
Crystal structure of C₂₀H₂₆O₂ — she1009

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Abstract

The crystal structure of C₂₀H₂₆O₂ is reported.

Comment

The crystallographic asymmetric unit consists of four molecules of C₂₀H₂₆O₂. The molecules are grouped into pairs: the coordinates of atoms of molecule two are very similar to the coordinates of the corresponding atoms of molecule one after a translation of 0.5 in y and 0.5 in z, and likewise for molecules four and three.

Experimental

The compound was prepared by MFS and was crystallised from hexane/methanol. The sample ID is MFSB187-HPLC-F1.

Computing details

Data collection: *COLLECT* (Nonius, 2001).; cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-II* (Johnson 1976) in *TEXSAN* (MSC, 1992-1997); software used to prepare material for publication: *CRYSTALS* (Betteridge *et al.*, 2003).

References

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National Laboratory, Oak Ridge, Tennessee, USA.

(she1009)

Crystal data

| | |
|---------------------------------|---|
| $C_{20}H_{26}O_2$ | $Z = 8$ |
| $M_r = 298.43$ | $F(000) = 1296$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.221 \text{ Mg m}^{-3}$ |
| $a = 7.5138 (1) \text{ \AA}$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $b = 18.4879 (3) \text{ \AA}$ | Cell parameters from 14598 reflections |
| $c = 25.3033 (4) \text{ \AA}$ | $\theta = 2.6\text{--}27.5^\circ$ |
| $\alpha = 111.1710 (7)^\circ$ | $\mu = 0.08 \text{ mm}^{-1}$ |
| $\beta = 90.369 (1)^\circ$ | $T = 200 \text{ K}$ |
| $\gamma = 97.4350 (9)^\circ$ | Needle, Colourless |
| $V = 3244.82 (9) \text{ \AA}^3$ | $0.36 \times 0.22 \times 0.10 \text{ mm}$ |

Data collection

| | |
|--|--|
| Area diffractometer | 10535 reflections with $I > 2.0\sigma(I)$ |
| graphite | $R_{\text{int}} = 0.036$ |
| φ & ω scans | $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.6^\circ$ |
| Absorption correction: Multi-scan <i>DENZO/SCALEPACK</i> (Otwinowski & Minor, 1997) | $h = -9 \rightarrow 9$ |
| $T_{\text{min}} = 0.91$, $T_{\text{max}} = 0.99$ | $k = -24 \rightarrow 23$ |
| 63495 measured reflections | $l = -32 \rightarrow 32$ |
| 14879 independent reflections | |

Refinement

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|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: Structure-invariant direct methods |
| Least-squares matrix: Full | Hydrogen site location: Inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.057$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.153$ | Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.06P)^2 + 1.85P]$, where $P = (\max(F_o^2, 0) + 2F_c^2)/3$ |
| $S = 0.98$ | $(\Delta/\sigma)_{\text{max}} = 0.043$ |
| 14879 reflections | $\Delta\rho_{\text{max}} = 0.69 \text{ e \AA}^{-3}$ |
| 854 parameters | $\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$ |
| 42 restraints | |

Special details

Refinement. The intensities of reflections with an even-value for $k+l$ are systematically significantly stronger than those with $k+l$ odd. As the packing of the structure might experience stacking faults, two scales were trialled: one for $k+l$ even and one for $k+l$ odd. In fact, the final values for the two scales were not significantly different from each other so only one scale was used for the refinement.

There is disorder at C217 and C218 of molecule three, seemingly arising from the presence of two alternative orientations for this group. Additional sites (C227 and C228) were added as indicated in difference electron density maps and the relative populations of sites

were refined. Restraints were imposed on bonded distances and angles so they should match values obtained in the rest of the structure. The displacement parameters of C217 and C227 were constrained to be equal as they are so close together and restraints were imposed on displacement parameters of bonded atoms in this section of this molecule so they would tend to be similar.

A similar disorder was observed at C317 and C318 of molecule four, but in this case there appear to be 3 sites for each atom. A similar procedure was used here as was used for molecule three.

H atoms attached to C were included at calculated locations and ride on the atoms to which they are bonded. H attached to O were included at positions indicated in difference electron density maps and then their positional parameters were allowed to refine while maintaining restraints on the O—H distances and C—O—H angles. No hydrogen was located for O222 and there are no convincing short intermolecular distances to this atom so it is possibly disordered over more than one site. It is not included in the final structure.

Most of the largest peaks in the final difference electron density map are located in the centre of six-membered rings of molecule three (i.e. atoms labelled C201 etc.). Possibly there is a disorder of the packing of this entire molecule but the population of the minor component is too small to identify meaningfully (estimated at about 6%) and so refinement has been terminated at this point.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|---------------|--------------|--------------|----------------------------------|-----------|
| O21 | 0.65517 (18) | 0.83083 (8) | 0.77798 (6) | 0.0392 | |
| O22 | 0.32659 (17) | 0.84575 (7) | 0.72905 (6) | 0.0377 | |
| O121 | 0.53404 (18) | 0.32015 (8) | 0.28481 (6) | 0.0432 | |
| O122 | 0.2669 (2) | 0.33927 (9) | 0.21745 (8) | 0.0638 | |
| O221 | 0.00595 (17) | 0.80777 (9) | 0.78332 (6) | 0.0412 | |
| O222 | 0.2401 (3) | 0.73902 (11) | 0.82764 (6) | 0.0716 | |
| O321 | -0.10677 (18) | 0.32298 (8) | 0.30603 (6) | 0.0414 | |
| O322 | 0.20979 (18) | 0.27324 (8) | 0.33608 (6) | 0.0399 | |
| C1 | 0.1957 (2) | 1.02727 (10) | 0.69822 (7) | 0.0301 | |
| C2 | 0.0717 (2) | 0.95802 (11) | 0.65368 (8) | 0.0386 | |
| C3 | 0.0463 (3) | 0.97007 (13) | 0.59775 (9) | 0.0467 | |
| C4 | 0.2213 (3) | 0.99719 (11) | 0.57811 (8) | 0.0400 | |
| C5 | 0.3714 (2) | 1.02745 (10) | 0.61088 (8) | 0.0325 | |
| C6 | 0.5426 (3) | 1.05651 (12) | 0.58966 (9) | 0.0426 | |
| C7 | 0.6016 (3) | 1.14324 (13) | 0.62384 (9) | 0.0481 | |
| C8 | 0.5972 (2) | 1.15942 (12) | 0.68610 (9) | 0.0401 | |
| C9 | 0.5007 (2) | 1.11385 (10) | 0.70884 (8) | 0.0315 | |
| C10 | 0.5122 (3) | 1.13035 (11) | 0.77179 (8) | 0.0369 | |
| C11 | 0.5523 (2) | 1.05828 (11) | 0.78390 (8) | 0.0367 | |
| C12 | 0.4312 (2) | 0.98360 (10) | 0.74500 (7) | 0.0290 | |
| C13 | 0.2384 (2) | 1.00284 (10) | 0.74793 (7) | 0.0298 | |
| C14 | 0.4716 (2) | 0.97129 (10) | 0.68321 (7) | 0.0295 | |
| C15 | 0.3836 (2) | 1.03705 (10) | 0.67280 (7) | 0.0276 | |
| C16 | 0.1267 (3) | 0.99881 (11) | 0.78716 (8) | 0.0400 | |
| C17 | 0.0965 (2) | 1.09771 (12) | 0.71471 (9) | 0.0400 | |
| C18 | 0.1122 (3) | 1.15466 (12) | 0.69543 (9) | 0.0455 | |
| C19 | 0.4493 (2) | 0.91299 (10) | 0.76170 (7) | 0.0306 | |
| C20 | 0.6334 (2) | 0.88722 (12) | 0.75330 (9) | 0.0389 | |
| C101 | 0.1690 (2) | 0.52522 (11) | 0.18723 (8) | 0.0364 | |
| C102 | 0.0684 (3) | 0.45796 (13) | 0.13553 (10) | 0.0549 | |
| C103 | 0.0837 (4) | 0.47421 (15) | 0.08080 (11) | 0.0657 | |
| C104 | 0.2720 (4) | 0.50492 (13) | 0.07343 (9) | 0.0556 | |
| C105 | 0.4013 (3) | 0.53495 (11) | 0.11471 (8) | 0.0409 | |

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|------|-------------|--------------|--------------|--------|-----------|
| C106 | 0.5840 (3) | 0.57075 (14) | 0.10597 (10) | 0.0559 | |
| C107 | 0.6178 (3) | 0.65706 (14) | 0.14370 (11) | 0.0554 | |
| C108 | 0.5789 (3) | 0.66723 (12) | 0.20381 (10) | 0.0439 | |
| C109 | 0.4694 (2) | 0.61607 (10) | 0.21844 (8) | 0.0335 | |
| C110 | 0.4404 (3) | 0.62690 (11) | 0.27957 (8) | 0.0411 | |
| C111 | 0.4636 (3) | 0.55274 (11) | 0.29159 (8) | 0.0399 | |
| C112 | 0.3647 (2) | 0.47898 (10) | 0.24505 (8) | 0.0325 | |
| C113 | 0.1742 (2) | 0.49517 (11) | 0.23606 (9) | 0.0387 | |
| C114 | 0.4466 (2) | 0.47309 (10) | 0.18858 (8) | 0.0335 | |
| C115 | 0.3724 (2) | 0.53953 (10) | 0.17491 (7) | 0.0317 | |
| C116 | 0.0336 (3) | 0.48300 (15) | 0.26469 (12) | 0.0590 | |
| C117 | 0.0696 (3) | 0.59510 (12) | 0.19985 (9) | 0.0454 | |
| C118 | 0.1074 (3) | 0.65629 (13) | 0.18516 (10) | 0.0502 | |
| C119 | 0.3642 (2) | 0.40547 (11) | 0.25997 (9) | 0.0384 | |
| C120 | 0.5489 (3) | 0.38762 (12) | 0.26941 (10) | 0.0452 | |
| C201 | 0.4294 (3) | 0.78910 (12) | 0.98363 (8) | 0.0414 | |
| C202 | 0.4662 (3) | 0.70336 (14) | 0.95425 (10) | 0.0566 | |
| C203 | 0.4397 (4) | 0.65662 (15) | 0.99313 (11) | 0.0679 | |
| C204 | 0.2694 (3) | 0.66917 (13) | 1.02316 (10) | 0.0549 | |
| C205 | 0.1754 (3) | 0.72674 (12) | 1.02775 (9) | 0.0445 | |
| C206 | 0.0106 (3) | 0.73856 (15) | 1.06139 (9) | 0.0528 | |
| C207 | 0.0446 (3) | 0.81637 (17) | 1.11109 (10) | 0.0614 | |
| C208 | 0.1168 (3) | 0.88055 (14) | 1.09083 (8) | 0.0461 | |
| C209 | 0.1999 (3) | 0.86935 (12) | 1.04287 (8) | 0.0407 | |
| C210 | 0.2623 (3) | 0.93620 (12) | 1.02336 (9) | 0.0471 | |
| C211 | 0.2014 (3) | 0.91635 (12) | 0.96069 (9) | 0.0470 | |
| C212 | 0.2364 (2) | 0.83267 (12) | 0.92361 (8) | 0.0382 | |
| C213 | 0.4290 (2) | 0.82651 (13) | 0.93859 (8) | 0.0412 | |
| C214 | 0.1250 (2) | 0.77570 (11) | 0.94583 (7) | 0.0345 | |
| C215 | 0.2295 (2) | 0.78831 (10) | 1.00213 (7) | 0.0319 | |
| C216 | 0.5736 (3) | 0.84549 (18) | 0.91417 (10) | 0.0660 | |
| C217 | 0.5837 (11) | 0.8295 (8) | 1.0279 (4) | 0.0442 | 0.523 (6) |
| C218 | 0.5791 (6) | 0.8377 (3) | 1.08102 (17) | 0.0532 | 0.523 (6) |
| C219 | 0.2040 (2) | 0.81531 (12) | 0.85990 (8) | 0.0373 | |
| C220 | 0.0160 (3) | 0.82043 (14) | 0.84272 (8) | 0.0445 | |
| C227 | 0.5447 (12) | 0.8332 (9) | 1.0392 (4) | 0.0442 | 0.477 (6) |
| C228 | 0.6830 (6) | 0.8870 (3) | 1.0481 (2) | 0.0617 | 0.477 (6) |
| C301 | 0.4126 (2) | 0.30532 (11) | 0.48751 (8) | 0.0372 | |
| C302 | 0.4825 (3) | 0.22993 (13) | 0.44891 (10) | 0.0478 | |
| C303 | 0.4889 (3) | 0.17029 (14) | 0.47759 (11) | 0.0609 | |
| C304 | 0.3269 (3) | 0.16364 (13) | 0.50998 (10) | 0.0536 | |
| C305 | 0.2061 (3) | 0.21287 (12) | 0.52317 (9) | 0.0427 | |
| C306 | 0.0516 (3) | 0.20458 (14) | 0.55884 (10) | 0.0551 | |
| C307 | 0.0660 (4) | 0.27614 (15) | 0.61352 (10) | 0.0612 | |
| C308 | 0.0964 (3) | 0.34954 (14) | 0.60067 (9) | 0.0522 | |
| C309 | 0.1605 (3) | 0.35400 (11) | 0.55302 (8) | 0.0401 | |
| C310 | 0.1742 (3) | 0.42868 (12) | 0.54081 (9) | 0.0472 | |
| C311 | 0.1035 (3) | 0.41434 (11) | 0.48046 (8) | 0.0405 | |
| C312 | 0.1746 (2) | 0.34283 (10) | 0.43725 (7) | 0.0313 | |
| C313 | 0.3772 (2) | 0.35267 (11) | 0.45061 (8) | 0.0347 | |
| C314 | 0.1027 (2) | 0.27099 (10) | 0.45185 (7) | 0.0323 | |
| C315 | 0.2200 (2) | 0.28358 (10) | 0.50596 (8) | 0.0339 | |

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|-------|-------------|--------------|--------------|---------|------------|
| C316 | 0.5008 (3) | 0.39400 (13) | 0.43234 (10) | 0.0483 | |
| C317 | 0.5723 (12) | 0.3421 (7) | 0.5299 (4) | 0.0397 | 0.379 (7) |
| C318 | 0.6523 (7) | 0.4123 (4) | 0.5530 (2) | 0.0457 | 0.379 (7) |
| C319 | 0.1300 (2) | 0.33462 (10) | 0.37591 (8) | 0.0319 | |
| C320 | -0.0686 (2) | 0.31635 (13) | 0.35924 (8) | 0.0401 | |
| C327 | 0.5298 (15) | 0.3494 (9) | 0.5426 (5) | 0.0397 | 0.376 (10) |
| C328 | 0.6958 (8) | 0.3546 (5) | 0.5514 (3) | 0.0609 | 0.376 (10) |
| C337 | 0.526 (2) | 0.3544 (13) | 0.5426 (7) | 0.0397 | 0.245 (9) |
| C338 | 0.5970 (17) | 0.3343 (6) | 0.5733 (4) | 0.0568 | 0.245 (9) |
| H21 | -0.0426 | 0.9528 | 0.6688 | 0.0463* | |
| H22 | 0.1236 | 0.9114 | 0.6465 | 0.0463* | |
| H31 | -0.0317 | 1.0083 | 0.6028 | 0.0560* | |
| H32 | -0.0061 | 0.9219 | 0.5697 | 0.0560* | |
| H41 | 0.2251 | 0.9924 | 0.5395 | 0.0480* | |
| H61 | 0.6344 | 1.0275 | 0.5933 | 0.0511* | |
| H62 | 0.5230 | 1.0493 | 0.5508 | 0.0511* | |
| H71 | 0.5227 | 1.1732 | 0.6140 | 0.0577* | |
| H72 | 0.7206 | 1.1578 | 0.6152 | 0.0577* | |
| H81 | 0.6686 | 1.2055 | 0.7112 | 0.0481* | |
| H101 | 0.6054 | 1.1726 | 0.7894 | 0.0442* | |
| H102 | 0.4009 | 1.1443 | 0.7870 | 0.0442* | |
| H111 | 0.5310 | 1.0660 | 0.8224 | 0.0441* | |
| H112 | 0.6747 | 1.0519 | 0.7774 | 0.0441* | |
| H141 | 0.5974 | 0.9775 | 0.6788 | 0.0355* | |
| H142 | 0.4185 | 0.9209 | 0.6582 | 0.0355* | |
| H161 | 0.1643 | 0.9830 | 0.8168 | 0.0480* | |
| H162 | 0.0089 | 1.0117 | 0.7858 | 0.0480* | |
| H171 | 0.0116 | 1.1009 | 0.7428 | 0.0480* | |
| H181 | 0.0410 | 1.1958 | 0.7096 | 0.0545* | |
| H182 | 0.1948 | 1.1551 | 0.6672 | 0.0545* | |
| H191 | 0.4249 | 0.9263 | 0.8006 | 0.0367* | |
| H201 | 0.7218 | 0.9317 | 0.7703 | 0.0467* | |
| H202 | 0.6496 | 0.8650 | 0.7137 | 0.0467* | |
| H1021 | -0.0551 | 0.4510 | 0.1430 | 0.0659* | |
| H1022 | 0.1177 | 0.4113 | 0.1306 | 0.0659* | |
| H1031 | 0.0078 | 0.5119 | 0.0816 | 0.0788* | |
| H1032 | 0.0460 | 0.4269 | 0.0496 | 0.0788* | |
| H1041 | 0.3017 | 0.5029 | 0.0365 | 0.0667* | |
| H1061 | 0.5908 | 0.5658 | 0.0674 | 0.0671* | |
| H1062 | 0.6726 | 0.5443 | 0.1153 | 0.0671* | |
| H1071 | 0.7399 | 0.6771 | 0.1423 | 0.0665* | |
| H1072 | 0.5419 | 0.6849 | 0.1304 | 0.0665* | |
| H1081 | 0.6361 | 0.7131 | 0.2332 | 0.0527* | |
| H1101 | 0.5251 | 0.6691 | 0.3032 | 0.0494* | |
| H1102 | 0.3221 | 0.6388 | 0.2879 | 0.0494* | |
| H1111 | 0.4162 | 0.5569 | 0.3271 | 0.0479* | |
| H1112 | 0.5880 | 0.5483 | 0.2930 | 0.0479* | |
| H1141 | 0.5742 | 0.4819 | 0.1926 | 0.0402* | |
| H1142 | 0.4079 | 0.4234 | 0.1599 | 0.0402* | |
| H1161 | -0.0809 | 0.4931 | 0.2553 | 0.0708* | |
| H1162 | 0.0474 | 0.4642 | 0.2946 | 0.0708* | |
| H1171 | -0.0338 | 0.5947 | 0.2212 | 0.0545* | |

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|-------|---------|--------|--------|---------|-------|
| H1181 | 0.0331 | 0.6965 | 0.1959 | 0.0602* | |
| H1182 | 0.2090 | 0.6604 | 0.1638 | 0.0602* | |
| H1191 | 0.3044 | 0.4139 | 0.2942 | 0.0460* | |
| H1201 | 0.6134 | 0.4311 | 0.2990 | 0.0542* | |
| H1202 | 0.6111 | 0.3778 | 0.2355 | 0.0542* | |
| H2021 | 0.5867 | 0.7040 | 0.9431 | 0.0679* | |
| H2022 | 0.3863 | 0.6784 | 0.9216 | 0.0679* | |
| H2031 | 0.5381 | 0.6728 | 1.0205 | 0.0815* | |
| H2032 | 0.4352 | 0.6025 | 0.9710 | 0.0815* | |
| H2041 | 0.2250 | 0.6329 | 1.0403 | 0.0658* | |
| H2061 | -0.0162 | 0.6972 | 1.0752 | 0.0634* | |
| H2062 | -0.0879 | 0.7388 | 1.0378 | 0.0634* | |
| H2071 | 0.1294 | 0.8130 | 1.1378 | 0.0737* | |
| H2072 | -0.0650 | 0.8277 | 1.1287 | 0.0737* | |
| H2081 | 0.1023 | 0.9327 | 1.1138 | 0.0554* | |
| H2101 | 0.2134 | 0.9814 | 1.0464 | 0.0566* | |
| H2102 | 0.3898 | 0.9467 | 1.0273 | 0.0566* | |
| H2111 | 0.0765 | 0.9193 | 0.9582 | 0.0564* | |
| H2112 | 0.2665 | 0.9531 | 0.9471 | 0.0564* | |
| H2141 | 0.0064 | 0.7882 | 0.9525 | 0.0414* | |
| H2142 | 0.1199 | 0.7232 | 0.9200 | 0.0414* | |
| H2161 | 0.6879 | 0.8360 | 0.9243 | 0.0792* | |
| H2162 | 0.5631 | 0.8686 | 0.8865 | 0.0792* | |
| H2171 | 0.6913 | 0.8502 | 1.0158 | 0.0530* | 0.523 |
| H2181 | 0.6811 | 0.8637 | 1.1062 | 0.0638* | 0.523 |
| H2182 | 0.4737 | 0.8178 | 1.0947 | 0.0638* | 0.523 |
| H2191 | 0.2842 | 0.8518 | 0.8499 | 0.0448* | |
| H2201 | -0.0141 | 0.8708 | 0.8640 | 0.0534* | |
| H2202 | -0.0656 | 0.7816 | 0.8497 | 0.0534* | |
| H2271 | 0.5107 | 0.8194 | 1.0708 | 0.0530* | 0.477 |
| H2281 | 0.7436 | 0.9101 | 1.0846 | 0.0742* | 0.477 |
| H2282 | 0.7235 | 0.9032 | 1.0182 | 0.0742* | 0.477 |
| H3021 | 0.6004 | 0.2436 | 0.4390 | 0.0574* | |
| H3022 | 0.4053 | 0.2065 | 0.4155 | 0.0574* | |
| H3031 | 0.5924 | 0.1860 | 0.5030 | 0.0731* | |
| H3032 | 0.4966 | 0.1205 | 0.4492 | 0.0731* | |
| H3041 | 0.3085 | 0.1205 | 0.5223 | 0.0644* | |
| H3061 | 0.0542 | 0.1590 | 0.5677 | 0.0661* | |
| H3062 | -0.0582 | 0.2000 | 0.5383 | 0.0661* | |
| H3071 | 0.1638 | 0.2754 | 0.6372 | 0.0734* | |
| H3072 | -0.0423 | 0.2750 | 0.6326 | 0.0734* | |
| H3081 | 0.0678 | 0.3963 | 0.6286 | 0.0626* | |
| H3101 | 0.1060 | 0.4638 | 0.5670 | 0.0566* | |
| H3102 | 0.2967 | 0.4516 | 0.5455 | 0.0566* | |
| H3111 | 0.1423 | 0.4593 | 0.4715 | 0.0486* | |
| H3112 | -0.0241 | 0.4051 | 0.4785 | 0.0486* | |
| H3141 | -0.0211 | 0.2702 | 0.4594 | 0.0388* | |
| H3142 | 0.1192 | 0.2237 | 0.4220 | 0.0388* | |
| H3161 | 0.6244 | 0.3962 | 0.4419 | 0.0579* | |
| H3162 | 0.4663 | 0.4216 | 0.4096 | 0.0579* | |
| H3171 | 0.6233 | 0.3056 | 0.5416 | 0.0479* | 0.379 |
| H3181 | 0.7525 | 0.4235 | 0.5792 | 0.0547* | 0.379 |

| | | | | | |
|-------|------------|-------------|------------|---------|-------|
| H3182 | 0.6115 | 0.4533 | 0.5440 | 0.0547* | 0.379 |
| H3191 | 0.1753 | 0.3824 | 0.3715 | 0.0383* | |
| H3201 | -0.1300 | 0.3519 | 0.3876 | 0.0481* | |
| H3202 | -0.1102 | 0.2643 | 0.3566 | 0.0481* | |
| H3271 | 0.4674 | 0.3772 | 0.5745 | 0.0479* | 0.377 |
| H3281 | 0.7505 | 0.3845 | 0.5881 | 0.0734* | 0.377 |
| H3282 | 0.7670 | 0.3284 | 0.5215 | 0.0734* | 0.377 |
| H3371 | 0.5390 | 0.4095 | 0.5521 | 0.0479* | 0.244 |
| H3381 | 0.6630 | 0.3720 | 0.6060 | 0.0681* | 0.244 |
| H3382 | 0.5905 | 0.2801 | 0.5666 | 0.0681* | 0.244 |
| H9021 | 0.589 (3) | 0.7914 (10) | 0.7605 (8) | 0.0500* | |
| H9022 | 0.234 (2) | 0.8482 (11) | 0.7451 (8) | 0.0500* | |
| H9121 | 0.637 (2) | 0.3147 (12) | 0.2900 (9) | 0.0500* | |
| H9122 | 0.352 (2) | 0.3256 (12) | 0.1940 (8) | 0.0500* | |
| H9221 | -0.099 (2) | 0.8096 (13) | 0.7751 (8) | 0.0500* | |
| H9321 | -0.066 (3) | 0.2889 (11) | 0.2813 (7) | 0.0500* | |
| H9322 | 0.313 (2) | 0.2921 (10) | 0.3318 (9) | 0.0500* | |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|-------------|-------------|-------------|--------------|-------------|
| O21 | 0.0389 (7) | 0.0432 (8) | 0.0431 (8) | 0.0105 (6) | -0.0016 (6) | 0.0234 (7) |
| O22 | 0.0323 (7) | 0.0321 (7) | 0.0493 (8) | 0.0013 (5) | 0.0032 (6) | 0.0169 (6) |
| O121 | 0.0344 (7) | 0.0451 (8) | 0.0617 (9) | 0.0100 (6) | 0.0015 (6) | 0.0318 (7) |
| O122 | 0.0732 (12) | 0.0398 (9) | 0.0792 (13) | -0.0028 (8) | -0.0192 (9) | 0.0267 (9) |
| O221 | 0.0320 (7) | 0.0613 (9) | 0.0366 (7) | 0.0065 (6) | -0.0030 (5) | 0.0255 (7) |
| O222 | 0.1024 (14) | 0.0796 (13) | 0.0353 (8) | 0.0500 (11) | 0.0009 (8) | 0.0114 (8) |
| O321 | 0.0392 (7) | 0.0466 (8) | 0.0455 (8) | 0.0094 (6) | -0.0038 (6) | 0.0241 (7) |
| O322 | 0.0346 (7) | 0.0463 (8) | 0.0370 (7) | 0.0097 (6) | 0.0059 (6) | 0.0117 (6) |
| C1 | 0.0232 (8) | 0.0302 (9) | 0.0366 (9) | 0.0027 (6) | 0.0003 (7) | 0.0122 (8) |
| C2 | 0.0289 (9) | 0.0388 (11) | 0.0461 (11) | -0.0031 (7) | -0.0050 (8) | 0.0159 (9) |
| C3 | 0.0431 (11) | 0.0445 (12) | 0.0470 (12) | -0.0036 (9) | -0.0172 (9) | 0.0139 (10) |
| C4 | 0.0509 (11) | 0.0370 (10) | 0.0328 (10) | 0.0082 (8) | -0.0047 (8) | 0.0130 (8) |
| C5 | 0.0390 (9) | 0.0288 (9) | 0.0337 (9) | 0.0102 (7) | 0.0049 (7) | 0.0143 (8) |
| C6 | 0.0444 (11) | 0.0497 (12) | 0.0426 (11) | 0.0142 (9) | 0.0118 (9) | 0.0250 (10) |
| C7 | 0.0461 (11) | 0.0496 (13) | 0.0560 (13) | -0.0001 (9) | 0.0085 (10) | 0.0304 (11) |
| C8 | 0.0331 (9) | 0.0363 (10) | 0.0527 (12) | -0.0018 (8) | -0.0020 (8) | 0.0206 (9) |
| C9 | 0.0264 (8) | 0.0293 (9) | 0.0392 (10) | 0.0026 (7) | -0.0021 (7) | 0.0133 (8) |
| C10 | 0.0384 (10) | 0.0303 (10) | 0.0375 (10) | -0.0040 (7) | -0.0073 (8) | 0.0104 (8) |
| C11 | 0.0372 (10) | 0.0349 (10) | 0.0366 (10) | -0.0014 (8) | -0.0074 (8) | 0.0137 (8) |
| C12 | 0.0262 (8) | 0.0300 (9) | 0.0320 (9) | 0.0035 (6) | 0.0007 (7) | 0.0129 (7) |
| C13 | 0.0281 (8) | 0.0247 (8) | 0.0336 (9) | 0.0015 (6) | 0.0013 (7) | 0.0078 (7) |
| C14 | 0.0260 (8) | 0.0298 (9) | 0.0353 (9) | 0.0057 (7) | 0.0037 (7) | 0.0143 (7) |
| C15 | 0.0260 (8) | 0.0271 (8) | 0.0301 (9) | 0.0041 (6) | 0.0005 (6) | 0.0108 (7) |
| C16 | 0.0383 (10) | 0.0418 (11) | 0.0422 (11) | 0.0100 (8) | 0.0105 (8) | 0.0165 (9) |
| C17 | 0.0330 (9) | 0.0418 (11) | 0.0476 (11) | 0.0132 (8) | 0.0070 (8) | 0.0165 (9) |
| C18 | 0.0427 (11) | 0.0421 (12) | 0.0534 (13) | 0.0152 (9) | 0.0042 (9) | 0.0164 (10) |
| C19 | 0.0308 (9) | 0.0320 (9) | 0.0312 (9) | 0.0033 (7) | 0.0017 (7) | 0.0146 (7) |
| C20 | 0.0314 (9) | 0.0411 (11) | 0.0526 (12) | 0.0068 (8) | 0.0032 (8) | 0.0265 (9) |
| C101 | 0.0312 (9) | 0.0339 (10) | 0.0454 (11) | 0.0032 (7) | -0.0031 (8) | 0.0165 (8) |
| C102 | 0.0501 (12) | 0.0420 (12) | 0.0687 (15) | -0.0052 (9) | -0.0206 (11) | 0.0198 (11) |
| C103 | 0.0800 (18) | 0.0484 (14) | 0.0578 (15) | 0.0018 (12) | -0.0308 (13) | 0.0094 (12) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|-------------|
| C104 | 0.0916 (18) | 0.0442 (13) | 0.0315 (11) | 0.0253 (12) | -0.0028 (11) | 0.0092 (9) |
| C105 | 0.0588 (12) | 0.0344 (10) | 0.0337 (10) | 0.0188 (9) | 0.0088 (9) | 0.0131 (8) |
| C106 | 0.0646 (14) | 0.0685 (16) | 0.0546 (14) | 0.0318 (12) | 0.0264 (11) | 0.0383 (12) |
| C107 | 0.0440 (12) | 0.0638 (15) | 0.0739 (16) | 0.0049 (10) | 0.0115 (11) | 0.0442 (13) |
| C108 | 0.0365 (10) | 0.0393 (11) | 0.0586 (13) | -0.0007 (8) | -0.0040 (9) | 0.0231 (10) |
| C109 | 0.0321 (9) | 0.0309 (9) | 0.0374 (10) | 0.0067 (7) | -0.0016 (7) | 0.0118 (8) |
| C110 | 0.0480 (11) | 0.0336 (10) | 0.0376 (10) | 0.0035 (8) | -0.0044 (8) | 0.0089 (8) |
| C111 | 0.0455 (11) | 0.0415 (11) | 0.0338 (10) | 0.0075 (8) | 0.0003 (8) | 0.0147 (9) |
| C112 | 0.0300 (9) | 0.0332 (9) | 0.0377 (10) | 0.0047 (7) | 0.0029 (7) | 0.0169 (8) |
| C113 | 0.0322 (9) | 0.0354 (10) | 0.0529 (12) | 0.0045 (7) | 0.0042 (8) | 0.0216 (9) |
| C114 | 0.0366 (9) | 0.0307 (9) | 0.0339 (9) | 0.0085 (7) | 0.0036 (7) | 0.0115 (8) |
| C115 | 0.0339 (9) | 0.0298 (9) | 0.0327 (9) | 0.0068 (7) | 0.0018 (7) | 0.0119 (7) |
| C116 | 0.0383 (11) | 0.0709 (16) | 0.0902 (18) | 0.0151 (10) | 0.0170 (11) | 0.0534 (15) |
| C117 | 0.0352 (10) | 0.0492 (12) | 0.0576 (13) | 0.0108 (9) | 0.0004 (9) | 0.0250 (11) |
| C118 | 0.0476 (12) | 0.0454 (12) | 0.0604 (14) | 0.0160 (9) | 0.0004 (10) | 0.0196 (11) |
| C119 | 0.0364 (10) | 0.0391 (11) | 0.0451 (11) | 0.0057 (8) | 0.0028 (8) | 0.0219 (9) |
| C120 | 0.0377 (10) | 0.0454 (12) | 0.0655 (14) | 0.0114 (9) | 0.0111 (9) | 0.0338 (11) |
| C201 | 0.0373 (10) | 0.0509 (12) | 0.0357 (10) | 0.0123 (9) | -0.0001 (8) | 0.0136 (9) |
| C202 | 0.0639 (14) | 0.0625 (15) | 0.0467 (13) | 0.0336 (12) | 0.0059 (11) | 0.0155 (11) |
| C203 | 0.094 (2) | 0.0522 (15) | 0.0599 (15) | 0.0352 (14) | -0.0066 (14) | 0.0145 (12) |
| C204 | 0.0763 (16) | 0.0400 (12) | 0.0527 (13) | 0.0058 (11) | -0.0070 (11) | 0.0231 (10) |
| C205 | 0.0499 (12) | 0.0456 (12) | 0.0376 (11) | -0.0029 (9) | -0.0089 (9) | 0.0181 (9) |
| C206 | 0.0453 (12) | 0.0727 (16) | 0.0458 (12) | -0.0069 (11) | -0.0020 (9) | 0.0331 (12) |
| C207 | 0.0495 (13) | 0.097 (2) | 0.0429 (13) | 0.0161 (13) | 0.0077 (10) | 0.0301 (13) |
| C208 | 0.0446 (11) | 0.0592 (14) | 0.0324 (10) | 0.0202 (10) | 0.0022 (8) | 0.0097 (10) |
| C209 | 0.0425 (10) | 0.0429 (11) | 0.0335 (10) | 0.0112 (8) | -0.0044 (8) | 0.0086 (9) |
| C210 | 0.0612 (13) | 0.0347 (11) | 0.0421 (11) | 0.0103 (9) | -0.0013 (10) | 0.0089 (9) |
| C211 | 0.0553 (13) | 0.0410 (12) | 0.0478 (12) | 0.0081 (9) | -0.0004 (10) | 0.0195 (10) |
| C212 | 0.0333 (9) | 0.0490 (12) | 0.0358 (10) | 0.0052 (8) | -0.0001 (7) | 0.0200 (9) |
| C213 | 0.0320 (9) | 0.0572 (13) | 0.0359 (10) | 0.0052 (8) | -0.0001 (8) | 0.0193 (9) |
| C214 | 0.0332 (9) | 0.0391 (10) | 0.0291 (9) | 0.0030 (7) | -0.0023 (7) | 0.0106 (8) |
| C215 | 0.0335 (9) | 0.0334 (9) | 0.0283 (9) | 0.0051 (7) | -0.0008 (7) | 0.0104 (7) |
| C216 | 0.0361 (11) | 0.118 (2) | 0.0585 (15) | 0.0096 (13) | 0.0032 (10) | 0.0502 (16) |
| C217 | 0.026 (3) | 0.072 (2) | 0.035 (3) | 0.015 (3) | 0.006 (2) | 0.017 (3) |
| C218 | 0.038 (2) | 0.078 (3) | 0.041 (2) | 0.013 (2) | -0.0058 (17) | 0.016 (2) |
| C219 | 0.0355 (9) | 0.0469 (11) | 0.0338 (10) | 0.0087 (8) | 0.0025 (7) | 0.0187 (9) |
| C220 | 0.0371 (10) | 0.0625 (14) | 0.0370 (11) | 0.0055 (9) | -0.0002 (8) | 0.0223 (10) |
| C227 | 0.026 (3) | 0.072 (2) | 0.035 (3) | 0.015 (3) | 0.006 (2) | 0.017 (3) |
| C228 | 0.045 (3) | 0.071 (4) | 0.068 (4) | -0.008 (2) | -0.016 (2) | 0.029 (3) |
| C301 | 0.0355 (9) | 0.0336 (10) | 0.0420 (11) | 0.0035 (7) | -0.0066 (8) | 0.0139 (8) |
| C302 | 0.0437 (11) | 0.0461 (12) | 0.0571 (13) | 0.0147 (9) | -0.0016 (9) | 0.0203 (10) |
| C303 | 0.0709 (16) | 0.0452 (13) | 0.0713 (16) | 0.0238 (11) | -0.0086 (13) | 0.0216 (12) |
| C304 | 0.0693 (15) | 0.0378 (12) | 0.0585 (14) | 0.0014 (10) | -0.0193 (11) | 0.0257 (11) |
| C305 | 0.0517 (12) | 0.0365 (11) | 0.0407 (11) | -0.0057 (9) | -0.0165 (9) | 0.0193 (9) |
| C306 | 0.0612 (14) | 0.0539 (14) | 0.0559 (14) | -0.0131 (11) | -0.0124 (11) | 0.0345 (12) |
| C307 | 0.0672 (15) | 0.0727 (17) | 0.0478 (13) | -0.0083 (12) | -0.0025 (11) | 0.0332 (13) |
| C308 | 0.0639 (14) | 0.0531 (13) | 0.0361 (11) | 0.0009 (11) | 0.0015 (10) | 0.0146 (10) |
| C309 | 0.0464 (11) | 0.0366 (10) | 0.0337 (10) | -0.0001 (8) | -0.0031 (8) | 0.0104 (8) |
| C310 | 0.0661 (14) | 0.0333 (11) | 0.0374 (11) | 0.0090 (9) | 0.0064 (10) | 0.0066 (9) |
| C311 | 0.0484 (11) | 0.0348 (10) | 0.0418 (11) | 0.0135 (8) | 0.0094 (9) | 0.0154 (9) |
| C312 | 0.0311 (9) | 0.0302 (9) | 0.0345 (9) | 0.0072 (7) | 0.0023 (7) | 0.0131 (8) |
| C313 | 0.0323 (9) | 0.0304 (9) | 0.0398 (10) | 0.0022 (7) | -0.0022 (7) | 0.0118 (8) |

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|------|-------------|-------------|-------------|-------------|-------------|-------------|
| C314 | 0.0329 (9) | 0.0318 (9) | 0.0323 (9) | 0.0038 (7) | -0.0011 (7) | 0.0121 (8) |
| C315 | 0.0391 (10) | 0.0288 (9) | 0.0325 (9) | -0.0003 (7) | -0.0052 (7) | 0.0115 (8) |
| C316 | 0.0350 (10) | 0.0491 (13) | 0.0640 (14) | -0.0013 (9) | -0.0035 (9) | 0.0271 (11) |
| C317 | 0.030 (3) | 0.048 (2) | 0.038 (3) | 0.006 (2) | 0.0026 (18) | 0.011 (2) |
| C318 | 0.029 (3) | 0.059 (4) | 0.044 (3) | -0.001 (2) | 0.002 (2) | 0.015 (3) |
| C319 | 0.0316 (9) | 0.0316 (9) | 0.0369 (10) | 0.0074 (7) | 0.0050 (7) | 0.0167 (8) |
| C320 | 0.0324 (9) | 0.0529 (12) | 0.0406 (11) | 0.0081 (8) | 0.0026 (8) | 0.0231 (9) |
| C327 | 0.030 (3) | 0.048 (2) | 0.038 (3) | 0.006 (2) | 0.0026 (18) | 0.011 (2) |
| C328 | 0.023 (3) | 0.095 (6) | 0.046 (4) | 0.004 (3) | -0.001 (3) | 0.005 (4) |
| C337 | 0.030 (3) | 0.048 (2) | 0.038 (3) | 0.006 (2) | 0.0026 (18) | 0.011 (2) |
| C338 | 0.063 (8) | 0.045 (6) | 0.047 (6) | 0.018 (5) | -0.020 (5) | -0.004 (4) |

Geometric parameters (Å, °)

| | | | |
|------------|------------|------------|------------|
| O21—C20 | 1.420 (2) | C201—C202 | 1.552 (3) |
| O21—H9021 | 0.803 (15) | C201—C213 | 1.532 (3) |
| O22—C19 | 1.425 (2) | C201—C215 | 1.576 (3) |
| O22—H9022 | 0.809 (15) | C201—C217 | 1.520 (9) |
| O121—C120 | 1.427 (2) | C201—C227 | 1.539 (10) |
| O121—H9121 | 0.809 (15) | C202—C203 | 1.525 (3) |
| O122—C119 | 1.413 (3) | C202—H2021 | 0.950 |
| O122—H9122 | 0.875 (15) | C202—H2022 | 0.950 |
| O221—C220 | 1.435 (2) | C203—C204 | 1.493 (4) |
| O221—H9221 | 0.821 (15) | C203—H2031 | 0.950 |
| O222—C219 | 1.414 (3) | C203—H2032 | 0.950 |
| O321—C320 | 1.426 (2) | C204—C205 | 1.323 (3) |
| O321—H9321 | 0.807 (15) | C204—H2041 | 0.950 |
| O322—C319 | 1.421 (2) | C205—C206 | 1.501 (3) |
| O322—H9322 | 0.831 (15) | C205—C215 | 1.516 (3) |
| C1—C2 | 1.553 (2) | C206—C207 | 1.520 (3) |
| C1—C13 | 1.527 (2) | C206—H2061 | 0.950 |
| C1—C15 | 1.572 (2) | C206—H2062 | 0.950 |
| C1—C17 | 1.513 (2) | C207—C208 | 1.497 (3) |
| C2—C3 | 1.525 (3) | C207—H2071 | 0.950 |
| C2—H21 | 0.950 | C207—H2072 | 0.950 |
| C2—H22 | 0.950 | C208—C209 | 1.329 (3) |
| C3—C4 | 1.498 (3) | C208—H2081 | 0.950 |
| C3—H31 | 0.950 | C209—C210 | 1.512 (3) |
| C3—H32 | 0.950 | C209—C215 | 1.527 (3) |
| C4—C5 | 1.327 (3) | C210—C211 | 1.544 (3) |
| C4—H41 | 0.950 | C210—H2101 | 0.950 |
| C5—C6 | 1.507 (3) | C210—H2102 | 0.950 |
| C5—C15 | 1.513 (2) | C211—C212 | 1.550 (3) |
| C6—C7 | 1.525 (3) | C211—H2111 | 0.950 |
| C6—H61 | 0.950 | C211—H2112 | 0.950 |
| C6—H62 | 0.950 | C212—C213 | 1.523 (3) |
| C7—C8 | 1.495 (3) | C212—C214 | 1.527 (3) |
| C7—H71 | 0.950 | C212—C219 | 1.537 (3) |
| C7—H72 | 0.950 | C213—C216 | 1.323 (3) |
| C8—C9 | 1.329 (3) | C214—C215 | 1.549 (2) |
| C8—H81 | 0.950 | C214—H2141 | 0.950 |

| | | | |
|------------|-----------|------------|------------|
| C9—C10 | 1.509 (3) | C214—H2142 | 0.950 |
| C9—C15 | 1.534 (2) | C216—H2161 | 0.950 |
| C10—C11 | 1.536 (3) | C216—H2162 | 0.950 |
| C10—H101 | 0.950 | C217—C218 | 1.299 (9) |
| C10—H102 | 0.950 | C217—H2171 | 0.950 |
| C11—C12 | 1.545 (2) | C218—H2181 | 0.950 |
| C11—H111 | 0.950 | C218—H2182 | 0.950 |
| C11—H112 | 0.950 | C219—C220 | 1.500 (3) |
| C12—C13 | 1.532 (2) | C219—H2191 | 0.950 |
| C12—C14 | 1.535 (2) | C220—H2201 | 0.950 |
| C12—C19 | 1.532 (2) | C220—H2202 | 0.950 |
| C13—C16 | 1.320 (2) | C227—C228 | 1.299 (11) |
| C14—C15 | 1.556 (2) | C227—H2271 | 0.950 |
| C14—H141 | 0.950 | C228—H2281 | 0.950 |
| C14—H142 | 0.950 | C228—H2282 | 0.950 |
| C16—H161 | 0.950 | C301—C302 | 1.545 (3) |
| C16—H162 | 0.950 | C301—C313 | 1.535 (3) |
| C17—C18 | 1.304 (3) | C301—C315 | 1.571 (3) |
| C17—H171 | 0.950 | C301—C317 | 1.516 (10) |
| C18—H181 | 0.950 | C301—C327 | 1.536 (10) |
| C18—H182 | 0.950 | C301—C337 | 1.538 (13) |
| C19—C20 | 1.512 (2) | C302—C303 | 1.528 (3) |
| C19—H191 | 0.950 | C302—H3021 | 0.950 |
| C20—H201 | 0.950 | C302—H3022 | 0.950 |
| C20—H202 | 0.950 | C303—C304 | 1.488 (4) |
| C101—C102 | 1.548 (3) | C303—H3031 | 0.950 |
| C101—C113 | 1.529 (3) | C303—H3032 | 0.950 |
| C101—C115 | 1.570 (2) | C304—C305 | 1.328 (3) |
| C101—C117 | 1.511 (3) | C304—H3041 | 0.950 |
| C102—C103 | 1.521 (3) | C305—C306 | 1.501 (3) |
| C102—H1021 | 0.950 | C305—C315 | 1.512 (3) |
| C102—H1022 | 0.950 | C306—C307 | 1.522 (3) |
| C103—C104 | 1.494 (4) | C306—H3061 | 0.950 |
| C103—H1031 | 0.950 | C306—H3062 | 0.950 |
| C103—H1032 | 0.950 | C307—C308 | 1.496 (3) |
| C104—C105 | 1.331 (3) | C307—H3071 | 0.950 |
| C104—H1041 | 0.950 | C307—H3072 | 0.950 |
| C105—C106 | 1.499 (3) | C308—C309 | 1.327 (3) |
| C105—C115 | 1.513 (3) | C308—H3081 | 0.950 |
| C106—C107 | 1.521 (3) | C309—C310 | 1.511 (3) |
| C106—H1061 | 0.950 | C309—C315 | 1.533 (3) |
| C106—H1062 | 0.950 | C310—C311 | 1.531 (3) |
| C107—C108 | 1.499 (3) | C310—H3101 | 0.950 |
| C107—H1071 | 0.950 | C310—H3102 | 0.950 |
| C107—H1072 | 0.950 | C311—C312 | 1.541 (2) |
| C108—C109 | 1.328 (3) | C311—H3111 | 0.950 |
| C108—H1081 | 0.950 | C311—H3112 | 0.950 |
| C109—C110 | 1.507 (3) | C312—C313 | 1.531 (2) |
| C109—C115 | 1.531 (2) | C312—C314 | 1.537 (2) |
| C110—C111 | 1.538 (3) | C312—C319 | 1.534 (2) |
| C110—H1101 | 0.950 | C313—C316 | 1.318 (3) |
| C110—H1102 | 0.950 | C314—C315 | 1.551 (2) |

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| C111—C112 | 1.538 (3) | C314—H3141 | 0.950 |
| C111—H1111 | 0.950 | C314—H3142 | 0.950 |
| C111—H1112 | 0.950 | C316—H3161 | 0.950 |
| C112—C113 | 1.532 (2) | C316—H3162 | 0.950 |
| C112—C114 | 1.533 (2) | C317—C318 | 1.278 (11) |
| C112—C119 | 1.536 (2) | C317—H3171 | 0.950 |
| C113—C116 | 1.325 (3) | C318—H3181 | 0.950 |
| C114—C115 | 1.556 (2) | C318—H3182 | 0.950 |
| C114—H1141 | 0.950 | C319—C320 | 1.510 (2) |
| C114—H1142 | 0.950 | C319—H3191 | 0.950 |
| C116—H1161 | 0.950 | C320—H3201 | 0.950 |
| C116—H1162 | 0.950 | C320—H3202 | 0.950 |
| C117—C118 | 1.312 (3) | C327—C328 | 1.251 (12) |
| C117—H1171 | 0.950 | C327—H3271 | 0.950 |
| C118—H1181 | 0.950 | C328—H3281 | 0.950 |
| C118—H1182 | 0.950 | C328—H3282 | 0.950 |
| C119—C120 | 1.504 (3) | C337—H3371 | 0.950 |
| C119—H1191 | 0.950 | C338—H3381 | 0.950 |
| C120—H1201 | 0.950 | C338—H3382 | 0.950 |
| C120—H1202 | 0.950 | | |
| O21...O22 ⁱ | 2.734 (2) | O221...O321 ⁱⁱⁱ | 2.842 (2) |
| O21...O121 ⁱⁱ | 2.842 (2) | O221...O322 ⁱⁱⁱ | 3.168 (2) |
| O21...O322 ⁱⁱ | 3.097 (2) | O221...C16 | 3.497 (3) |
| O21...C220 ⁱ | 3.221 (3) | O221...C20 ^{iv} | 3.523 (3) |
| O21...O122 ⁱⁱ | 3.314 (2) | O221...C320 ⁱⁱⁱ | 3.581 (2) |
| O21...C216 | 3.423 (3) | O222...O321 ⁱⁱⁱ | 3.258 (2) |
| O22...O221 | 2.913 (2) | O222...C120 ⁱⁱ | 3.299 (3) |
| O22...O321 ⁱⁱⁱ | 3.146 (2) | O321...C120 ^{iv} | 3.248 (3) |
| O22...O121 ⁱⁱ | 3.269 (2) | O321...C116 | 3.522 (4) |
| O22...C320 ⁱⁱⁱ | 3.367 (2) | O322...C20 ⁱⁱ | 3.376 (2) |
| O121...O321 ⁱ | 2.739 (2) | C11...C218 ^v | 3.485 (4) |
| O121...O322 | 2.946 (2) | C110...C338 ⁱⁱ | 3.55 (1) |
| O121...O222 ⁱⁱ | 3.235 (2) | C111...C338 ⁱⁱ | 3.371 (9) |
| O121...C316 | 3.504 (3) | C208...C228 ^{iv} | 3.458 (5) |
| O121...C320 ⁱ | 3.542 (2) | C308...C328 ^{iv} | 3.276 (7) |
| O122...O221 ⁱⁱⁱ | 3.180 (2) | C309...C328 ^{iv} | 3.493 (7) |
| O122...C220 ⁱⁱⁱ | 3.262 (2) | C311...C311 ⁱⁱⁱ | 3.530 (4) |
| C20—O21—H9021 | 107.9 (13) | C201—C202—H2021 | 108.7 |
| C19—O22—H9022 | 107.2 (13) | C203—C202—H2021 | 108.7 |
| C120—O121—H9121 | 104.3 (13) | C201—C202—H2022 | 108.7 |
| C119—O122—H9122 | 99.2 (13) | C203—C202—H2022 | 108.7 |
| C220—O221—H9221 | 106.4 (12) | H2021—C202—H2022 | 109.5 |
| C320—O321—H9321 | 108.9 (13) | C202—C203—C204 | 111.35 (19) |
| C319—O322—H9322 | 107.3 (13) | C202—C203—H2031 | 109.0 |
| C2—C1—C13 | 107.96 (14) | C204—C203—H2031 | 109.0 |
| C2—C1—C15 | 108.72 (14) | C202—C203—H2032 | 109.0 |
| C13—C1—C15 | 103.49 (13) | C204—C203—H2032 | 109.0 |
| C2—C1—C17 | 107.08 (14) | H2031—C203—H2032 | 109.5 |
| C13—C1—C17 | 113.42 (15) | C203—C204—C205 | 125.2 (2) |
| C15—C1—C17 | 115.88 (14) | C203—C204—H2041 | 117.4 |

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| C1—C2—C3 | 112.57 (15) | C205—C204—H2041 | 117.4 |
| C1—C2—H21 | 108.7 | C204—C205—C206 | 122.4 (2) |
| C3—C2—H21 | 108.7 | C204—C205—C215 | 123.1 (2) |
| C1—C2—H22 | 108.7 | C206—C205—C215 | 114.43 (18) |
| C3—C2—H22 | 108.7 | C205—C206—C207 | 109.43 (18) |
| H21—C2—H22 | 109.5 | C205—C206—H2061 | 109.5 |
| C2—C3—C4 | 111.75 (15) | C207—C206—H2061 | 109.5 |
| C2—C3—H31 | 108.9 | C205—C206—H2062 | 109.5 |
| C4—C3—H31 | 108.9 | C207—C206—H2062 | 109.5 |
| C2—C3—H32 | 108.9 | H2061—C206—H2062 | 109.5 |
| C4—C3—H32 | 108.9 | C206—C207—C208 | 110.17 (18) |
| H31—C3—H32 | 109.5 | C206—C207—H2071 | 109.3 |
| C3—C4—C5 | 124.62 (18) | C208—C207—H2071 | 109.3 |
| C3—C4—H41 | 117.7 | C206—C207—H2072 | 109.3 |
| C5—C4—H41 | 117.7 | C208—C207—H2072 | 109.3 |
| C4—C5—C6 | 122.67 (17) | H2071—C207—H2072 | 109.5 |
| C4—C5—C15 | 122.81 (16) | C207—C208—C209 | 124.3 (2) |
| C6—C5—C15 | 114.51 (15) | C207—C208—H2081 | 117.8 |
| C5—C6—C7 | 110.55 (16) | C209—C208—H2081 | 117.8 |
| C5—C6—H61 | 109.2 | C208—C209—C210 | 121.80 (19) |
| C7—C6—H61 | 109.2 | C208—C209—C215 | 122.80 (19) |
| C5—C6—H62 | 109.2 | C210—C209—C215 | 115.31 (16) |
| C7—C6—H62 | 109.2 | C209—C210—C211 | 111.51 (17) |
| H61—C6—H62 | 109.5 | C209—C210—H2101 | 109.0 |
| C6—C7—C8 | 110.75 (16) | C211—C210—H2101 | 109.0 |
| C6—C7—H71 | 109.2 | C209—C210—H2102 | 109.0 |
| C8—C7—H71 | 109.2 | C211—C210—H2102 | 109.0 |
| C6—C7—H72 | 109.2 | H2101—C210—H2102 | 109.5 |
| C8—C7—H72 | 109.2 | C210—C211—C212 | 110.69 (16) |
| H71—C7—H72 | 109.5 | C210—C211—H2111 | 109.2 |
| C7—C8—C9 | 124.58 (18) | C212—C211—H2111 | 109.2 |
| C7—C8—H81 | 117.7 | C210—C211—H2112 | 109.2 |
| C9—C8—H81 | 117.7 | C212—C211—H2112 | 109.2 |
| C8—C9—C10 | 122.02 (17) | H2111—C211—H2112 | 109.5 |
| C8—C9—C15 | 122.57 (17) | C211—C212—C213 | 106.64 (16) |
| C10—C9—C15 | 115.17 (14) | C211—C212—C214 | 107.24 (16) |
| C9—C10—C11 | 111.26 (15) | C213—C212—C214 | 103.17 (15) |
| C9—C10—H101 | 109.0 | C211—C212—C219 | 112.17 (16) |
| C11—C10—H101 | 109.0 | C213—C212—C219 | 111.99 (15) |
| C9—C10—H102 | 109.0 | C214—C212—C219 | 114.91 (16) |
| C11—C10—H102 | 109.0 | C201—C213—C212 | 109.40 (15) |
| H101—C10—H102 | 109.5 | C201—C213—C216 | 124.69 (19) |
| C10—C11—C12 | 110.81 (14) | C212—C213—C216 | 125.78 (19) |
| C10—C11—H111 | 109.1 | C212—C214—C215 | 102.94 (14) |
| C12—C11—H111 | 109.1 | C212—C214—H2141 | 111.1 |
| C10—C11—H112 | 109.1 | C215—C214—H2141 | 111.1 |
| C12—C11—H112 | 109.1 | C212—C214—H2142 | 111.1 |
| H111—C11—H112 | 109.5 | C215—C214—H2142 | 111.1 |
| C11—C12—C13 | 107.02 (14) | H2141—C214—H2142 | 109.5 |
| C11—C12—C14 | 108.10 (14) | C214—C215—C209 | 105.62 (14) |
| C13—C12—C14 | 102.31 (13) | C214—C215—C205 | 115.17 (15) |
| C11—C12—C19 | 111.91 (14) | C209—C215—C205 | 110.87 (16) |

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| C13—C12—C19 | 112.47 (14) | C214—C215—C201 | 101.58 (14) |
| C14—C12—C19 | 114.35 (14) | C209—C215—C201 | 110.65 (15) |
| C12—C13—C1 | 109.20 (14) | C205—C215—C201 | 112.44 (15) |
| C12—C13—C16 | 125.38 (17) | C213—C216—H2161 | 120.0 |
| C1—C13—C16 | 125.41 (16) | C213—C216—H2162 | 120.0 |
| C12—C14—C15 | 102.72 (13) | H2161—C216—H2162 | 120.0 |
| C12—C14—H141 | 111.1 | C201—C217—C218 | 124.8 (6) |
| C15—C14—H141 | 111.1 | C201—C217—H2171 | 117.6 |
| C12—C14—H142 | 111.1 | C218—C217—H2171 | 117.6 |
| C15—C14—H142 | 111.1 | C217—C218—H2181 | 120.0 |
| H141—C14—H142 | 109.5 | C217—C218—H2182 | 120.0 |
| C9—C15—C14 | 105.26 (13) | H2181—C218—H2182 | 120.0 |
| C9—C15—C5 | 111.58 (14) | C212—C219—O222 | 110.34 (15) |
| C14—C15—C5 | 113.04 (14) | C212—C219—C220 | 114.27 (15) |
| C9—C15—C1 | 111.86 (14) | O222—C219—C220 | 107.10 (17) |
| C14—C15—C1 | 100.64 (13) | C212—C219—H2191 | 108.3 |
| C5—C15—C1 | 113.69 (14) | O222—C219—H2191 | 108.3 |
| C13—C16—H161 | 120.0 | C220—C219—H2191 | 108.3 |
| C13—C16—H162 | 120.0 | C219—C220—O221 | 108.87 (15) |
| H161—C16—H162 | 120.0 | C219—C220—H2201 | 109.6 |
| C1—C17—C18 | 128.57 (18) | O221—C220—H2201 | 109.6 |
| C1—C17—H171 | 115.7 | C219—C220—H2202 | 109.6 |
| C18—C17—H171 | 115.7 | O221—C220—H2202 | 109.6 |
| C17—C18—H181 | 120.0 | H2201—C220—H2202 | 109.5 |
| C17—C18—H182 | 120.0 | C201—C227—C228 | 127.8 (8) |
| H181—C18—H182 | 120.0 | C201—C227—H2271 | 116.1 |
| C12—C19—O22 | 112.00 (13) | C228—C227—H2271 | 116.1 |
| C12—C19—C20 | 113.71 (14) | C227—C228—H2281 | 120.0 |
| O22—C19—C20 | 105.44 (14) | C227—C228—H2282 | 120.0 |
| C12—C19—H191 | 108.5 | H2281—C228—H2282 | 120.0 |
| O22—C19—H191 | 108.5 | C302—C301—C313 | 107.56 (16) |
| C20—C19—H191 | 108.5 | C302—C301—C315 | 109.43 (15) |
| C19—C20—O21 | 112.11 (14) | C313—C301—C315 | 103.03 (14) |
| C19—C20—H201 | 108.8 | C302—C301—C317 | 100.1 (4) |
| O21—C20—H201 | 108.8 | C313—C301—C317 | 113.8 (5) |
| C19—C20—H202 | 108.8 | C315—C301—C317 | 122.3 (4) |
| O21—C20—H202 | 108.8 | C302—C301—C327 | 113.4 (5) |
| H201—C20—H202 | 109.5 | C313—C301—C327 | 116.5 (7) |
| C102—C101—C113 | 107.30 (16) | C315—C301—C327 | 106.3 (6) |
| C102—C101—C115 | 109.40 (16) | C302—C301—C337 | 116.5 (7) |
| C113—C101—C115 | 103.41 (14) | C313—C301—C337 | 113.1 (9) |
| C102—C101—C117 | 107.54 (16) | C315—C301—C337 | 106.3 (8) |
| C113—C101—C117 | 113.45 (17) | C301—C302—C303 | 112.70 (19) |
| C115—C101—C117 | 115.44 (15) | C301—C302—H3021 | 108.7 |
| C101—C102—C103 | 112.81 (18) | C303—C302—H3021 | 108.7 |
| C101—C102—H1021 | 108.6 | C301—C302—H3022 | 108.7 |
| C103—C102—H1021 | 108.6 | C303—C302—H3022 | 108.7 |
| C101—C102—H1022 | 108.6 | H3021—C302—H3022 | 109.5 |
| C103—C102—H1022 | 108.6 | C302—C303—C304 | 112.31 (18) |
| H1021—C102—H1022 | 109.5 | C302—C303—H3031 | 108.8 |
| C102—C103—C104 | 111.82 (19) | C304—C303—H3031 | 108.8 |
| C102—C103—H1031 | 108.9 | C302—C303—H3032 | 108.8 |

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| C104—C103—H1031 | 108.9 | C304—C303—H3032 | 108.8 |
| C102—C103—H1032 | 108.9 | H3031—C303—H3032 | 109.5 |
| C104—C103—H1032 | 108.9 | C303—C304—C305 | 125.5 (2) |
| H1031—C103—H1032 | 109.5 | C303—C304—H3041 | 117.2 |
| C103—C104—C105 | 124.9 (2) | C305—C304—H3041 | 117.2 |
| C103—C104—H1041 | 117.6 | C304—C305—C306 | 122.26 (19) |
| C105—C104—H1041 | 117.6 | C304—C305—C315 | 122.4 (2) |
| C104—C105—C106 | 122.6 (2) | C306—C305—C315 | 115.31 (18) |
| C104—C105—C115 | 122.6 (2) | C305—C306—C307 | 109.88 (18) |
| C106—C105—C115 | 114.67 (18) | C305—C306—H3061 | 109.4 |
| C105—C106—C107 | 109.98 (17) | C307—C306—H3061 | 109.4 |
| C105—C106—H1061 | 109.3 | C305—C306—H3062 | 109.4 |
| C107—C106—H1061 | 109.3 | C307—C306—H3062 | 109.4 |
| C105—C106—H1062 | 109.3 | H3061—C306—H3062 | 109.5 |
| C107—C106—H1062 | 109.3 | C306—C307—C308 | 110.24 (18) |
| H1061—C106—H1062 | 109.5 | C306—C307—H3071 | 109.3 |
| C106—C107—C108 | 110.28 (17) | C308—C307—H3071 | 109.3 |
| C106—C107—H1071 | 109.3 | C306—C307—H3072 | 109.3 |
| C108—C107—H1071 | 109.3 | C308—C307—H3072 | 109.3 |
| C106—C107—H1072 | 109.3 | H3071—C307—H3072 | 109.5 |
| C108—C107—H1072 | 109.3 | C307—C308—C309 | 124.7 (2) |
| H1071—C107—H1072 | 109.5 | C307—C308—H3081 | 117.7 |
| C107—C108—C109 | 124.0 (2) | C309—C308—H3081 | 117.7 |
| C107—C108—H1081 | 118.0 | C308—C309—C310 | 121.92 (19) |
| C109—C108—H1081 | 118.0 | C308—C309—C315 | 122.58 (19) |
| C108—C109—C110 | 122.23 (18) | C310—C309—C315 | 115.48 (16) |
| C108—C109—C115 | 122.71 (18) | C309—C310—C311 | 112.39 (16) |
| C110—C109—C115 | 114.96 (15) | C309—C310—H3101 | 108.7 |
| C109—C110—C111 | 111.69 (16) | C311—C310—H3101 | 108.7 |
| C109—C110—H1101 | 108.9 | C309—C310—H3102 | 108.7 |
| C111—C110—H1101 | 108.9 | C311—C310—H3102 | 108.7 |
| C109—C110—H1102 | 108.9 | H3101—C310—H3102 | 109.5 |
| C111—C110—H1102 | 108.9 | C310—C311—C312 | 110.65 (15) |
| H1101—C110—H1102 | 109.5 | C310—C311—H3111 | 109.2 |
| C110—C111—C112 | 111.07 (15) | C312—C311—H3111 | 109.2 |
| C110—C111—H1111 | 109.1 | C310—C311—H3112 | 109.2 |
| C112—C111—H1111 | 109.1 | C312—C311—H3112 | 109.2 |
| C110—C111—H1112 | 109.1 | H3111—C311—H3112 | 109.5 |
| C112—C111—H1112 | 109.1 | C311—C312—C313 | 107.09 (15) |
| H1111—C111—H1112 | 109.5 | C311—C312—C314 | 107.44 (14) |
| C111—C112—C113 | 107.36 (15) | C313—C312—C314 | 103.00 (14) |
| C111—C112—C114 | 107.79 (15) | C311—C312—C319 | 111.70 (14) |
| C113—C112—C114 | 102.29 (14) | C313—C312—C319 | 112.21 (14) |
| C111—C112—C119 | 112.12 (15) | C314—C312—C319 | 114.76 (15) |
| C113—C112—C119 | 112.17 (14) | C301—C313—C312 | 108.96 (14) |
| C114—C112—C119 | 114.43 (15) | C301—C313—C316 | 125.79 (17) |
| C112—C113—C101 | 109.33 (15) | C312—C313—C316 | 125.24 (17) |
| C112—C113—C116 | 125.79 (18) | C312—C314—C315 | 102.51 (14) |
| C101—C113—C116 | 124.85 (18) | C312—C314—H3141 | 111.2 |
| C112—C114—C115 | 102.80 (14) | C315—C314—H3141 | 111.2 |
| C112—C114—H1141 | 111.1 | C312—C314—H3142 | 111.2 |
| C115—C114—H1141 | 111.1 | C315—C314—H3142 | 111.2 |

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| C112—C114—H1142 | 111.1 | H3141—C314—H3142 | 109.5 |
| C115—C114—H1142 | 111.1 | C309—C315—C314 | 106.06 (15) |
| H1141—C114—H1142 | 109.5 | C309—C315—C305 | 111.13 (16) |
| C109—C115—C114 | 105.35 (14) | C314—C315—C305 | 114.17 (14) |
| C109—C115—C105 | 111.62 (15) | C309—C315—C301 | 111.06 (15) |
| C114—C115—C105 | 113.03 (14) | C314—C315—C301 | 101.14 (14) |
| C109—C115—C101 | 111.60 (14) | C305—C315—C301 | 112.72 (16) |
| C114—C115—C101 | 101.08 (14) | C313—C316—H3161 | 120.0 |
| C105—C115—C101 | 113.45 (15) | C313—C316—H3162 | 120.0 |
| C113—C116—H1161 | 120.0 | H3161—C316—H3162 | 120.0 |
| C113—C116—H1162 | 120.0 | C301—C317—C318 | 133.1 (10) |
| H1161—C116—H1162 | 120.0 | C301—C317—H3171 | 113.5 |
| C101—C117—C118 | 128.5 (2) | C318—C317—H3171 | 113.5 |
| C101—C117—H1171 | 115.8 | C317—C318—H3181 | 120.0 |
| C118—C117—H1171 | 115.8 | C317—C318—H3182 | 120.0 |
| C117—C118—H1181 | 120.0 | H3181—C318—H3182 | 120.0 |
| C117—C118—H1182 | 120.0 | C312—C319—O322 | 111.83 (14) |
| H1181—C118—H1182 | 120.0 | C312—C319—C320 | 113.76 (14) |
| C112—C119—O122 | 110.80 (16) | O322—C319—C320 | 105.77 (15) |
| C112—C119—C120 | 113.91 (15) | C312—C319—H3191 | 108.4 |
| O122—C119—C120 | 108.98 (17) | O322—C319—H3191 | 108.4 |
| C112—C119—H1191 | 107.6 | C320—C319—H3191 | 108.4 |
| O122—C119—H1191 | 107.6 | C319—C320—O321 | 111.98 (15) |
| C120—C119—H1191 | 107.6 | C319—C320—H3201 | 108.8 |
| C119—C120—O121 | 109.59 (15) | O321—C320—H3201 | 108.8 |
| C119—C120—H1201 | 109.4 | C319—C320—H3202 | 108.8 |
| O121—C120—H1201 | 109.4 | O321—C320—H3202 | 108.8 |
| C119—C120—H1202 | 109.4 | H3201—C320—H3202 | 109.5 |
| O121—C120—H1202 | 109.4 | C301—C327—C328 | 129.4 (10) |
| H1201—C120—H1202 | 109.5 | C301—C327—H3271 | 115.3 |
| C202—C201—C213 | 108.13 (17) | C328—C327—H3271 | 115.3 |
| C202—C201—C215 | 108.91 (17) | C327—C328—H3281 | 120.0 |
| C213—C201—C215 | 102.91 (14) | C327—C328—H3282 | 120.0 |
| C202—C201—C217 | 105.7 (5) | H3281—C328—H3282 | 120.0 |
| C213—C201—C217 | 110.9 (5) | C301—C337—C338 | 129.3 (17) |
| C215—C201—C217 | 119.9 (3) | C301—C337—H3371 | 115.3 |
| C202—C201—C227 | 112.8 (6) | C338—C337—H3371 | 115.3 |
| C213—C201—C227 | 118.6 (6) | C337—C338—H3381 | 119.8 |
| C215—C201—C227 | 104.7 (3) | C337—C338—H3382 | 120.2 |
| C201—C202—C203 | 112.39 (18) | H3381—C338—H3382 | 120.0 |
| O21—C20—C19—O22 | -66.9 (2) | C201—C215—C205—C204 | -14.5 (2) |
| O21—C20—C19—C12 | 170.0 (1) | C201—C215—C205—C206 | 162.7 (1) |
| O22—C19—C12—C11 | 175.0 (1) | C201—C215—C209—C208 | -133.1 (2) |
| O22—C19—C12—C13 | 54.5 (2) | C201—C215—C209—C210 | 50.2 (2) |
| O22—C19—C12—C14 | -61.7 (2) | C201—C215—C214—C212 | -44.9 (2) |
| O121—C120—C119—O122 | -57.6 (2) | C202—C201—C213—C212 | 105.0 (2) |
| O121—C120—C119—C112 | 178.1 (1) | C202—C201—C213—C216 | -70.9 (3) |
| O122—C119—C112—C111 | 177.9 (1) | C202—C201—C215—C205 | 42.3 (2) |
| O122—C119—C112—C113 | 57.0 (2) | C202—C201—C215—C209 | 166.9 (2) |
| O122—C119—C112—C114 | -59.0 (2) | C202—C201—C215—C214 | -81.3 (2) |
| O221—C220—C219—O222 | -60.9 (2) | C202—C201—C217—C218 | -95 (1) |

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|---------------------|------------|---------------------|------------|
| O221—C220—C219—C212 | 176.6 (2) | C202—C201—C227—C228 | 106 (1) |
| O222—C219—C212—C211 | 179.1 (2) | C202—C203—C204—C205 | -16.1 (3) |
| O222—C219—C212—C213 | 59.2 (2) | C203—C202—C201—C213 | -170.8 (2) |
| O222—C219—C212—C214 | -58.1 (2) | C203—C202—C201—C215 | -59.7 (2) |
| O321—C320—C319—O322 | -67.3 (2) | C203—C202—C201—C217 | 70.4 (5) |
| O321—C320—C319—C312 | 169.5 (1) | C203—C202—C201—C227 | 56.1 (5) |
| O322—C319—C312—C311 | 174.5 (1) | C203—C204—C205—C206 | -176.5 (2) |
| O322—C319—C312—C313 | 54.2 (2) | C203—C204—C205—C215 | 0.4 (3) |
| O322—C319—C312—C314 | -63.0 (2) | C204—C205—C206—C207 | 115.8 (3) |
| C1—C2—C3—C4 | 46.3 (2) | C204—C205—C215—C209 | -138.9 (2) |
| C1—C13—C12—C11 | 95.4 (2) | C204—C205—C215—C214 | 101.3 (2) |
| C1—C13—C12—C14 | -18.2 (2) | C205—C206—C207—C208 | 50.6 (3) |
| C1—C13—C12—C19 | -141.3 (1) | C205—C215—C201—C213 | 156.9 (1) |
| C1—C15—C5—C4 | -13.8 (3) | C205—C215—C201—C217 | -79.5 (7) |
| C1—C15—C5—C6 | 165.0 (2) | C205—C215—C201—C227 | -78.5 (7) |
| C1—C15—C9—C8 | -137.2 (2) | C205—C215—C209—C208 | -7.7 (3) |
| C1—C15—C9—C10 | 48.2 (2) | C205—C215—C209—C210 | 175.7 (2) |
| C1—C15—C14—C12 | -46.5 (1) | C205—C215—C214—C212 | -166.7 (1) |
| C2—C1—C13—C12 | 104.7 (1) | C206—C205—C215—C209 | 38.2 (2) |
| C2—C1—C13—C16 | -75.2 (2) | C206—C205—C215—C214 | -81.6 (2) |
| C2—C1—C15—C5 | 41.0 (2) | C206—C207—C208—C209 | -22.7 (3) |
| C2—C1—C15—C9 | 168.5 (2) | C207—C206—C205—C215 | -61.4 (3) |
| C2—C1—C15—C14 | -80.2 (2) | C207—C208—C209—C210 | 177.1 (2) |
| C2—C1—C17—C18 | -97.2 (2) | C207—C208—C209—C215 | 0.7 (4) |
| C2—C3—C4—C5 | -17.2 (3) | C208—C209—C210—C211 | -130.7 (2) |
| C3—C2—C1—C13 | -170.1 (1) | C208—C209—C215—C214 | 117.7 (2) |
| C3—C2—C1—C15 | -58.4 (2) | C209—C210—C211—C212 | -45.5 (2) |
| C3—C2—C1—C17 | 67.4 (2) | C209—C215—C201—C213 | -78.5 (2) |
| C3—C4—C5—C6 | -177.8 (2) | C209—C215—C201—C217 | 45.1 (7) |
| C3—C4—C5—C15 | 0.9 (3) | C209—C215—C201—C227 | 46.0 (7) |
| C4—C5—C6—C7 | 120.1 (2) | C209—C215—C214—C212 | 70.6 (2) |
| C4—C5—C15—C9 | -141.5 (2) | C210—C209—C215—C214 | -58.9 (2) |
| C4—C5—C15—C14 | 100.1 (2) | C210—C211—C212—C213 | -48.5 (2) |
| C5—C6—C7—C8 | 48.1 (3) | C210—C211—C212—C214 | 61.5 (2) |
| C5—C15—C1—C13 | 155.6 (1) | C210—C211—C212—C219 | -171.5 (2) |
| C5—C15—C1—C17 | -79.6 (2) | C211—C210—C209—C215 | 46.0 (3) |
| C5—C15—C9—C8 | -8.6 (2) | C211—C212—C213—C216 | -88.8 (3) |
| C5—C15—C9—C10 | 176.9 (2) | C211—C212—C214—C215 | -73.8 (2) |
| C5—C15—C14—C12 | -168.2 (1) | C211—C212—C219—C220 | -60.2 (2) |
| C6—C5—C15—C9 | 37.4 (2) | C212—C213—C201—C215 | -10.1 (2) |
| C6—C5—C15—C14 | -81.0 (2) | C212—C213—C201—C217 | -139.5 (5) |
| C6—C7—C8—C9 | -21.5 (3) | C212—C213—C201—C227 | -125.0 (5) |
| C7—C6—C5—C15 | -58.7 (2) | C213—C201—C215—C214 | 33.2 (2) |
| C7—C8—C9—C10 | 175.5 (2) | C213—C201—C217—C218 | 148 (1) |
| C7—C8—C9—C15 | 1.3 (3) | C213—C201—C227—C228 | -22 (1) |
| C8—C9—C10—C11 | -126.9 (2) | C213—C212—C214—C215 | 38.6 (2) |
| C8—C9—C15—C14 | 114.4 (2) | C213—C212—C219—C220 | 179.9 (2) |
| C9—C10—C11—C12 | -46.2 (2) | C214—C212—C213—C216 | 158.4 (2) |
| C9—C15—C1—C13 | -76.9 (2) | C214—C212—C219—C220 | 62.6 (2) |
| C9—C15—C1—C17 | 47.9 (2) | C214—C215—C201—C217 | 156.8 (7) |
| C9—C15—C14—C12 | 69.8 (1) | C214—C215—C201—C227 | 157.8 (7) |
| C10—C9—C15—C14 | -60.2 (2) | C215—C201—C213—C216 | 173.9 (2) |

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| C10—C11—C12—C13 | -48.3 (2) | C215—C201—C217—C218 | 28 (2) |
| C10—C11—C12—C14 | 61.2 (2) | C215—C201—C227—C228 | -136 (1) |
| C10—C11—C12—C19 | -172.0 (1) | C215—C214—C212—C219 | 160.8 (1) |
| C11—C10—C9—C15 | 47.8 (2) | C216—C213—C201—C217 | 44.6 (5) |
| C11—C12—C13—C16 | -84.7 (2) | C216—C213—C201—C227 | 59.1 (5) |
| C11—C12—C14—C15 | -72.7 (2) | C216—C213—C212—C219 | 34.3 (3) |
| C11—C12—C19—C20 | -65.6 (2) | C301—C302—C303—C304 | 42.0 (2) |
| C12—C13—C1—C15 | -10.5 (2) | C301—C313—C312—C311 | 96.9 (2) |
| C12—C13—C1—C17 | -136.9 (1) | C301—C313—C312—C314 | -16.2 (2) |
| C13—C1—C15—C14 | 34.4 (1) | C301—C313—C312—C319 | -140.2 (1) |
| C13—C1—C17—C18 | 143.8 (2) | C301—C315—C305—C304 | -16.4 (3) |
| C13—C12—C14—C15 | 40.0 (1) | C301—C315—C305—C306 | 160.5 (2) |
| C13—C12—C19—C20 | 173.9 (1) | C301—C315—C309—C308 | -129.9 (2) |
| C14—C12—C13—C16 | 161.7 (2) | C301—C315—C309—C310 | 52.0 (2) |
| C14—C12—C19—C20 | 57.8 (2) | C301—C315—C314—C312 | -46.4 (2) |
| C14—C15—C1—C17 | 159.2 (1) | C302—C301—C313—C312 | 103.3 (2) |
| C15—C1—C13—C16 | 169.6 (2) | C302—C301—C313—C316 | -75.5 (2) |
| C15—C1—C17—C18 | 24.3 (3) | C302—C301—C315—C305 | 43.7 (2) |
| C15—C14—C12—C19 | 161.9 (1) | C302—C301—C315—C309 | 169.2 (2) |
| C16—C13—C1—C17 | 43.2 (2) | C302—C301—C315—C314 | -78.6 (2) |
| C16—C13—C12—C19 | 38.6 (2) | C302—C301—C317—C318 | 137.9 (9) |
| C101—C102—C103—C104 | 45.5 (3) | C302—C301—C327—C328 | 32 (2) |
| C101—C113—C112—C111 | 94.4 (2) | C302—C301—C337—C338 | -41 (2) |
| C101—C113—C112—C114 | -18.9 (2) | C302—C303—C304—C305 | -12.9 (3) |
| C101—C113—C112—C119 | -142.0 (2) | C303—C302—C301—C313 | -169.0 (2) |
| C101—C115—C105—C104 | -14.1 (3) | C303—C302—C301—C315 | -57.8 (2) |
| C101—C115—C105—C106 | 162.9 (2) | C303—C302—C301—C317 | 71.9 (5) |
| C101—C115—C109—C108 | -134.4 (2) | C303—C302—C301—C327 | 60.7 (7) |
| C101—C115—C109—C110 | 49.2 (2) | C303—C302—C301—C337 | 62.7 (9) |
| C101—C115—C114—C112 | -46.0 (1) | C303—C304—C305—C306 | -176.5 (2) |
| C102—C101—C113—C112 | 106.3 (2) | C303—C304—C305—C315 | 0.2 (3) |
| C102—C101—C113—C116 | -71.8 (2) | C304—C305—C306—C307 | 117.3 (2) |
| C102—C101—C115—C105 | 40.5 (2) | C304—C305—C315—C309 | -141.8 (2) |
| C102—C101—C115—C109 | 167.7 (2) | C304—C305—C315—C314 | 98.3 (2) |
| C102—C101—C115—C114 | -80.7 (2) | C305—C306—C307—C308 | 49.5 (3) |
| C102—C101—C117—C118 | -98.7 (2) | C305—C315—C301—C313 | 157.9 (1) |
| C102—C103—C104—C105 | -17.3 (4) | C305—C315—C301—C317 | -72.6 (6) |
| C103—C102—C101—C113 | -169.2 (2) | C305—C315—C301—C327 | -79.1 (7) |
| C103—C102—C101—C115 | -57.6 (3) | C305—C315—C301—C337 | -83 (1) |
| C103—C102—C101—C117 | 68.4 (2) | C305—C315—C309—C308 | -3.5 (3) |
| C103—C104—C105—C106 | -175.0 (2) | C305—C315—C309—C310 | 178.3 (2) |
| C103—C104—C105—C115 | 1.6 (4) | C305—C315—C314—C312 | -167.7 (1) |
| C104—C105—C106—C107 | 117.4 (3) | C306—C305—C315—C309 | 35.1 (2) |
| C104—C105—C115—C109 | -141.2 (2) | C306—C305—C315—C314 | -84.8 (2) |
| C104—C105—C115—C114 | 100.3 (2) | C306—C307—C308—C309 | -20.8 (3) |
| C105—C106—C107—C108 | 50.9 (3) | C307—C306—C305—C315 | -59.6 (3) |
| C105—C115—C101—C113 | 154.7 (1) | C307—C308—C309—C310 | 175.1 (2) |
| C105—C115—C101—C117 | -80.9 (2) | C307—C308—C309—C315 | -3.0 (4) |
| C105—C115—C109—C108 | -6.2 (3) | C308—C309—C310—C311 | -134.0 (2) |
| C105—C115—C109—C110 | 177.3 (2) | C308—C309—C315—C314 | 121.1 (2) |
| C105—C115—C114—C112 | -167.6 (1) | C309—C310—C311—C312 | -45.1 (2) |
| C106—C105—C115—C109 | 35.7 (2) | C309—C315—C301—C313 | -76.6 (2) |

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| C106—C105—C115—C114 | -82.8 (2) | C309—C315—C301—C317 | 52.9 (6) |
| C106—C107—C108—C109 | -23.8 (3) | C309—C315—C301—C327 | 46.4 (7) |
| C107—C106—C105—C115 | -59.5 (3) | C309—C315—C301—C337 | 43 (1) |
| C107—C108—C109—C110 | 177.3 (2) | C309—C315—C314—C312 | 69.6 (2) |
| C107—C108—C109—C115 | 1.1 (3) | C310—C309—C315—C314 | -57.1 (2) |
| C108—C109—C110—C111 | -129.8 (2) | C310—C311—C312—C313 | -48.0 (2) |
| C108—C109—C115—C114 | 116.8 (2) | C310—C311—C312—C314 | 62.1 (2) |
| C109—C110—C111—C112 | -45.5 (2) | C310—C311—C312—C319 | -171.3 (2) |
| C109—C115—C101—C113 | -78.2 (2) | C311—C310—C309—C315 | 44.2 (2) |
| C109—C115—C101—C117 | 46.3 (2) | C311—C312—C313—C316 | -84.3 (2) |
| C109—C115—C114—C112 | 70.3 (1) | C311—C312—C314—C315 | -74.2 (2) |
| C110—C109—C115—C114 | -59.6 (2) | C311—C312—C319—C320 | -65.8 (2) |
| C110—C111—C112—C113 | -48.7 (2) | C312—C313—C301—C315 | -12.3 (2) |
| C110—C111—C112—C114 | 60.8 (2) | C312—C313—C301—C317 | -146.8 (4) |
| C110—C111—C112—C119 | -172.3 (2) | C312—C313—C301—C327 | -128.2 (5) |
| C111—C110—C109—C115 | 46.7 (2) | C312—C313—C301—C337 | -126.5 (7) |
| C111—C112—C113—C116 | -87.5 (2) | C313—C301—C315—C314 | 35.6 (2) |
| C111—C112—C114—C115 | -73.0 (2) | C313—C301—C317—C318 | 23 (1) |
| C111—C112—C119—C120 | -58.8 (2) | C313—C301—C327—C328 | -93 (2) |
| C112—C113—C101—C115 | -9.3 (2) | C313—C301—C337—C338 | -166 (2) |
| C112—C113—C101—C117 | -135.1 (1) | C313—C312—C314—C315 | 38.7 (1) |
| C113—C101—C115—C114 | 33.4 (1) | C313—C312—C319—C320 | 173.9 (2) |
| C113—C101—C117—C118 | 142.8 (2) | C314—C312—C313—C316 | 162.6 (2) |
| C113—C112—C114—C115 | 40.0 (1) | C314—C312—C319—C320 | 56.8 (2) |
| C113—C112—C119—C120 | -179.8 (2) | C314—C315—C301—C317 | 165.1 (6) |
| C114—C112—C113—C116 | 159.2 (2) | C314—C315—C301—C327 | 158.6 (7) |
| C114—C112—C119—C120 | 64.3 (2) | C314—C315—C301—C337 | 155 (1) |
| C114—C115—C101—C117 | 157.8 (2) | C315—C301—C313—C316 | 168.9 (2) |
| C115—C101—C113—C116 | 172.5 (2) | C315—C301—C317—C318 | -101 (1) |
| C115—C101—C117—C118 | 23.7 (3) | C315—C301—C327—C328 | 152 (2) |
| C115—C114—C112—C119 | 161.5 (1) | C315—C301—C337—C338 | 82 (2) |
| C116—C113—C101—C117 | 46.8 (2) | C315—C314—C312—C319 | 161.0 (1) |
| C116—C113—C112—C119 | 36.1 (2) | C316—C313—C301—C317 | 34.4 (5) |
| C201—C202—C203—C204 | 45.9 (2) | C316—C313—C301—C327 | 53.0 (5) |
| C201—C213—C212—C211 | 95.3 (2) | C316—C313—C301—C337 | 54.7 (7) |
| C201—C213—C212—C214 | -17.5 (2) | C316—C313—C312—C319 | 38.6 (2) |
| C201—C213—C212—C219 | -141.6 (2) | | |

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x, -y+1, -z+1$; (iv) $x-1, y, z$; (v) $-x+1, -y+2, -z+2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|----------|-------------|-------------|---------------|
| O21—H9021 \cdots O121 ⁱⁱ | 0.80 (2) | 2.05 (2) | 2.842 (4) | 168 (2) |
| O21—H9021 \cdots O22 | 0.80 (2) | 2.57 (2) | 2.844 (4) | 102 (2) |
| O22—H9022 \cdots O221 | 0.81 (2) | 2.15 (2) | 2.913 (4) | 157 (2) |
| O121—H9121 \cdots O321 ⁱ | 0.81 (2) | 1.94 (2) | 2.739 (4) | 169 (2) |
| O221—H9221 \cdots O21 ^{iv} | 0.82 (2) | 1.94 (2) | 2.734 (4) | 164 (2) |
| O321—H9321 \cdots O221 ⁱⁱⁱ | 0.81 (2) | 2.04 (2) | 2.842 (4) | 170 (2) |
| O321—H9321 \cdots O322 | 0.81 (2) | 2.59 (2) | 2.851 (4) | 101 (2) |
| O322—H9322 \cdots O121 | 0.83 (2) | 2.17 (2) | 2.946 (4) | 156 (2) |

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x, -y+1, -z+1$; (iv) $x-1, y, z$.