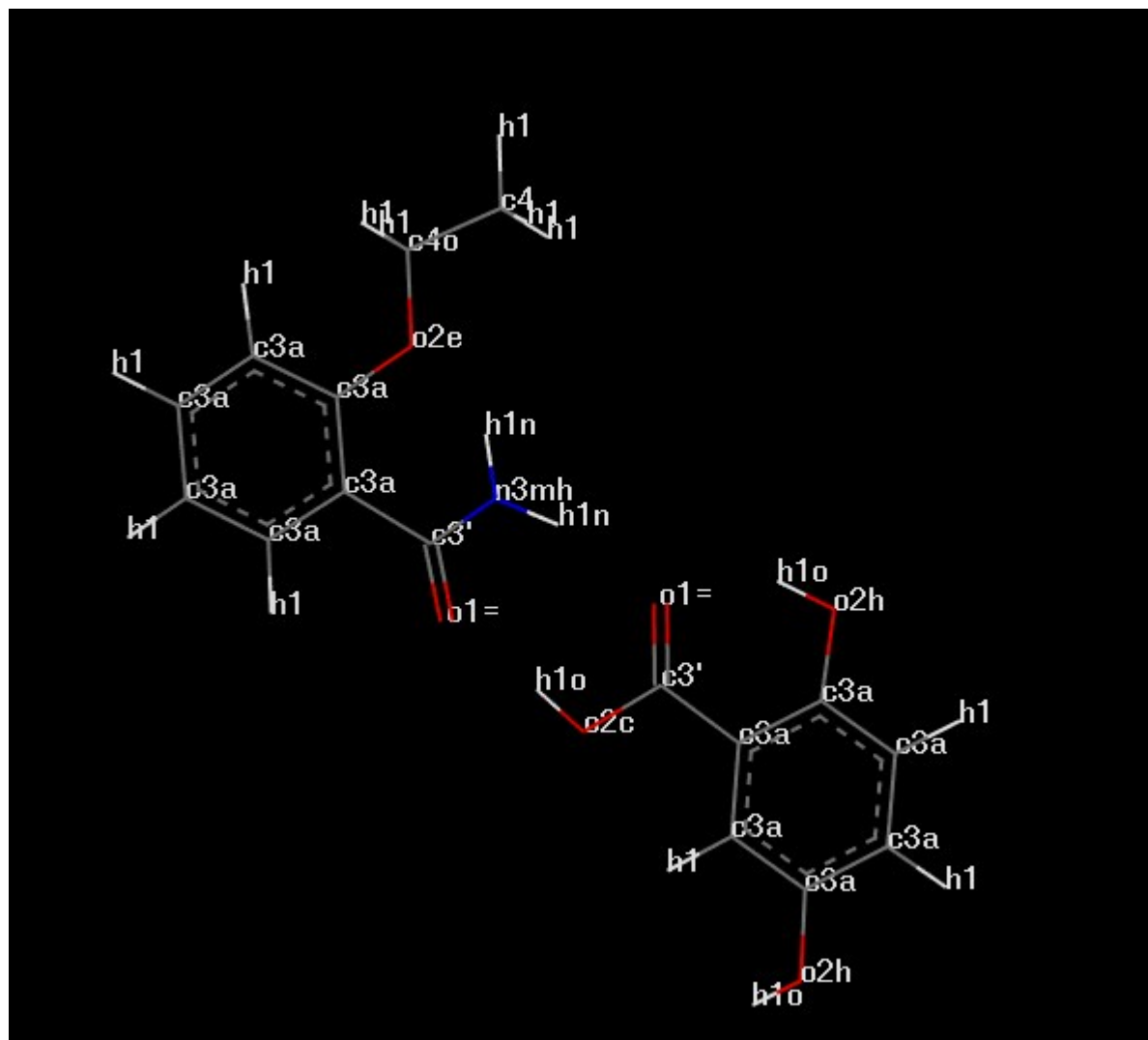
Fig. S6. QULLUF02 optimized asymmetric unit calculated using correct atom types.