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_0m_a

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Bond precision:   C-C = 0.0167 A          Wavelength=0.71073

Cell:             a=9.967(4)     b=20.023(8)          c=12.654(6)
                  alpha=90       beta=111.958(9)      gamma=90
Temperature:      300 K
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	Calculated	Reported
Volume	2342.2(17)	2342.3(18)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	K N8 O23 Pr, 4(C7 H14 N O), O	K N8 O24 Pr, 4(C7 H14 N O)
Sum formula	C28 H56 K N12 O28 Pr	C28 H56 K N12 O28 Pr
Mr	1188.86	1188.85
Dx,g cm-3	1.686	1.686
Z	2	2
Mu (mm-1)	1.234	1.234
F000	1220.0	1220.0
F000'	1220.66	
h,k,lmax	12,25,15	12,25,15
Nref	9578[4933]	9554
Tmin,Tmax	0.873,0.884	0.612,0.746
Tmin'	0.873	

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Correction method= # Reported T Limits: Tmin=0.612 Tmax=0.746
AbsCorr = NONE

Data completeness= 1.94/1.00        Theta(max)= 26.370

R(reflections)= 0.0439( 8452)                    wR2(reflections)=
                                                 0.1085( 9554)
S = 1.048                  Npar= 668
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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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PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: K N8 O23 Pr, 4(C7 H14 N O), O
             Rep.: K N8 O24 Pr, 4(C7 H14 N O)
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       7.38 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.48 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference O8       --N10      .       0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O18 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O28 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Pr1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         K1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N8 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         N3 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C14 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01671 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H1A      ..H29      .       2.11 Ang.
                                                x,y,1+z  =      1_556 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D       H15      ..H29      .       2.11 Ang.
                                              1+x,y,1+z  =      1_656 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         18 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          74 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         8 Report
             H7    H11   H3    H15   H5    H29   H13   H31
PLAT115_ALERT_5_G ADDSYM Detects Noncrystallographic Inversion ...        87% Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          4 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU 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
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pr1      --O32      .        7.3 s.u.
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             O2      O3      O5      O13     O19     O25     O27     O33
             N2      N7      N9      N14
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         21% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    6)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    7)        100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         O9 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O21 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3       ..C16      .       2.52 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O19      ..C18      .       2.53 Ang.
                                                x,y,z  =      1_555 Check
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PLAT432_ALERT_2_G Short Inter X...Y Contact  O19      ..C16      .       2.90 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O21      ..C25      .       2.46 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O21      ..C23      .       2.59 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O21      ..C24      .       2.86 Ang.
                                                   -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O23      ..C25      .       2.44 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O23      ..C13      .       2.44 Ang.
                                                      x,y,z  =      1_555 Check
PLAT480_ALERT_4_G Long H...A H-Bond Reported H4B      ..O34      .       2.62 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H8A      ..O12      .       2.63 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H7A      ..O3       .       2.61 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H17A     ..O26      .       2.64 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H11B     ..O10      .       2.63 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H27A     ..O22      .       2.65 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Pr1       (III)     .       3.91 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       482 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        3 Note
               1  7 15,   2  7 14,   2  9 14,
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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
14 **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

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

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_0m_a - ellipsoid plot