checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dmwmsv6-26_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: dmwmsv6-26_sq

Bond precision: C-C = 0.0050 A Wavelength=0.68890

Cell: a=32.8649(2) b=29.89225(18) c=40.5389(4)
alpha=90 beta=95.9164(7) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	39613.5(5)	39613.5(4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C336 H264 Co8 N72, 3.492(C9 H10 O2), B2 F5, 12.338(B F4) [+ sol	C336 H264 Co8 N72, 16(B F4), 28(C H4 O), 3.5(C9 H10 O2)
Sum formula	C367.43 H298.92 B14.34 Co8 F54.35 N72 O6.98 [+ solvent]	C395.50 H411 B16 Co8 F64 N72 O35
Mr	7493.73	8593.34
Dx,g cm-3	1.257	1.441
Z	4	4
Mu (mm-1)	0.379	0.401
F000	15360.9	17760.0
F000’	15378.39	
h,k,lmax	47,43,58	47,43,58
Nref	63152	63039
Tmin,Tmax		0.951,1.000
Tmin’		

Correction method= # Reported T Limits: Tmin=0.951 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.998 Theta(max)= 29.947

R(reflections)= 0.0853(32955) wR2(reflections)= 0.3169(63039)

S = 1.065 Npar= 2426

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

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PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          3 Check
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Alert level C

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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.32 Report
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.8 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O23H      0.116 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F92      0.113 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F22      0.117 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F32      0.145 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F42      0.155 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F52      0.154 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F62      0.182 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       F72      0.157 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C336 H264 Co8 N72
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -1.866 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         50 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          4 Check
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:C395.5 H411 B16 Co8 F64 N72 O35
            Atom count from the _atom_site data:  C367.4280 H298.9200 B14.338 Co8
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  C395.50 H411 B16 Co8 F64 N72 O35
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C       1582.00   1469.71  112.29
           H       1644.00   1195.68  448.32
           B         64.00     57.35    6.65
           Co        32.00     32.00    0.00
           F        256.00    217.41   38.59
           N        288.00    288.00    0.00
           O        140.00     27.94  112.06
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        248 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        265 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
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.19 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 ..............    0.00018 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00040 Ang.
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records         34 Report
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PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  2         20.31 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  3         16.36 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  9          4.18 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 10          3.77 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 11          2.89 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 . #        761 Check
             B91  -F92  -B91     2.856   1.555   1.555            40.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        762 Check
             B91  -F94  -B91     1.555   1.555   2.856            42.20 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C9 H10 O2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
             B2 F5
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         10 Note
             B F4
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       1.52 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)      .       1.53 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co3       (II)      .       1.54 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co4       (II)      .       1.49 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          7 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       6014 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         65 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         21 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
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  52 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
  34 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT934_dmwmsv6-26_sq
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          3 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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 07/08/2019; check.def file version of 30/07/2019

Datablock dmwmsv6-26_sq - ellipsoid plot