checkCIF/PLATON report

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

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: mo_r3hq_prk_353k_0m_a

Bond precision: C-C = 0.0108 A Wavelength=0.71073

Cell: a=9.9188(6) b=24.426(2) c=9.8593(8)
alpha=90 beta=90 gamma=90
Temperature: 353 K

	Calculated	Reported
Volume	2388.7(3)	2388.6(3)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	N6 O18 Pr, 4(C7 N O), 2(N O3), K	K N8 O24 Pr, 4(C7 N O)
Sum formula	C28 K N12 O28 Pr	C28 K N12 O28 Pr
Mr	1132.41	1132.41
Dx,g cm-3	1.574	1.574
Z	2	2
Mu (mm-1)	1.207	1.207
F000	1108.0	1108.0
F000'	1108.66	
h,k,lmax	11,29,11	11,29,11
Nref	4394[2515]	4371
Tmin,Tmax	0.876,0.886	0.396,0.745
Tmin'	0.876	

Correction method= # Reported T Limits: Tmin=0.396 Tmax=0.745
AbsCorr = NONE

Data completeness= 1.74/0.99 Theta(max)= 25.416

R(reflections)= 0.0665(2276) wR2(reflections)= 0.2100(4371)

S = 0.988 Npar= 427

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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PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ........       5.89 Note
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Alert level C

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.163
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.490
          From the CIF: _refine_ls_abs_structure_Flack_su    0.050
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: N6 O18 Pr, 4(C7 N O), 2(N O3), K
             Rep.: K N8 O24 Pr, 4(C7 N O)
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Pr1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         C1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O5      0.191 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O11      0.213 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O2      0.137 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O9      0.133 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O5 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O19 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O11 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O21 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0108 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         29 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          48 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.163 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.490 Note
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          7 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         15 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 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          5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          5 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0100 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar      0.0200 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             O3      O4      O14     O16     O18     O20     O22     O23
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             O5      O19     C3      C7      C13     C15     O11     O21
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        32% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)        33% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)        11% 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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       2.08 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       1.92 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    6)       0.50 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2       ..C16      .       2.91 Ang.
                                                  x,y,1+z  =      1_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O7       ..C10      .       2.74 Ang.
                                                    x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O16      ..C12      .       3.02 Ang.
                                                1-x,1-y,z  =      2_665 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        727 Note
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          6 Note
               -5  2 10,  -3  4 11,   0  7 10,   0 25  3,   5  2 10,   6  2 10,
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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
  36 ALERT level G = General information/check it is not something unexpected

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

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_RINTA01_mo_r3hq_prk_353k_0m_a
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_STRVA01_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT090_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Poor Data / Parameter Ratio (Zmax > 18) ........       5.89 Note
RESPONSE: ...
;
_vrf_PLAT042_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
```

```
RESPONSE: ...
;
_vrf_PLAT241_mo_r3hq_prk_353k_0m_a
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of         O8 Check
RESPONSE: ...
;
_vrf_PLAT242_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        Pr1 Check
RESPONSE: ...
;
_vrf_PLAT244_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Low    'Solvent' Ueq as Compared to Neighbors of         C1 Check
RESPONSE: ...
;
_vrf_PLAT260_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Large Average Ueq of Residue Including        O5      0.191 Check
RESPONSE: ...
;
_vrf_PLAT309_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O5 Check
RESPONSE: ...
;
_vrf_PLAT342_mo_r3hq_prk_353k_0m_a
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............     0.0108 Ang.
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 22/08/2024; check.def file version of 21/08/2024

Datablock mo_r3hq_prk_353k_0m_a - ellipsoid plot