checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_li97i1_2_0m

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_li97i1_2_0m

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Bond precision:   C-C = 0.0074 A              Wavelength=0.71073

Cell:             a=10.3667(5)       b=26.2054(13)     c=28.8910(13)
                  alpha=75.959(2)    beta=79.942(2)    gamma=85.099(2)
Temperature:      150 K
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	Calculated	Reported
Volume	7489.5(6)	7489.5(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C144 H164 N12 O8, C143.20 H169.60 N12 O8, 4(C H Cl3), 0.8(C H3)	2(C H Cl3), C72 H86 N6 O4, C72 H82 N6 O4
Sum formula	C292 H340 Cl12 N24 O16 [+ solvent]	C146 H170 Cl6 N12 O8
Mr	4867.29	2433.63
Dx,g cm-3	1.079	1.079
Z	1	2
Mu (mm-1)	0.170	0.170
F000	2592.0	2592.0
F000'	2594.68	
h,k,lmax		12,31,34
Nref		26399
Tmin,Tmax	0.994,0.995	0.693,0.745
Tmin'	0.976	

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Correction method= # Reported T Limits: Tmin=0.693 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness=                      Theta(max)= 25.050
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R(reflections)= 0.1162(17237)   wR2(reflections)= 0.3355(26399)

S = 2.116   Npar= 1525

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**

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 =   2.116
PLAT082_ALERT_2_C High R1 Value .... 0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) .... 0.34 Report
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) .... 2.12 Check
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 1.52 eA-3
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   2 Check
          C04J   C04A
PLAT220_ALERT_2_C NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   4.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range   5.0 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of C03C Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of C03J Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of C03Q Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of C028 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of C03H Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of C03O Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of C022 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of C02B Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of Cl10 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of Cl11 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Cl9   0.102 Check
PLAT336_ALERT_2_C Long Bond Distance for ..... C23   -Cl03   1.860 Ang.
PLAT336_ALERT_2_C Long Bond Distance for ..... C04A   -Cl15   1.880 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00742 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   1 Note
          C144 H164 N12 O8
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ...... 3.506 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).   10 Note
          0 1 0,   0 2 0,   0 -1 1,   0 0 1,   0 1 1,   0 2 1,
          0 -1 2,   0 0 2,   0 1 2,   0 2 2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.596   150 Report
          2 0 0, -2 1 0, -3 2 0,   2 2 0,   2 4 0,   2 6 0,
         -2 11 0,   0 -6 1, -1 -5 1,   0 -5 1,   2 -5 1, -2 -4 1,
         -1 -4 1,   2 -3 1,   2 -2 1, -1 -1 1, -2 0 1,   2 0 1,
          1 2 1,   2 2 1,   3 3 1,   1 5 1, -1 12 1,   1 12 1,
          2-10 2, -5 -6 2,   0 -6 2, -2 -4 2,   1 -4 2,   1 -3 2,
          2 0 2, -1 3 2,   0 3 2,   2 3 2, -1 5 2,   2 6 2,
          4 6 2,   1 9 2, -2 -5 3, -1 -3 3,   1 -3 3, -1 -1 3,
          0 0 3, -2 2 3,   2 2 3, -1 3 3,   1 3 3, -1 4 3,
          2 4 3, -1 5 3,   2 6 3,   2 7 3,   3 7 3, -2 8 3,
          1 8 3,   2 8 3,   0 17 3, -2 -7 4, -2 -6 4, -1 -4 4,
         -5 -3 4,   1 -3 4,   1 -2 4, -1 -1 4,   1 1 4, -2 2 4,

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              -1  3  4,    0  6  4,    2  7  4,    4 -8  5,    0 -3  5,   -1 -1  5,
               0  1  5,   -2  2  5,    4  4  5,   -1  6  5,   -1 14  5,    3-11  6,
              -2 -8  6,    4 -4  6,   -2 -3  6,   -1 -1  6,   -3  0  6,   -2  0  6,
              -1  0  6,   -2  2  6,    1  2  6,    6  2  6,    2  6  6,    1  7  6,
               0  8  6,   -1 11  6,    1 -6  7,    0  2  7,    0  4  7,    3-12  8,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....        21 Note
               0  2  0,    2  2  0,    2  6  0,   -1 -5  1,   -2 -4  1,    2 -2  1,
               2  0  1,    2  2  1,    1  5  1,    1 -4  2,    1 -3  2,   -1 -3  3,
              -2  2  3,    2  2  3,    2  4  3,    2  6  3,    1 -3  4,   -2  2  4,
              -1 -1  5,   -2  2  5,    0  2  7,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         1 Check
               4 -9  3,
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🔘 Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        83 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
               Calc: C144 H164 N12 O8, C143.20 H169.60 N12 O8, 4(C H Cl3), 0.8(C
               Rep.: 2(C H Cl3), C72 H86 N6 O4, C72 H82 N6 O4
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    0.500 Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.002 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records       15 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       37 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       15 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C1B        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1C        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1D        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1E        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1F        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1G        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1H        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1I        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3         Constrained at       0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C11        Constrained at       0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C27        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C28        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29        Constrained at       0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C32          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C36          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C49          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C50          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C049         Constrained at        0.7 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C04C         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04D         Constrained at        0.7 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C04Q         Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H2B          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2C          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H4B          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4C          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H9C          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H27C         Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H48C          Constrained at          0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H49C          Constrained at          0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H50C          Constrained at          0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of Hf            Constrained at          0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hg            Constrained at          0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of Hk            Constrained at          0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H05R          Constrained at          0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H05U          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05V          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05W          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H1BB          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H1IB          Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H10B          Constrained at        0.3 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H16B          Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03X          Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03Y          Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ha            Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A           Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7            Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8            Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12           Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13           Constrained at       0.75 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C30           Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C02U          Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C039          Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0            Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C03E          Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C03S          Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C03X          Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C041          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C042          Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04F          Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04K          Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04L          Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04M          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04S          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04T          Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04U          Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04W          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04X          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04Y          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C051          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C058          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C059          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5            Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17           Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19           Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20           Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21           Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22           Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24           Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25           Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26           Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31           Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C33           Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C34           Constrained at       0.25 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C35          Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1           Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7B          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7C          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8A          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8B          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8C          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13C         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15C         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02H         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02I         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03A         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03B         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03D         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03E         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03F         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03G         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03H         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03J         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03K         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H03M         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04A         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04B         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04C         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04D         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04E         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04F         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04G         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04H         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04I         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04J         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04K         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04L         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04M         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04N         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04O         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04P         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04Q         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04R         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04S         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04T         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04U         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04V         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04W         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04X         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04Y         Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hm           Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04Z         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hp           Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hq           Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H04          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hr           Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of Hs          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ht          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hu          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05A        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05B        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05C        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05D        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05E        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05F        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05G        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05H        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H05I        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A         Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B         Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5C         Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19A        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19B        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20A        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20C        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21A        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22A        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22C        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24A        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24B        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24C        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25A        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25B        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25C        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26A        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26B        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26C        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33A        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33B        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33C        Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H34A        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H34B        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl9         Constrained at     0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl03        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C04J        Constrained at     0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9          Constrained at     0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23         Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl8         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl15        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hc          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6          Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A         Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B         Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6C         Constrained at      0.4 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       30% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       25% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3 )        50% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4 )        25% 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  2 )    332.80 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5 )      1.60 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C03J Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C03K Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for      C03N Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond C02O     - C03J    .      1.50 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond C037     - C03J    .      1.52 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O00G    .     14.6 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O00E    .    109.4 Degree
PLAT410_ALERT_2_G Short Intra H...H Contact  H01F    ..H21B    .      2.09 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H3      ..H02W    .      2.07 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H8      ..H03Z    .      1.70 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H46A    ..H03Z    .      1.95 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H7A     ..H025    .      1.88 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H15C    ..H027    .      2.07 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H01Y    ..H04E    .      2.13 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H024    ..Hm      .      2.14 Ang.
                                              x,y,z  =     1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H027    ..H04A    .      2.08 Ang.
                                              x,y,z  =     1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H01W    ..H6A     .      1.97 Ang.
                                              x,y,z  =     1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C01S    ..C6      .      2.59 Ang.
                                              x,y,z  =     1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C01W    ..C6      .      2.86 Ang.
                                              x,y,z  =     1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl6     ..Cl03    .      3.37 Ang.
                                              x,y,z  =     1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........        ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       317 Note
            O009    O00B    O00D    O00E    O00G    O00H    O00I    N00J
            N00K    N00L    N00N    O00O    N00P    N00Q    N00R    N00S
            N00T    C00U    N00V    C00W    C00X    C00Y    C00Z    N010
            C011    C012    C013    C014    N015    C016    C017    H017
            C018    C019    H019    C01A    C01B    H01A    H01B    C01C
            H01K    C01D    H01L    C01E    H01C    H01D    C01F    C01G
            H01G    C01H    H01H    C01I    C01J    C01K    C01L    H01M
            C01M    C01N    C01O    C01P    H01P    C01Q    H01E    H01F
            C01R    H01I    H01J    C01S    C01T    C01U    H01U    C01V
            H01V    C01W    H01W    C01X    H01N    H01O    C01Y    H01Y
            C01Z    H01Z    C020    H02A    H02B    C021    H021    C022
            C023    H02L    H02M    C024    H024    C025    H025    C026
            C027    H027    C028    H02N    H02O    C029    H029    C02A
            H02C    C02B    C02C    H02R    C02D    C02E    H02D    H02E
            C02F    H02F    H02G    C02G    C02H    H02S    C02I    C02J
            H02T    C02K    C02L    C02M    H02U    H02V    C02N    C02O
            C02P    H02P    C02Q    H02Q    C02S    C02T    H02W    C02U
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          H02H      H02I      C02V      H02J      H02K      C02W      H02X      H02Y
          C02X      C02Y      C02Z      H02Z      C030      H030      C031      C033
          H033      C034      H034      C035      C037      C038      C039      H03A
          H03B      C03B      H03C      C03C      H03N      H03O      C0        C03E
          H03D      H03E      C03G      H03Q      C03H      C03I      H03I      C03J
          C03K      C03L      H03L      C03M      H03R      H03S      H03T      C03N
          C03O      C03P      H03P      C03Q      H03U      H03V      H03W      H03X
          H03Y      Ha        C03R      C03S      H03F      H03G      H03H      C03V
          H03Z      C103      C03X      H03J      H03K      H03M      C040      C041
          H04A      H04B      H04C      C042      H04D      H04E      H04F      C043
          H043      C045      H045      C049      Hb        C04A      Hc        C04B
          Hd        He        C04C      C04D      Hf        C04E      C04F      H04G
          H04H      C04H      Hg        Hh        C04I      Hi        Hj        C04J
          C04K      H04I      H04J      H04K      C04L      H04L      H04M      H04N
          C04M      H04O      H04P      H04Q      C04Q      Hk        Hl        C04S
          H04R      H04S      H04T      C04T      H04U      H04V      H04W      C04U
          H04X      H04Y      Hm        C04V      Hn        Ho        C04W      H04Z
          Hp        Hq        C04X      H04       Hr        Hs        C04Y      Ht
          Hu        C050      H05J      H05K      H05L      C051      H05A      H05B
          H05C      C055      H05M      H05N      H05O      C056      H05P      H05Q
          H05R      C058      H05D      H05E      H05F      C059      H05G      H05H
          H05I      C05A      H05S      H05T      H05U      C05C      H05V      H05W
          H05X      H1BA      H1BB      H1IA      H1IB
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C35      --C6                1.86 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        3 Note
          C H Cl3
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       94 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       30% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File       92 Note
          -2  4 10,   3  7  3,   2 -5  1,   1  2  1,   0  8  6,  -1  3  4,
           0 -3 10,   1 12  1,   4 -4  6,  -1  9  9,  -1  5 11,   1  3 12,
          -1  3  2,  -5 -6  2,   2  3 10,   4  6  2,   0  2  1,   1  7  6,
           2  3  2,  -3  0  6,  -3  4 11,   0 -4 10,   1  4 12,   0  2  0,
           0  6  4,   0 -1  2,   2  3 13,   2 -4  9,   1  2  6,  -2  4  9,
           0  3  2,  -2  8  3,  -1 -4  4,   2  4  0,   4  0 13,   2-10  2,
           2  1  8,  -1 -1 15,   1  6 11,   4  4  8,   1  1  4,   3-12  8,
           3  3  1,   3  7 11,  -3  2  0,   5 -8 10,   2  8  3,   2 -3  8,
           2  6  6,  -3  0 12,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........      4.3 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..     50.1 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        4 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by        2 Check
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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
  30 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 362 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  40 ALERT type 2 Indicator that the structure model may be wrong or deficient
  29 ALERT type 3 Indicator that the structure quality may be low
 316 ALERT type 4 Improvement, methodology, query or suggestion
   3 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* 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 14/11/2023; check.def file version of 14/09/2023