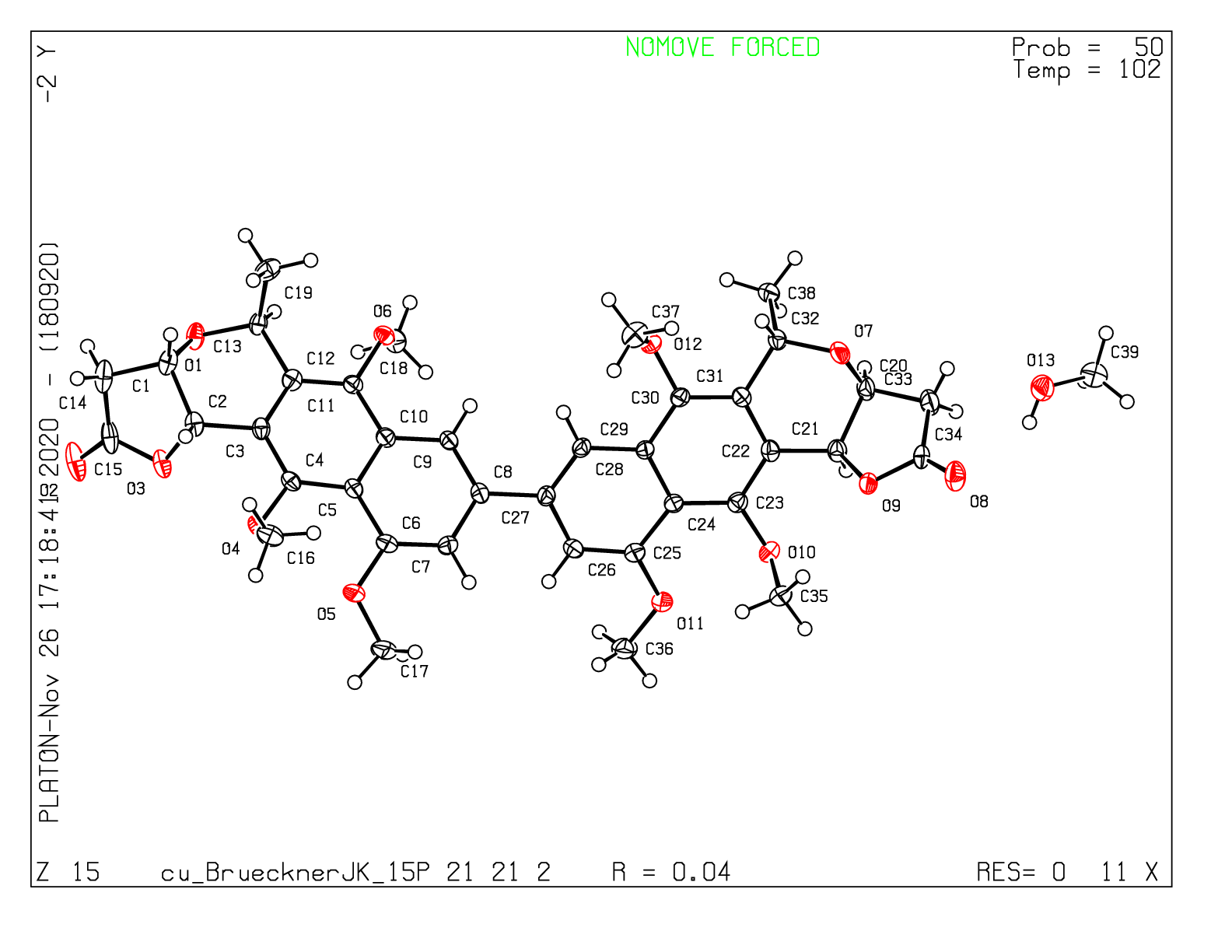
# Structure Tables



**The following text is only a suggestion:** [No crystallization method was given]. The data for cu\_BruecknerJK\_153F40\_0m were collected from a shock-cooled single crystal at 102(2) K on a [No measurement device type given] [No measurement device given] with a [No radiation source given] using [No monochromator type given] as monochromator and a [No detector type given] detector. The diffractometer was equipped with a low temperature device and used Cu*Kα* radiation (λ = 1.54178 Å). All data were integrated with SAINT and a multi-scan absorption correction using SADABS was applied.[1,2] The structure were solved by direct methods using SHELXT and refined by full-matrix least-squares methods against *F*2 by SHELXL-2018/3.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their *U*iso values constrained to 1.5 times the *U*eq of their pivot atoms for terminal sp3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC 1979688 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/​structures. This report and the CIF file were generated using FinalCif.[6]

## Table 1. Crystal data and structure refinement for cu\_BruecknerJK\_153F40\_0m

|  |  |
| --- | --- |
| CCDC number | 1979688 |
| Empirical formula | C38.50H40O12.50 |
| Formula weight | 702.70 |
| Temperature [K] | 102(2) |
| Crystal system | orthorhombic |
| Space group (number) | (18) |
| *a* [Å] | 19.678(3) |
| *b* [Å] | 37.0229(9) |
| *c* [Å] | 4.7720(4) |
| α [Å] | 90 |
| β [Å] | 90 |
| γ [Å] | 90 |
| Volume [Å3] | 3476.6(7) |
| *Z* | 4 |
| *ρ*calc [g/cm3] | 1.343 |
| *μ* [mm-1] | 0.838 |
| *F*(000) | 1484 |
| Crystal size [mm3] | 0.220×0.100×0.040 |
| Crystal colour | colourless |
| Crystal shape | plate |
| Radiation | Cu*Kα* (λ=1.54178 Å) |
| 2ϴ range [°] | 4.77 to 156.95 (0.79 Å) |
| Index ranges | -24 ≤ h ≤ 24 -47 ≤ k ≤ 46 -5 ≤ l ≤ 5 |
| Reflections collected | 51638 |
| Independent reflections | 7338 *R*int = 0.0302 *R*sigma = 0.0149 |
| Completeness to  θ = 67.679° | 99.9 % |
| Data / Restraints / Parameters | 7338/5/479 |
| Goodness-of-fit on *F*2 | 1.198 |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0364 w*R*2 = 0.0917 |
| Final *R* indexes  [all data] | *R*1 = 0.0368 w*R*2 = 0.0919 |
| Largest peak/hole [eÅ3] | 0.26/-0.21 |
| Flack X parameter | 0.04(2) |

## Table 2. Atomic coordinates and *U*eq [Å2] for cu\_BruecknerJK\_153F40\_0m

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | ***z*** | ***U*eq** |
| C1 | 0.00232(11) | 0.37061(7) | 0.3615(5) | 0.0240(5) |
| H1 | -0.004416 | 0.382450 | 0.547826 | 0.029 |
| O1 | 0.02619(8) | 0.39536(5) | 0.1512(4) | 0.0239(4) |
| C2 | 0.04929(11) | 0.33785(7) | 0.3773(5) | 0.0222(5) |
| H2 | 0.041865 | 0.324706 | 0.557764 | 0.027 |
| O2 | -0.06534(10) | 0.30877(7) | -0.1251(5) | 0.0444(5) |
| C3 | 0.12367(11) | 0.34684(6) | 0.3437(5) | 0.0188(4) |
| O3 | 0.02748(9) | 0.31504(5) | 0.1395(4) | 0.0280(4) |
| C4 | 0.17159(12) | 0.31982(6) | 0.3825(5) | 0.0191(4) |
| O4 | 0.14805(8) | 0.28609(4) | 0.4503(4) | 0.0215(3) |
| O5 | 0.27337(9) | 0.26484(4) | 0.3552(5) | 0.0296(4) |
| C5 | 0.24236(11) | 0.32684(6) | 0.3402(5) | 0.0191(4) |
| O6 | 0.23152(8) | 0.42552(4) | 0.1932(3) | 0.0192(3) |
| C6 | 0.29485(12) | 0.29983(6) | 0.3375(6) | 0.0235(5) |
| O7 | 0.73086(9) | 0.47914(4) | 0.6156(4) | 0.0278(4) |
| C7 | 0.36205(12) | 0.30935(6) | 0.3087(6) | 0.0246(5) |
| H7 | 0.395856 | 0.291035 | 0.307928 | 0.030 |
| O8 | 0.89175(9) | 0.42106(5) | 0.7874(4) | 0.0336(4) |
| C8 | 0.38186(12) | 0.34604(6) | 0.2800(6) | 0.0222(5) |
| O9 | 0.80099(8) | 0.40908(4) | 0.5219(4) | 0.0222(4) |
| C9 | 0.33258(11) | 0.37240(6) | 0.2656(5) | 0.0199(4) |
| H9 | 0.345488 | 0.396914 | 0.240601 | 0.024 |
| O10 | 0.71633(8) | 0.36267(4) | 0.1160(4) | 0.0267(4) |
| C10 | 0.26263(12) | 0.36330(6) | 0.2877(5) | 0.0195(4) |
| O11 | 0.61510(9) | 0.31944(5) | -0.0335(4) | 0.0284(4) |
| C11 | 0.21156(11) | 0.39014(6) | 0.2511(5) | 0.0180(4) |
| O12 | 0.52253(8) | 0.45508(4) | 0.5609(3) | 0.0189(3) |
| C12 | 0.14374(12) | 0.38230(6) | 0.2726(5) | 0.0194(4) |
| C13 | 0.09056(11) | 0.41131(6) | 0.2202(5) | 0.0202(5) |
| H13 | 0.105712 | 0.425160 | 0.051506 | 0.024 |
| C14 | -0.06280(13) | 0.35437(8) | 0.2459(6) | 0.0323(6) |
| H14A | -0.092167 | 0.345114 | 0.398248 | 0.039 |
| H14B | -0.088559 | 0.372267 | 0.134159 | 0.039 |
| C15 | -0.03688(13) | 0.32419(8) | 0.0651(6) | 0.0319(6) |
| C16 | 0.16202(14) | 0.27563(7) | 0.7376(6) | 0.0278(5) |
| H16A | 0.157773 | 0.249358 | 0.755926 | 0.042 |
| H16B | 0.129459 | 0.287461 | 0.862909 | 0.042 |
| H16C | 0.208276 | 0.282987 | 0.787893 | 0.042 |
| C17 | 0.32322(15) | 0.23737(6) | 0.3063(8) | 0.0377(7) |
| H17A | 0.300883 | 0.213739 | 0.298159 | 0.057 |
| H17B | 0.356507 | 0.237497 | 0.459030 | 0.057 |
| H17C | 0.346375 | 0.242092 | 0.128199 | 0.057 |
| C18 | 0.24752(12) | 0.43131(7) | -0.0987(5) | 0.0240(5) |
| H18A | 0.252400 | 0.457250 | -0.134199 | 0.036 |
| H18B | 0.210834 | 0.421604 | -0.215474 | 0.036 |
| H18C | 0.290174 | 0.418994 | -0.144651 | 0.036 |
| C19 | 0.08325(14) | 0.43854(7) | 0.4585(6) | 0.0286(5) |
| H19A | 0.126943 | 0.450553 | 0.490553 | 0.043 |
| H19B | 0.069194 | 0.425955 | 0.629616 | 0.043 |
| H19C | 0.048924 | 0.456593 | 0.408303 | 0.043 |
| C20 | 0.77127(12) | 0.46820(7) | 0.3822(6) | 0.0275(5) |
| H20 | 0.764914 | 0.484217 | 0.215471 | 0.033 |
| C21 | 0.75888(11) | 0.42840(6) | 0.3143(5) | 0.0214(5) |
| H21 | 0.775876 | 0.423023 | 0.121291 | 0.026 |
| C22 | 0.68592(11) | 0.41693(6) | 0.3385(5) | 0.0192(4) |
| C23 | 0.66612(11) | 0.38373(6) | 0.2329(5) | 0.0203(5) |
| C24 | 0.59663(11) | 0.37266(6) | 0.2381(5) | 0.0193(4) |
| C25 | 0.56976(12) | 0.34054(6) | 0.1056(6) | 0.0223(5) |
| C26 | 0.50150(12) | 0.33263(6) | 0.1204(6) | 0.0238(5) |
| H26 | 0.484940 | 0.311299 | 0.033398 | 0.029 |
| C27 | 0.45523(11) | 0.35571(6) | 0.2630(5) | 0.0210(5) |
| C28 | 0.47865(11) | 0.38691(6) | 0.3818(5) | 0.0195(4) |
| H28 | 0.447679 | 0.402561 | 0.474499 | 0.023 |
| C29 | 0.54863(11) | 0.39632(6) | 0.3689(5) | 0.0172(4) |
| C30 | 0.57071(11) | 0.43045(6) | 0.4717(5) | 0.0178(4) |
| C31 | 0.63779(11) | 0.44097(6) | 0.4568(5) | 0.0179(4) |
| C32 | 0.65905(11) | 0.47805(6) | 0.5607(5) | 0.0212(5) |
| H32 | 0.635558 | 0.482025 | 0.743976 | 0.025 |
| C33 | 0.84430(13) | 0.46775(7) | 0.4856(8) | 0.0366(7) |
| H33A | 0.876675 | 0.470540 | 0.328242 | 0.044 |
| H33B | 0.852403 | 0.487182 | 0.624163 | 0.044 |
| C34 | 0.85057(11) | 0.43104(6) | 0.6186(5) | 0.0226(5) |
| C35 | 0.74027(13) | 0.33415(7) | 0.2969(7) | 0.0340(6) |
| H35A | 0.777024 | 0.320965 | 0.203420 | 0.051 |
| H35B | 0.702804 | 0.317537 | 0.337910 | 0.051 |
| H35C | 0.757238 | 0.344594 | 0.472124 | 0.051 |
| C36 | 0.58889(14) | 0.28982(7) | -0.1954(6) | 0.0308(6) |
| H36A | 0.626565 | 0.277149 | -0.286890 | 0.046 |
| H36B | 0.557544 | 0.299040 | -0.338024 | 0.046 |
| H36C | 0.564690 | 0.273068 | -0.071573 | 0.046 |
| C37 | 0.50029(14) | 0.45070(7) | 0.8456(6) | 0.0291(5) |
| H37A | 0.460892 | 0.466274 | 0.880081 | 0.044 |
| H37B | 0.537214 | 0.457407 | 0.973257 | 0.044 |
| H37C | 0.487593 | 0.425446 | 0.877807 | 0.044 |
| C38 | 0.63748(12) | 0.50904(6) | 0.3660(6) | 0.0242(5) |
| H38A | 0.587772 | 0.510127 | 0.356932 | 0.036 |
| H38B | 0.655813 | 0.504821 | 0.177915 | 0.036 |
| H38C | 0.655101 | 0.531940 | 0.439052 | 0.036 |
| O13 | 0.9588(2) | 0.48086(11) | 1.0443(9) | 0.0337(9) |
| H13A | 0.955437 | 0.460236 | 0.972254 | 0.051 |
| C39 | 1.0123(4) | 0.5002(5) | 0.9115(11) | 0.030(2) |
| H39A | 1.012625 | 0.525207 | 0.978836 | 0.045 |
| H39B | 1.005378 | 0.499988 | 0.708113 | 0.045 |
| H39C | 1.055913 | 0.488733 | 0.955932 | 0.045 |

*U*eq is defined as 1/3 of the trace of the orthogonalized *Uij* tensor.

## Table 3. Bond lengths and angles for cu\_BruecknerJK\_153F40\_0m

|  |  |
| --- | --- |
| **Atom–Atom** | **Length [Å]** |
| C1–O1 | 1.438(3) |
| C1–C14 | 1.519(3) |
| C1–C2 | 1.527(3) |
| O1–C13 | 1.436(3) |
| C2–O3 | 1.478(3) |
| C2–C3 | 1.510(3) |
| O2–C15 | 1.210(4) |
| C3–C4 | 1.387(3) |
| C3–C12 | 1.412(3) |
| O3–C15 | 1.358(3) |
| C4–O4 | 1.371(3) |
| C4–C5 | 1.431(3) |
| O4–C16 | 1.451(3) |
| O5–C6 | 1.365(3) |
| O5–C17 | 1.432(3) |
| C5–C10 | 1.430(3) |
| C5–C6 | 1.438(3) |
| O6–C11 | 1.395(3) |
| O6–C18 | 1.444(3) |
| C6–C7 | 1.376(3) |
| O7–C20 | 1.427(3) |
| O7–C32 | 1.438(3) |
| C7–C8 | 1.419(3) |
| O8–C34 | 1.201(3) |
| C8–C9 | 1.378(3) |
| C8–C27 | 1.490(3) |
| O9–C34 | 1.351(3) |
| O9–C21 | 1.476(3) |
| C9–C10 | 1.421(3) |
| O10–C23 | 1.377(3) |
| O10–C35 | 1.443(3) |
| C10–C11 | 1.424(3) |
| O11–C25 | 1.359(3) |
| O11–C36 | 1.437(3) |
| C11–C12 | 1.370(3) |
| O12–C30 | 1.382(3) |
| O12–C37 | 1.437(3) |
| C12–C13 | 1.520(3) |
| C13–C19 | 1.526(3) |
| C14–C15 | 1.501(4) |
| C20–C33 | 1.520(3) |
| C20–C21 | 1.528(3) |
| C21–C22 | 1.502(3) |
| C22–C23 | 1.384(3) |
| C22–C31 | 1.417(3) |
| C23–C24 | 1.428(3) |
| C24–C29 | 1.431(3) |
| C24–C25 | 1.447(3) |
| C25–C26 | 1.377(3) |
| C26–C27 | 1.422(3) |
| C27–C28 | 1.367(3) |
| C28–C29 | 1.422(3) |
| C29–C30 | 1.424(3) |
| C30–C31 | 1.378(3) |
| C31–C32 | 1.518(3) |
| C32–C38 | 1.536(3) |
| C33–C34 | 1.505(3) |
| O13–C39 | 1.423(11) |
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## Table 4. Torsion angles for cu\_BruecknerJK\_153F40\_0m

|  |  |
| --- | --- |
| **Atom–Atom–Atom–Atom** | **Torsion Angle [°]** |
| C14–C1–O1–C13 | -175.9(2) |
| C2–C1–O1–C13 | -66.0(3) |
| O1–C1–C2–O3 | -80.0(2) |
| C14–C1–C2–O3 | 32.3(2) |
| O1–C1–C2–C3 | 38.6(3) |
| C14–C1–C2–C3 | 150.9(2) |
| O3–C2–C3–C4 | -70.9(3) |
| C1–C2–C3–C4 | 173.5(2) |
| O3–C2–C3–C12 | 108.9(2) |
| C1–C2–C3–C12 | -6.7(3) |
| C3–C2–O3–C15 | -143.1(2) |
| C1–C2–O3–C15 | -21.2(2) |
| C12–C3–C4–O4 | -179.8(2) |
| C2–C3–C4–O4 | -0.1(3) |
| C12–C3–C4–C5 | -2.6(4) |
| C2–C3–C4–C5 | 177.2(2) |
| C3–C4–O4–C16 | -108.9(2) |
| C5–C4–O4–C16 | 73.9(3) |
| O4–C4–C5–C10 | -176.1(2) |
| C3–C4–C5–C10 | 6.8(3) |
| O4–C4–C5–C6 | 6.0(4) |
| C3–C4–C5–C6 | -171.1(2) |
| C17–O5–C6–C7 | -7.9(4) |
| C17–O5–C6–C5 | 169.9(3) |
| C10–C5–C6–O5 | -172.6(2) |
| C4–C5–C6–O5 | 5.3(4) |
| C10–C5–C6–C7 | 5.2(4) |
| C4–C5–C6–C7 | -176.8(3) |
| O5–C6–C7–C8 | 177.5(3) |
| C5–C6–C7–C8 | -0.2(4) |
| C6–C7–C8–C9 | -3.6(4) |
| C6–C7–C8–C27 | 177.1(3) |
| C7–C8–C9–C10 | 1.9(4) |
| C27–C8–C9–C10 | -178.7(2) |
| C8–C9–C10–C11 | -175.1(2) |
| C8–C9–C10–C5 | 3.3(4) |
| C4–C5–C10–C9 | 175.1(2) |
| C6–C5–C10–C9 | -6.8(3) |
| C4–C5–C10–C11 | -6.4(3) |
| C6–C5–C10–C11 | 171.7(2) |
| C18–O6–C11–C12 | -98.9(2) |
| C18–O6–C11–C10 | 81.4(3) |
| C9–C10–C11–C12 | -179.6(2) |
| C5–C10–C11–C12 | 1.9(4) |
| C9–C10–C11–O6 | 0.0(3) |
| C5–C10–C11–O6 | -178.5(2) |
| O6–C11–C12–C3 | -177.2(2) |
| C10–C11–C12–C3 | 2.5(4) |
| O6–C11–C12–C13 | 2.9(3) |
| C10–C11–C12–C13 | -177.4(2) |
| C4–C3–C12–C11 | -2.2(3) |
| C2–C3–C12–C11 | 178.1(2) |
| C4–C3–C12–C13 | 177.8(2) |
| C2–C3–C12–C13 | -2.0(3) |
| C1–O1–C13–C12 | 56.3(2) |
| C1–O1–C13–C19 | -71.7(2) |
| C11–C12–C13–O1 | 158.6(2) |
| C3–C12–C13–O1 | -21.3(3) |
| C11–C12–C13–C19 | -75.2(3) |
| C3–C12–C13–C19 | 104.9(3) |
| O1–C1–C14–C15 | 84.1(2) |
| C2–C1–C14–C15 | -31.2(3) |
| C2–O3–C15–O2 | -179.6(2) |
| C2–O3–C15–C14 | 0.8(3) |
| C1–C14–C15–O2 | -159.6(3) |
| C1–C14–C15–O3 | 19.9(3) |
| C32–O7–C20–C33 | -174.99(18) |
| C32–O7–C20–C21 | -65.1(2) |
| C34–O9–C21–C22 | -144.3(2) |
| C34–O9–C21–C20 | -21.7(2) |
| O7–C20–C21–O9 | -80.1(2) |
| C33–C20–C21–O9 | 32.3(3) |
| O7–C20–C21–C22 | 39.9(3) |
| C33–C20–C21–C22 | 152.4(2) |
| O9–C21–C22–C23 | -75.8(3) |
| C20–C21–C22–C23 | 167.9(2) |
| O9–C21–C22–C31 | 107.2(2) |
| C20–C21–C22–C31 | -9.1(3) |
| C35–O10–C23–C22 | 101.2(2) |
| C35–O10–C23–C24 | -80.8(3) |
| C31–C22–C23–O10 | 178.4(2) |
| C21–C22–C23–O10 | 1.5(3) |
| C31–C22–C23–C24 | 0.4(4) |
| C21–C22–C23–C24 | -176.6(2) |
| O10–C23–C24–C29 | 179.0(2) |
| C22–C23–C24–C29 | -3.1(3) |
| O10–C23–C24–C25 | -5.3(4) |
| C22–C23–C24–C25 | 172.6(2) |
| C36–O11–C25–C26 | 6.6(4) |
| C36–O11–C25–C24 | -172.6(2) |
| C23–C24–C25–O11 | 0.2(4) |
| C29–C24–C25–O11 | 175.9(2) |
| C23–C24–C25–C26 | -179.1(2) |
| C29–C24–C25–C26 | -3.4(3) |
| O11–C25–C26–C27 | -178.7(2) |
| C24–C25–C26–C27 | 0.5(4) |
| C25–C26–C27–C28 | 1.8(4) |
| C25–C26–C27–C8 | -178.8(2) |
| C9–C8–C27–C28 | 36.1(4) |
| C7–C8–C27–C28 | -144.5(3) |
| C9–C8–C27–C26 | -143.3(3) |
| C7–C8–C27–C26 | 36.1(4) |
| C26–C27–C28–C29 | -1.0(4) |
| C8–C27–C28–C29 | 179.5(2) |
| C27–C28–C29–C30 | 174.3(2) |
| C27–C28–C29–C24 | -1.9(4) |
| C23–C24–C29–C28 | -179.9(2) |
| C25–C24–C29–C28 | 4.1(3) |
| C23–C24–C29–C30 | 3.9(3) |
| C25–C24–C29–C30 | -172.2(2) |
| C37–O12–C30–C31 | -102.1(2) |
| C37–O12–C30–C29 | 84.8(3) |
| C28–C29–C30–C31 | -178.4(2) |
| C24–C29–C30–C31 | -2.1(3) |
| C28–C29–C30–O12 | -5.4(3) |
| C24–C29–C30–O12 | 170.9(2) |
| O12–C30–C31–C22 | -173.6(2) |
| C29–C30–C31–C22 | -0.6(3) |
| O12–C30–C31–C32 | 5.2(3) |
| C29–C30–C31–C32 | 178.2(2) |
| C23–C22–C31–C30 | 1.5(3) |
| C21–C22–C31–C30 | 178.5(2) |
| C23–C22–C31–C32 | -177.3(2) |
| C21–C22–C31–C32 | -0.3(3) |
| C20–O7–C32–C31 | 54.4(3) |
| C20–O7–C32–C38 | -73.0(2) |
| C30–C31–C32–O7 | 160.4(2) |
| C22–C31–C32–O7 | -20.8(3) |
| C30–C31–C32–C38 | -73.5(3) |
| C22–C31–C32–C38 | 105.2(2) |
| O7–C20–C33–C34 | 84.5(3) |
| C21–C20–C33–C34 | -31.2(3) |
| C21–O9–C34–O8 | -179.1(2) |
| C21–O9–C34–C33 | 1.4(3) |
| C20–C33–C34–O8 | -160.0(3) |
| C20–C33–C34–O9 | 19.6(3) |

Bonds to hydrogen atoms were omitted.

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