checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_20240708a_1_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: cu_20240708a_1_a

Bond precision: C-C = 0.0186 A Wavelength=1.54178

Cell: a=30.283(1) b=32.1268(12) c=36.5647(14)
alpha=90 beta=94.511(2) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	35464(2)	35463(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C144 H140 N8 O12 Rh6), 7(C F3 O3 S) [+ solvent]	2(C144 H140 N8 O12 Rh6), 7(C F3 O3 S), 11.5[CF3SO3], 1[CH3OH]
Sum formula	C295 H280 F21 N16 O45 Rh12 S7 [+ solvent]	C307.50 H284 F55.50 N16 O80.50 Rh12 S18.50
Mr	6627.71	8374.02
Dx,g cm-3	1.241	1.568
Z	4	4
Mu (mm-1)	5.369	6.342
F000	13452.0	16882.0
F000'	13504.08	
h,k,lmax	33,35,40	33,35,40
Nref	51466	51070
Tmin,Tmax	0.444,0.386	
Tmin'	0.336	

Correction method= Not given

Data completeness= 0.992 Theta(max)= 59.256

R(reflections)= 0.1055(21206)

wR2(reflections)= 0.2598(51070)

S = 1.094 Npar= 3409

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.186
THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5574
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.186 Report
PLAT260_ALERT_2_B Large Average Ueq of Residue Including S3 0.384 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including S5 0.327 Check

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Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 42% Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.26 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 4.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 5.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh9 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S1 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S2 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S3 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S4 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S5 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S6 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S7 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 8) 2.7 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Rh1 0.144 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Rh2 0.126 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S1 0.220 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S2 0.251 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S4 0.239 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S6 0.213 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S7 0.240 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01859 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C232 - C258 . 1.53 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H216 ..H230 . 1.99 Ang.

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                                                  x,y,z  =      1_555 Check
PLAT434_ALERT_2_C Short Inter HL..HL Contact F15      ..F20      .       2.50 Ang.
                                       3/2-x,-1/2+y,3/2-z  =      2_646 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -14.687 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.216 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.557        395 Report
                2  0  0,   1  1  0,   1  2  0,   2  2  0,   3  2  0,   5  2  0,
                6  3  0,  33  7  0,   1 10  0,  32 11  0,  15 32  0,  13 33  0,
                7 35  0, -31  0  1,   1  0  1,  -5  1  1,  -3  1  1,   1  1  1,
                3  1  1,  -2  2  1,  -1  2  1,   0  2  1,   5  2  1,   9  3  1,
                2  5  1,   4  5  1,  33  6  1, -33  7  1,  11  9  1, -31 14  1,
               30 16  1,  29 18  1,  15 32  1, -13 33  1,  -7 35  1,   7 35  1,
                0  0  2,   2  0  2,  -2  1  2,  -1  1  2,   0  1  2,   1  2  2,
               -3  3  2,  -1  3  2,   0  3  2,   4  4  2,   6  4  2,  33  5  2,
               33  6  2, -31 14  2, -28 20  2,  -7 35  2,  -1  0  3,   1  0  3,
               33  0  3,  -2  1  3,  -3  2  3,   0  2  3,   2  2  3,  13  2  3,
               -1  3  3,   4  3  3,  33  5  3,  32 10  3,  31 13  3, -31 14  3,
              -28 20  3,  18 30  3, -13 33  3,  10 34  3,   0  0  4,  -4  3  4,
               33  3  4,   3  4  4,  33  4  4,  32  9  4, -31 14  4,  28 19  4,
              -15 32  4,   6 35  4,  33  0  5,  -7  1  5,  33  1  5,   1  2  5,
               33  2  5, -33  7  5, -31 14  5,  29 17  5,  16 31  5,  12 33  5,
              -10 34  5,  -6 35  5,  -5  1  6,  -1  1  6,   8  3  6, -33  7  6,
PLAT977_ALERT_2_C Check Negative Difference Density on H28H      .      -0.34 eA-3
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C307.5 H284 F55.5 N16 O80.5 R
           Atom count from _chemical_formula_moiety:C306.5 H280 F55.5 N16 O79.5 R
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C307.5 H284 F55.5 N16 O80.5 Rh12
           Atom count from the _atom_site data:  C295 H280 F21 N16 O45 Rh12 S7
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C307.50 H284 F55.50 N16 O80.50 Rh1
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C       1230.00   1180.00   50.00
          H       1136.00   1120.00   16.00
          F        222.00     84.00  138.00
          N         64.00     64.00    0.00
          O        322.00    180.00  142.00
          Rh        48.00     48.00    0.00
          S         74.00     28.00   46.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        161 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         396 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C295 H280 F21 N16 O45 Rh12 S7
             Rep.: C307.50 H284 F55.50 N16 O80.50 Rh12 S18.50
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C144 H140 N8 O12 Rh6), 7(C F3 O3 S)
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              Rep.: 2(C144 H140 N8 O12 Rh6), 7(C F3 O3 S), 11.5[CF
                    3SO3], 1[CH3OH]
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      15.34 %
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     200.00 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         54 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         61 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         10 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         82 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         18 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         17 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         C9 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        C73 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       C147 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       C289 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       C293 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       C145 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       C291 Check
PLAT344_ALERT_2_G Unusual sp3       Angle Range in Solvent/Ion for        C73 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C2 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C245 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C273 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C233 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C257 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C33 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C285 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C237 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C59 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C61 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C253 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C265 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C277 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C69 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C71 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C235 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C117 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C247 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C243 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C123 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C255 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C127 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C267 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C263 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C133 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C275 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C137 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C283 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C143 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C193 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C5 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C11 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C217 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C21 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C205 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C27 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C43 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C197 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C49 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C51 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C213 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C225 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C87 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C85 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C195 Check
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PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C97 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C207 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C203 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C103 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C215 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C107 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C227 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C223 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C113 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C175 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C169 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C171 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C173 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F11      ..C34      .       2.86 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F19      ..C139     .       2.86 Ang.
                                    -1/2+x,1/2-y,1/2+z  =      4_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F19      ..C287     .       2.95 Ang.
                                    -1/2+x,1/2-y,1/2+z  =      4_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O15      ..C183     .       2.99 Ang.
                                                  x,1+y,z  =      1_565 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5       ..F6       .       2.73 Ang.
                                                      x,y,z  =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       6161 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         53 Note
               -7  1  5,  -7  4  9,  -5  1  1,  -5  1  6,  -4  3  4,  -3  1  1,
               -3  2  3,  -3  3  2,  -2  1  2,  -2  1  3,  -2  1  7,  -2  2  1,
               -1  0  3,  -1  1  2,  -1  1  6,  -1  2  1,  -1  3  2,  -1  3  3,
                0  0  2,   0  0  4,   0  1  2,   0  2  1,   0  2  3,   0  3  2,
                0 10  6,   1  0  1,   1  0  3,   1  1  0,   1  1  1,   1  2  0,
                1  2  2,   1  2  5,   1 10  0,   2  0  0,   2  0  2,   2  2  0,
                2  2  3,   2  5  1,   3  1  1,   3  2  0,   3  4  4,   4  3  3,
                4  4  2,   4  5  1,   5  2  0,   5  2  1,   6  3  0,   6  4  2,
                7  4  8,   8  3  6,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.847 Note
             Predicted wR2: Based on SigI**2 14.07 or SHELX Weight 23.76
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   5 ALERT level B = A potentially serious problem, consider carefully
  40 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 145 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  38 ALERT type 2 Indicator that the structure model may be wrong or deficient
  61 ALERT type 3 Indicator that the structure quality may be low
  82 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock cu_20240708a_1_a - ellipsoid plot