checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: ce20

Bond precision: C-C = 0.0050 A   Wavelength=0.71073

Cell: a=15.4784(3)   b=21.5356(6)   c=22.0470(5)
                   alpha=90   beta=90   gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	7349.1(3)	7349.1(3)
Space group	P 21 21 21	P212121
Hall group	P 2ac 2ab	?
Moiety formula	4(C58 H96 N4 O28), C10 H24	?
Sum formula	C242 H408 N16 O112	C60.50 H102 N4 O28
Mr	5333.87	1333.46
Dx,g cm-3	1.205	1.205
Z	1	4
Mu (mm-1)	0.095	0.095
F000	2868.0	2868.0
F000'	2869.72	
h,k,lmax	19,27,28	19,27,28
Nref	8745[16056]	14608
Tmin,Tmax	0.992,0.994	
Tmin'	0.970	

Correction method= Not given

Data completeness= 1.67/0.91   Theta(max)= 27.000

R(reflections)= 0.0495(7646)   wR2(reflections)= 0.1386(14608)

S = 0.615   Npar= 839

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 A**
PLAT213_ALERT_2_A Atom C18   has ADP max/min Ratio .....   5.9 prola
PLAT222_ALERT_3_A Large Non-Solvent   H   Uiso(max)/Uiso(min) ..   10.0 Ratio

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🔴 Alert level B

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PLAT035_ALERT_1_B No _chemical_absolute_configuration info given .         ?
PLAT220_ALERT_2_B Large Non-Solvent    C      Ueq(max)/Ueq(min) ...     10.0 Ratio
PLAT220_ALERT_2_B Large Non-Solvent    O      Ueq(max)/Ueq(min) ...      4.2 Ratio
PLAT220_ALERT_2_B Large Non-Solvent    C      Ueq(max)/Ueq(min) ...      4.3 Ratio
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for       O13
PLAT413_ALERT_2_B Short Inter XH3 .. XHn      H18B   .. H19A    ..     1.97 Ang.
PLAT413_ALERT_2_B Short Inter XH3 .. XHn      H57B   .. H71E    ..     2.06 Ang.
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🟡 Alert level C

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DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =       0.669
           Test value =       0.600
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =       0.615
STRVA01_ALERT_4_C          Flack parameter is too small
           From the CIF: _refine_ls_abs_structure_Flack   -0.300
           From the CIF: _refine_ls_abs_structure_Flack_su    0.800
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......     0.969
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....     3.03
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density    0.67 eA-3
PLAT213_ALERT_2_C Atom O13           has ADP max/min Ratio .....      3.5 prola
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.0050 Ang
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .      56 A**3
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⚪ Alert level G

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REFLT03_ALERT_4_G  ALERT: MoKa measured Friedel data cannot be used to
               determine absolute structure in a light-atom
               study EXCEPT under VERY special conditions.
               It is preferred that Friedel data is merged in such cases.
           From the CIF: _diffrn_reflns_theta_max         27.00
           From the CIF: _reflns_number_total            14608
           Count of symmetry unique reflns        8745
           Completeness (_total/calc)         167.04%
           TEST3: Check Friedels for noncentro structure
           Estimate of Friedel pairs measured      5863
           Fraction of Friedel pairs measured     0.670
           Are heavy atom types Z>Si present         no
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....        ?
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .    0.800
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............    0.25 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.    0.12
PLAT242_ALERT_2_G Check Low       Ueq as Compared to Neighbors for    C72A
PLAT242_ALERT_2_G Check Low       Ueq as Compared to Neighbors for    C74A
PLAT242_ALERT_2_G Check Low       Ueq as Compared to Neighbors for    C75A
PLAT242_ALERT_2_G Check Low       Ueq as Compared to Neighbors for    C75B
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................      3 Perc.
PLAT791_ALERT_4_G Note: The Model has Chirality at C1      (Verify)     R
PLAT791_ALERT_4_G Note: The Model has Chirality at C2      (Verify)     R
PLAT791_ALERT_4_G Note: The Model has Chirality at C3      (Verify)     R
PLAT791_ALERT_4_G Note: The Model has Chirality at C4      (Verify)     S
PLAT791_ALERT_4_G Note: The Model has Chirality at C5      (Verify)     R
PLAT791_ALERT_4_G Note: The Model has Chirality at C11     (Verify)     R
PLAT791_ALERT_4_G Note: The Model has Chirality at C12     (Verify)     R
PLAT791_ALERT_4_G Note: The Model has Chirality at C13     (Verify)     R
PLAT791_ALERT_4_G Note: The Model has Chirality at C14     (Verify)     S
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PLAT791_ALERT_4_G Note: The Model has Chirality at C15       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C21       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C22       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C23       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C24       (Verify)           S
PLAT791_ALERT_4_G Note: The Model has Chirality at C25       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C31       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C32       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C33       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C34       (Verify)           S
PLAT791_ALERT_4_G Note: The Model has Chirality at C35       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C41       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C42       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C43       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C44       (Verify)           S
PLAT791_ALERT_4_G Note: The Model has Chirality at C45       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C51       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C52       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C53       (Verify)           R
PLAT791_ALERT_4_G Note: The Model has Chirality at C54       (Verify)           S
PLAT791_ALERT_4_G Note: The Model has Chirality at C55       (Verify)           R
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   7 ALERT level B = A potentially serious problem, consider carefully
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  40 ALERT level G = General information/check it is not something unexpected

   3 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
   4 ALERT type 3 Indicator that the structure quality may be low
  33 ALERT type 4 Improvement, methodology, query or suggestion
   1 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*, 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 04/07/2012; check.def file version of 28/06/2012

NOMOVE FORCED

Prob = 50
Temp = 120

-9 Y

PLATON-Aug 10 14:49:48 2012 - (40712)

Z 162 ce20 P212121 R = 0.05 RES= 0 -91 X