checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dmwmsv6-25_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: dmwmsv6-25_sq

Bond precision: C-C = 0.0044 A   Wavelength=0.68890

Cell: a=32.56923(10)   b=30.16165(10)   c=40.83634(17)
               alpha=90   beta=95.9061(3)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	39902.3(2)	39902.31(19)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C336 H264 Co8 N72), 8.9(C9 H10 O), 2(B2 F5), 24.905(B F4), 1.	C336 H264 Co8 N72, 6.226(B2 F8), B2 F5, 2.226(C18 H20 O2), 0.41
Sum formula	C752.10 H617 B28.91 Co16 F109.62 N144 O10.56 [+ solvent]	C407.80 H417.66 B16 Co8 F64 N72 O31.03
Mr	15179.24	8684.25
Dx,g cm-3	1.263	1.446
Z	2	4
Mu (mm-1)	0.377	0.398
F000	15570.4	17955.0
F000'	15587.94	
h,k,lmax	47,43,59	47,43,59
Nref	63592	63534
Tmin,Tmax		0.973,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.973 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.999   Theta(max)= 29.947

R(reflections)= 0.0827(37629)   wR2(reflections)= 0.2981(63534)

S = 1.083   Npar= 2727

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
PLAT214_ALERT_2_B Atom F73A   (Anion/Solvent) ADP max/min Ratio   5.3 prolat
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..   7 Check

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🟡 Alert level C
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.30 Report
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.1 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.6 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   O22G   0.105 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   O22I   0.111 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F92   0.105 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F22   0.141 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F32   0.125 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F42   0.131 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F52   0.113 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F52A   0.118 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F72   0.168 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F22A   0.179 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F62   0.115 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F72A   0.150 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   O16   0.152 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ....   O22G Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   1 Note
            C336 H264 Co8 N72
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   22 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   8 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.09A   From O22G   0.90 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.69A   From O22G   0.81 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Info

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⚪ Alert level G
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: C407.8 H417.66 B16 Co8 F64 N7
          Atom count from _chemical_formula_moiety:C376.0679 H308.5199 B14.452 C
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:C407.8 H417.66 B16 Co8 F64 N72 O
          Atom count from the _atom_site data: C376.0501 H308.5 B14.45260 Co8 F
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 C407.80 H417.66 B16 Co8 F64 N72 O3
          TEST: Compare cell contents of formula and atom_site data

          atom   Z*formula cif sites diff
          C   1631.20   1504.20 127.00
          H   1670.64   1234.00 436.64
          B   64.00   57.81   6.19

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            Co          32.00     32.00     0.00
            F          256.00    219.24    36.76
            N          288.00    288.00     0.00
            O          124.12     21.12   103.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        280 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        299 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       0.19 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 ..............  0.00010 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............  0.00017 Ang.
PLAT145_ALERT_4_G s.u. on beta     Small or Missing ..............   0.0003 Degree
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records         39 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
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        B31 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        B41 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O22H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16H      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23J      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23K      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23L      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31D      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31E      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31F      Constrained at     0.6396 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O22I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16I      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23M      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23N      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23O      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31G      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31H      Constrained at     0.3604 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31I      Constrained at     0.3604 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of F22        Constrained at     0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F23        Constrained at     0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F24        Constrained at     0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F25        Constrained at     0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B21        Constrained at     0.6 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 F52A       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F53A       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F54A       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F55A       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B51A       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F72        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F73        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F74        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F75        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B71        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F22A       Constrained at     0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F23A       Constrained at     0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F24A       Constrained at     0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F25A       Constrained at     0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B21A       Constrained at     0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F72A       Constrained at  0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F73A       Constrained at  0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F74A       Constrained at  0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F75A       Constrained at  0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B71A       Constrained at  0.3333 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  4  )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )    100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )    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     12.80 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  3     12.79 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  4     11.70 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  5      7.21 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 11      2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 12      2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 13      2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 15      1.97 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 16      1.67 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 17      0.41 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    O16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C31G Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C23G Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C31H Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C23H Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C31J Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C23J Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F34      ..C15H        2.90 Ang.
                                                 x,y,z =    1_555 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure    ! Info
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PLAT773_ALERT_2_G Check long C-C Bond in CIF: C21J      --C23J            1.73 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      779 Check
             B91  -F93 -B91     1.555   1.555   2.856        38.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      780 Check
             B91  -F94 -B91     2.856   1.555   1.555        32.50 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        2 Note
             C9 H10 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        4 Note
             C9 H10 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        5 Note
             C9 H10 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        6 Note
             B2 F5
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
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       11 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       12 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       13 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       14 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       15 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       16 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       17 Note
             O
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)    .    1.52 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)    .    1.54 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co3       (II)    .    1.52 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      8 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............  7141 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 !
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     36 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....     2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...    12 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
   2 ALERT level B = A potentially serious problem, consider carefully
  23 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 156 ALERT level G = General information/check it is not something unexpected

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  28 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
 130 ALERT type 4 Improvement, methodology, query or suggestion
   5 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_PLAT214_dmwmsv6-25_sq
;
PROBLEM: Atom F73A      (Anion/Solvent) ADP max/min Ratio        5.3 prolat
RESPONSE: ...
;
_vrf_PLAT934_dmwmsv6-25_sq
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..        7 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

65 Y

NOMOVE FORCED

Prob = 50
Temp = 100

PLATON-Oct 31 14:22:55 2019 - (70316)

Z 73 dmwmsv6-25C 1 2/c 1 R = 0.08 RES= 0 35 X