checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dmwmsv6-45_sq

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: dmwmsv6-45_sq

Bond precision: C-C = 0.0035 A Wavelength=0.68890

Cell: a=33.04569(13) b=30.13654(16) c=39.97965(19)
alpha=90 beta=96.4337(4) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	39564.3(3)	39564.3(2)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C336 H264 Co8 N72), 2(C10 H8 O3), 29(B F4), 10(C H3 O) [+ sol	C336 H264 Co8 N72, 16(B F4), 30(C H4 O), C10 H8 O3
Sum formula	C702 H574 B29 Co16 F116 N144 O16 [+ solvent]	C376 H392 B16 Co8 F64 N72 O33
Mr	14743.46	8307.99
Dx,g cm-3	1.238	1.395
Z	2	4
Mu (mm-1)	0.379	0.398
F000	15086.0	17152.0
F000’	15103.66	
h,k,lmax	47,43,57	47,43,57
Nref	63071	62978
Tmin,Tmax		0.987,1.000
Tmin’		

Correction method= # Reported T Limits: Tmin=0.987 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.999 Theta(max)= 29.947

R(reflections)= 0.0719(42192) wR2(reflections)= 0.2596(62978)

S = 1.079 Npar= 2517

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 C

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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.26 Report
PLAT214_ALERT_2_C Atom F64       (Anion/Solvent) ADP max/min Ratio        4.3 prolat
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O16G      0.195 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F72      0.123 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      F82A      0.149 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O11S      0.104 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O11S Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O21S Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O31S Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O41S Check
PLAT431_ALERT_2_C Short Inter HL..A Contact  F23      ..O31S     .       2.84 Ang.
                                                     x,y,z  =      1_555 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         72 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          9 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.73A   From O31S            1.39 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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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:C376 H392 B16 Co8 F64 N72 O33
           Atom count from the _atom_site data:  C351 H287 B14.5 Co8 F58 N72 O8
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
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  C376 H392 B16 Co8 F64 N72 O33
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C       1504.00   1404.00  100.00
           H       1568.00   1148.00  420.00
           B         64.00     58.00    6.00
           Co        32.00     32.00    0.00
           F        256.00    232.00   24.00
           N        288.00    288.00    0.00
           O        132.00     32.00  100.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        251 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        279 Report
PLAT014_ALERT_1_G N.O.K.   _shelx_fab_checksum Found in CIF ......     Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.17 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.68890 Ang.
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............    0.00016 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00019 Ang.
PLAT145_ALERT_4_G s.u. on beta     Small or Missing ..............     0.0004 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
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PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records         36 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT244_ALERT_4_G Low    Solvent Ueq as Compared to Neighbors of        B11 Check
PLAT244_ALERT_4_G Low    Solvent Ueq as Compared to Neighbors of        B21 Check
PLAT244_ALERT_4_G Low    Solvent Ueq as Compared to Neighbors of        B31 Check
PLAT244_ALERT_4_G Low    Solvent Ueq as Compared to Neighbors of        B41 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O16G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O17G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O25G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24G       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26M       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26N       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26O       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F94        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B91        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F52        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F53        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F54        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F55        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B51        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F72        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F73        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F74        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F75        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B71        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O11S       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12S       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O21S       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22S       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O31S       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32S       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32A       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32B       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32C       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O41S       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41S       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41A       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41B       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41C       Constrained at       0.35 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        40% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 14  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 16  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 17  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )     10.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  8  )      2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  9  )      3.75 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 10  )      2.80 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 11  )      0.81 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 12  )      1.69 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 13  )      2.20 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 14  )      3.75 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 15  )      3.75 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 16  )      3.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 17  )      1.75 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #       779 Check
             B91  -F92  -B91     2.656   1.555   1.555            29.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #       780 Check
             B91  -F93  -B91     1.555   1.555   2.656            32.90 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        20 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .      1.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)      .      1.85 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co3       (II)      .      1.86 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co4       (II)      .      1.83 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         5 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      6651 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        20 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        36 Note
PLAT984_ALERT_1_G The Co-f'=    0.3538 Deviates from the B&C-Value    0.3480 Check
PLAT985_ALERT_1_G The Co-f"=    0.9121 Deviates from the B&C-Value    0.9239 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         1 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 116 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  95 ALERT type 4 Improvement, methodology, query or suggestion
   5 ALERT type 5 Informative message, check
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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 22/12/2019; check.def file version of 13/12/2019

Datablock dmwmsv6-45_sq - ellipsoid plot