checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_mcg23_139_0m, mcg2267, mcg22_131-depnfeetbenzene, mcg22_167

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.

Datablock: mcg2267

R(reflections) = 0.0960(5333)

S = 1.050

| Bond precision: | C-C = 0.0056 A | Ţ | Wavelength | =1.54178 |
|---|-------------------|-----------|-------------|-------------------|
| Cell: | a=13.3694(18) | | | |
| Temperature: | alpha=90 150 K | beta=103. | .86(1) | gamma=90 |
| | Calculated | | Reported | |
| Volume | 4276.8(8) | | 4276.8(8) | |
| Space group | P 21/c | | P 1 21/c | 1 |
| Hall group | | | -P 2ybc | |
| Moiety formula | C48 H36 B2 N2 O4, | C H2 C12 | С48 Н36 В | 2 N2 O4, C H2 C12 |
| Sum formula | C49 H38 B2 C12 N2 | 04 | С49 Н38 В | 2 C12 N2 O4 |
| Mr | 811.33 | | 811.33 | |
| Dx,g cm-3 | 1.260 | | 1.260 | |
| Ζ | 4 | | 4 | |
| Mu (mm-1) | 1.735 | | 1.735 | |
| F000 | 1688.0 | | 1688.0 | |
| F000' | 1695.36 | | | |
| h,k,lmax | | | 15,25,18 | |
| Nref | | | 7629 | |
| Tmin, Tmax | 0.855,0.949 | | 0.589,0.7 | 46 |
| Tmin' | 0.848 | | | |
| | | | | |
| Correction method= # Reported T Limits: Tmin=0.589 Tmax=0.746 | | | | |
| AbsCorr = NUMERICAL | | | | |
| | | | | |
| Data completenes | ss= | Theta(ma | ax) = 67.07 | 5 |
| | | | | |

Npar= 711

wR2(reflections)=

0.3080 (7629)

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

PLAT260_ALERT_2_B Large Average Ueq of Residue Including

Cl1B

0.313 Check

Author Response: This is caused by the large amount of disorder present within the interstitial methylene chloride solvent molecule.

Alert level C

Author Response: This is caused by the large amount of disorder present within the interstitial methylene chloride solvent molecule.

| PLAT340_ALERT_3_C | Low Bond Precision on C-C Bonds | 0.00564 Ang. |
|-------------------|--|-------------------|
| PLAT420_ALERT_2_C | D-H Bond Without Acceptor Cl2BH49A . | Please Check |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | 3.577 Check |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= 0.597 | 7 Report |
| 3 | 2 0, -3 3 1, -9 2 7, -8 0 8, -9 1 9, | -13 2 12 , |
| -11 | 9 14, | |
| PLAT918_ALERT_3_C | Reflection(s) with I(obs) much Smaller I(calc) . | 3 Check |
| PLAT922_ALERT_1_C | wR2 in the CIF and FCF Differ by | 0.0028 Check |

Alert level G

| PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite | 58 Note |
|--|---------------|
| PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms | 42 Report |
| PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms | 2 Report |
| H49A H49B | |
| PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large | 0.20 Report |
| PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records | 1 Report |
| PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records | 73 Report |
| PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records | 2 Report |
| PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records | 3 Report |
| PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used | 0.0010 Report |
| PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used | 0.0010 Report |
| PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par | 0.0010 Report |
| PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar | 0.0010 Report |
| PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par | 0.0010 Report |
| PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar | 0.0010 Report |
| PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par | 0.0010 Report |
| PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar | 0.0010 Report |
| PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used | 0.0400 Report |
| PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used | 0.0400 Report |
| PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used | 0.0400 Report |
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                       0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
{\tt PLAT191\_ALERT\_3\_G~A~Non-default~SADI~Restraint~Value~has~been~used}
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191 ALERT 3 G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1A
                                                Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2A
                                                  Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C49A
                                                                         0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H49C
                                                  Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H49D
                                                  Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1B
                                                  Constrained at
                                                                         0.5 Check
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2B
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of C49B
                                                   Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H49A
                                                  Constrained at
                                                                         0.5 Check
PLAT300 ALERT 4 G Atom Site Occupancy of H49B
                                                  Constrained at
                                                                         0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ......(Resd 1 )
                                                                         50% Note
{\tt 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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2 )
                                                                       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 3 )
                                                                       2.50 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1A .
                                                                       103.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2A
                                                                       103.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3A .
                                                                       102.5 Degree
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PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4A
                                                                           102.6 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1B
                                                                             96.9 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2B PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3B PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4B
                                                                            102.8 Degree
                                                                            97.2 Degree
                                                                             98.4 Degree
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....
                                                                                ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
                                                                               355 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still
                                                                             45% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).
                                                                                 1 Note
                 1 0 0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File
                                                                                 3 Note
                -3 3 1, 1 0 0, 3 2 0,
                                                                                11 Info
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.
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0 ALERT level A = Most likely a serious problem - resolve or explain
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- 1 ALERT level B = A potentially serious problem, consider carefully
- 9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
- 88 ALERT level G = General information/check it is not something unexpected
- 2 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
- 59 ALERT type 3 Indicator that the structure quality may be low
- 18 ALERT type 4 Improvement, methodology, query or suggestion
- 2 ALERT type 5 Informative message, check

Datablock: cu_mcg23_139_0m

Bond precision: C-C = 0.0049 A Wavelength=1.54178

Cell: a=13.1490(12) b=21.651(2) c=15.2429(17)

alpha=90 beta=102.590(6) gamma=90

Temperature: 100 K

| | | - <u>+</u> | | |
|---|-------------------------|-------------------------|--|--|
| Volume | 4235.1(7) | 4235.2(8) | | |
| Space group | P 21/c | P 1 21/c 1 | | |
| Hall group | -P 2ybc | -P 2ybc | | |
| Moiety formula | C48 H36 B2 N2 O4, C7 H8 | C48 H36 B2 N2 O4, C7 H8 | | |
| Sum formula | C55 H44 B2 N2 O4 | C55 H44 B2 N2 O4 | | |
| Mr | 818.54 | 817.53 | | |
| Dx,g cm-3 | 1.284 | 1.282 | | |
| Z | 4 | 4 | | |
| Mu (mm-1) | 0.625 | 0.625 | | |
| F000 | 1720.0 | 1716.0 | | |
| F000' | 1724.84 | | | |
| h,k,lmax | | 15,25,18 | | |
| Nref | | 7496 | | |
| Tmin, Tmax | 0.878,0.901 | 0.628,0.754 | | |
| Tmin' | 0.878 | | | |
| | | | | |
| Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.754 | | | | |
| AbsCorr = MULTI-SCAN | | | | |
| | | | | |
| Data completeness= Theta(max) = 67.068 | | | | |

Reported

R(reflections) = 0.0825(6013)

wR2(reflections) = 0.2384(7496)

S = 1.023 Npar= 753

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.

Calculated

Alert level B

PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor 4.2 Note

Author Response: This is caused by the large amount of disorder present within the interstitial toluene and DEPN molecules.

Alert level C

CHEMW01_ALERT_1_C The difference between the given and expected weight for compound is greater 1 mass unit. Check that all hydrogen atoms have been taken into account.

| PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of | 2.750 Sigma |
|---|--------------|
| PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by | 1.01 Check |
| PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing) | Please Check |
| PLAT088_ALERT_3_C Poor Data / Parameter Ratio | 9.95 Note |

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PLAT234_ALERT_4_C Large Hirshfeld Difference C54A --C55A .
                                                              0.20 Ang.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C49A
                                                            0.155 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including
                                                    C49B
                                                             0.166 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ...... 0.00488 Ang.
PLAT721_ALERT_1_C Bond Calc 1.40(5), Rep 1.38650 Dev...
                                                             0.01 Ang.
                                 C54B
                   -C53B
PLAT723_ALERT_1_C Torsion Calc
                                1(5), Rep -0.10 Dev...
                                                             1.10 Sigma
           C55B-C54B-C53B-C52B 1_555 1_555 1_555 # 235 Check
PLAT723_ALERT_1_C Torsion Calc
                              -1(4), Rep 0.10 Dev...
                                                            1.10 Sigma
           C54B-C53B-C52B-C51B 1_555 1_555 1_555 # 236 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....
                                                           4.873 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597
                                                             73 Report
             2 0 0, 3 0 0, 2 2 0, 2 3 0, -2 3 1, 2 4 1,
            -2 0 2, 0 0 2,
                                2 0 2, -2 1 2, 2 1 2, -2 1 3,
             0 3 3, 0 4 3, 0 5 3, 2 24 3, -14 1 11, -13 1 11,
            -14 2 11, -14 3 11, -13 0 12, -11 0 12, -8 0 12, -13 1 12,
            -12 1 12, -13 2 12, -12 2 12, -13 3 12, -12 3 12, -13 4 12,
            -13 1 13, -12 1 13, -11 1 13, -9 1 13, -13 2 13, -12 2 13,
            -13 3 13, -12 3 13, -12 0 14, -11 0 14, -10 0 14, -9 0 14,
            -12 1 14, -11 1 14, -12 2 14, -10 2 14, -8 2 14, -12 3 14,
            -10 3 14, -11 1 15, -10 1 15, -9 1 15, -11 2 15, -10 2 15,
            -9 2 15, -7 2 15, -11 3 15, -9 3 15, -10 0 16, -9 0 16,
            -8 0 16, -6 0 16, -5 0 16, -10 1 16, -9 1 16, -7 1 16,
-6 1 16, -10 2 16, -8 3 16, -8 3 17, -7 3 17, -5 3 17,
            -5 4 17,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....
                                                               10 Note
             2 3 0, -2 3 1, -2 0 2, 0 0 2, 2 0 2, -2 1 2,
             2 1 2, -2 1 3, 0 3 3,
                                        0 4 3,
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Alert level G

| PLAT002_ALERT_2_G Number of Distance or Angle Restraints on A | Site | 62 | Note |
|---|-------|--------|--------|
| PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atom | 3 | 67 | Report |
| PLAT005_ALERT_5_G No Embedded Refinement Details Found in the | e CIF | Please | Do ! |
| PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually | large | 0.12 | Report |
| PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C52AC53A | | 10.9 | s.u. |
| PLAT300_ALERT_4_G Atom Site Occupancy of C49A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C50A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C51A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C52A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C53A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C54A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C55A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H49A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H49B Constraine | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H49C Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H51A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H52A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H53A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H54A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of H55A Constrained | ed at | 0.85 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C49B Constraine | ed at | 0.15 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C50B Constraine | ed at | 0.15 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C51B Constraine | ed at | 0.15 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C52B Constraine | ed at | 0.15 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C53B Constrained | ed at | 0.15 | Check |
| PLAT300_ALERT_4_G Atom Site Occupancy of C54B Constrained | ed at | 0.15 | Check |
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PLAT300_ALERT_4_G Atom Site Occupancy of C55B
                                                  Constrained at
                                                                        0.15 Check
                                                                        0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H49D
                                                   Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H49E
                                                   Constrained at
                                                                        0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H49F
                                                   Constrained at
                                                                        0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H51B
                                                   Constrained at
                                                                        0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52B
                                                   Constrained at
                                                                        0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53B
                                                  Constrained at
                                                                        0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54B
                                                  Constrained at
                                                                        0.15 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H55B
                                                                       0.15 Check
PLAT301_ALERT_3_G Main Residue Disorder ......(Resd 1 )
                                                                        54% Note
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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2 )
                                                                      12.75 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 3 )
                                                                       2.25 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1A
                                                                      103.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2A
                                                                      104.6 Degree
PLAT395 ALERT 2 G Deviating X-O-Y Angle From 120 for O3A
                                                                      104.3 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4A
                                                                      104.6 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1B
                                                                      102.4 Degree
PLAT395_ALERT_2_G Deviating X-O-Y
                                    Angle From 120 for O2B
                                                                      106.5 Degree
PLAT395_ALERT_2_G Deviating X-O-Y
                                                                      104.7 Degree
                                    Angle From 120 for O3B
PLAT395_ALERT_2_G Deviating X-O-Y
                                   Angle From 120 for O4B
                                                                      104.9 Degree
PLAT411_ALERT_2_G Short Inter H...H Contact H21
                                                                       1.87 Ang.
                                                    ..H53B
                                                                   3_656 Check
                                                1-x, -y, 1-z =
PLAT411_ALERT_2_G Short Inter H...H Contact
                                            Н33
                                                     ..H52B
                                                                        0.72 Ang.
                                                                   1_555 Check
                                                     x, y, z =
                                                                        0.95 Ang.
PLAT413_ALERT_2_G Short Inter XH3 .. XHn
                                            H26
                                                     ..H49D
                                                 -x, -y, 1-z =
                                                                   3_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                            C13
                                                    ..C2B
                                                                        3.09 Ang.
                                            x, 1/2-y, -1/2+z =
                                                                   4_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                            C14
                                                   ..C2B
                                                                        3.19 Ang.
                                            x, 1/2-y, -1/2+z =
                                                                   4_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                                    ..C49B
                                                                        2.63 Ang.
                                            C26
                                                                   3_556 Check
                                                 -x, -y, 1-z =
                                            C33
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                                     ..C52B
                                                                        2.24 Ang.
                                                     x, y, z =
                                                                   1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                            C33
                                                     ..C53B
                                                                        2.95 Ang.
                                                                   1_555 Check
                                                     x, y, z =
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                            C33
                                                     ..C51B
                                                                        3.18 Ang.
                                                     x, y, z =
                                                                   1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                           C34
                                                     ..C52B
                                                                        2.74 Ang.
                                                     x, y, z =
                                                                   1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C34
                                                     ..C51B
                                                                       3.11 Ang.
                                                     x, y, z =
                                                                   1_555 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....
                                                                          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
                                                                         613 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still
                                                                         59% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).
                                                                           1 Note
                1 0 0,
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.
                                                                          13 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by
                                                                           2 Check
```

⁰ **ALERT level A** = Most likely a serious problem - resolve or explain

¹ ALERT level ${\bf B}$ = A potentially serious problem, consider carefully

¹⁵ ALERT level C = Check. Ensure it is not caused by an omission or oversight

⁶⁵ **ALERT level G** = General information/check it is not something unexpected

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 26 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
- 37 ALERT type 4 Improvement, methodology, query or suggestion
- 3 ALERT type 5 Informative message, check

Datablock: mcg22_131-depnfeetbenzene

Bond precision: C-C = 0.0048 AWavelength=1.54178 Cell: a=13.0756(8)b=21.2676(11)c=15.4455(8)alpha=90 beta=102.211(4) gamma=90 Temperature: 100 K Calculated Reported Volume 4198.0(4) 4198.0(4) Space group P 21/c P 1 21/c 1 Hall group -P 2ybc -P 2ybc Moiety formula C48 H36 B2 N2 O4, C6 H6 C48 H36 B2 N2 O4, C6 H6 Sum formula C54 H42 B2 N2 O4 C54 H42 B2 N2 O4 804.21 804.52 Dx,g cm-3 1.273 1.272 0.622 0.622 Mu (mm-1)F000 1688.0 1687.0 F000' 1692.77 h,k,lmax 15, 25, 18 Nref 7504 0.647,0.754 Tmin, Tmax 0.923,0.949 Tmin' 0.872 Correction method= # Reported T Limits: Tmin=0.647 Tmax=0.754 AbsCorr = MULTI-SCAN Theta (max) = 67.069Data completeness= wR2 (reflections) = R(reflections) = 0.0918(6232)0.2662 (7504) Npar= 677 S = 1.042

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
```

Alert level C

```
DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00 _refine_diff_density_min given = -0.894 Test value = -0.800
```

Author Response: This is caused by disorder of the benzene substituent. Repeated attempts to model the disorder, accompanied by suitable constraints and restraints have been used without success. Difference map shows unequivocally that the peaks are those associated with benzene.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.33 eA-3

Author Response: This is caused by disorder of the benzene substituent. Repeated attempts to model the disorder, accompanied by suitable constraints and restraints have been used without success. Difference map shows unequivocally that the peaks are those associated with benzene.

PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -0.89 eA-3

Author Response: This is caused by disorder of the benzene substituent. Repeated attempts to model the disorder, accompanied by suitable constraints and restraints have been used without success. Difference map shows unequivocally that the peaks are those associated with benzene.

PLAT922_ALERT_1_B wR2 in the CIF and FCF Differ by 0.0095 Check

Author Response: This is caused by addition of the fcf into the cif file. Repeated attempts to resolve this issue by any method other than exclusion of the fcf from the cif have been unsuccessful.

```
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75

The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.
```

0.0400 Report

Alert level G PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 58 Note PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 69 Report PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.56 Why ? PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 11 Report PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 72 Report PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 4 Report ${\tt PLAT187_ALERT_4_G\ The\ CIF-Embedded\ .res\ File\ Contains\ RIGU\ Records}$ 5 Report PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0010 Report PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0010 Report PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0010 Report PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0010 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0020 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0020 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0050 Report PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0050 Report PLAT191 ALERT 3 G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191 ALERT 3 G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report

PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used

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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C1
                                                 Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3
                                                  Constrained at
                                                                        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4
                                                                        0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of C5
                                                  Constrained at
                                                                        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6
                                                  Constrained at
                                                                        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7
                                                  Constrained at
                                                                        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1
                                                                        0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H3
                                                                        0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H4
                                                                        0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H5
                                                                         0.5 Check
                                                   Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H6
                                                   Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7
                                                   Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cc
                                                   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 C8
                                                  Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9
                                                  Constrained at
                                                                         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10
                                                                         0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of C11
                                                  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 H2
                                                                        0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H8
                                                                        0.5 Check
                                                  Constrained at
PLAT300_ALERT_4_G Atom Site Occupancy of H9
                                                  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 H11
                                                  Constrained at
                                                                        0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... (Resd 1 )
                                                                        50% Note
                                                                       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 )
                                                                       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3 )
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1A
                                                                      104.2 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2A
                                                                      103.6 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3A
                                                                      102.9 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4A
                                                                      103.4 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1B
                                                                      105.6 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2B PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3B PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4B
                                                                      101.1 Degree
                                                                        98.8 Degree
                                                                      101.4 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact C13
                                                 ..C5B
                                                                       3.11 Ang.
                                                                   4_575 Check
                                            x, 3/2-y, -1/2+z =
PLAT432_ALERT_2_G Short Inter X...Y Contact C14
                                                   ..C5B
                                                                       3.12 Ang.
                                            x, 3/2-y, -1/2+z =
                                                                   4_575 Check
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder
                                                                        ! Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....
                                                                           2 Note
              Сс
                     HС
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....
                                                                          ! Info
```

```
O ALERT level A = Most likely a serious problem - resolve or explain

4 ALERT level B = A potentially serious problem, consider carefully

9 ALERT level C = Check. Ensure it is not caused by an omission or oversight

112 ALERT level G = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

19 ALERT type 2 Indicator that the structure model may be wrong or deficient

66 ALERT type 3 Indicator that the structure quality may be low

32 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check
```

Datablock: mcg22_167

| Bond precision: | C-C = 0.0072 A Wavelength=1.54178 | | |
|-----------------|-----------------------------------|---------------------------------|---------------|
| Cell: | | b=21.8540(8) beta=102.053(2) | |
| Temperature: | 100 K | | |
| | Calculated | Reported | |
| Volume | 4291.3(3) | 4291.3(3) | |
| Space group | P 21/c | P 1 21/c 1 | |
| Hall group | -P 2ybc | -P 2ybc | |
| Moiety formula | C48 H36 B2 N2 O4, | C8 H10 C48 H36 B2 | N2 O4, C8 H10 |
| Sum formula | C56 H46 B2 N2 O4 | С56 Н46 В2 | N2 O4 |
| Mr | 832.57 | 832.57 | |
| Dx,g cm-3 | 1.289 | 1.289 | |
| Z | 4 | 4 | |
| Mu (mm-1) | 0.625 | 0.625 | |
| F000 | 1752.0 | 1752.0 | |
| F000' | 1756.91 | | |
| h,k,lmax | | 15,26,18 | |
| Nref | | 7657 | |
| Tmin, Tmax | 0.799,0.945 | 0.818,0.95 | 1 |
| Tmin' | 0.799 | | |

Correction method= # Reported T Limits: Tmin=0.818 Tmax=0.951 AbsCorr = MULTI-SCAN

Data completeness=

Theta(max) = 67.074

R(reflections) = 0.0998(6424)

wR2(reflections) = 0.2959(7657)

S = 1.055

Npar= 733

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

PLAT411_ALERT_2_A Short Inter H...H Contact H55B ...H55B . 1.68 Ang. $-x, 2-y, 1-z = 3_576$ Check

Author Response: This is caused by disorder of the ethylbenzene substituent. Repeated attempts to model the disorder, accompanied by suitable constraints and restraints have been used without success. Difference map shows unequivocally that the peaks are those associated with ethylbenzene.

PLAT412_ALERT_2_A Short Intra XH3 .. XHn H50 ..H56B . 1.58 Ang. x,y,z = 1_555 Check

Author Response: This is caused by disorder of the ethylbenzene substituent. Repeated attempts to model the disorder, accompanied by suitable constraints and restraints have been used without success. Difference map shows unequivocally that the peaks are those associated with ethylbenzene.

Alert level B

PLAT922_ALERT_1_B wR2 in the CIF and FCF Differ by 0.0118 Check

Author Response: This is caused by addition of the fcf into the cif file. Repeated attempts to resolve this issue by any method other than exclusion of the fcf from the cif have been unsuccessful.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75 The relevant atom site should be identified.

Author Response: This is caused by disorder of the ethylbenzene substituent. Repeated attempts to model the disorder, accompanied by suitable constraints and restraints have been used without success. Difference map shows unequivocally that the peaks are those associated with ethylbenzene.

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ...... 4.340 Check PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 10 Report 2 0 0, 2 3 0, -2 0 2, 0 0 2, -2 1 2, -2 1 3, 0 4 3, -1 0 14, 1 0 14, -4 2 18, PLAT921_ALERT_1_C R1 in the CIF and FCF Differ by ..... 0.0044 Check PLAT923_ALERT_1_C S Values in the CIF and FCF Differ by ..... 0.046 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite
                                                                           60 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
                                                                           66 Report
PLAT072 ALERT 2 G SHELXL First Parameter in WGHT Unusually Large
                                                                         0.18 Report
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records
                                                                           81 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records
                                                                            6 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par
                                                                       0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar
                                                                       0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par
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PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar
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PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par
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PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar
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PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par
                                                                       0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar
                                                                       0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par
                                                                       0.0200 Report
                                                                       0.0200 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par
                                                                       0.0050 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar
                                                                       0.0050 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                       0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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{\tt PLAT191\_ALERT\_3\_G~A~Non-default~SADI~Restraint~Value~has~been~used}
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
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{\tt PLAT191\_ALERT\_3\_G~A~Non-default~SADI~Restraint~Value~has~been~used}
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PLAT191 ALERT 3 G A Non-default SADI Restraint Value has been used
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used
                                                                      0.0400 Report
PLAT301_ALERT_3_G Main Residue Disorder ......(Resd 1 )
                                                                         52% Note
                                                                       104.5 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1A .
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2A
                                                                       104.7 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3A
                                                                       102.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4A
                                                                       103.7 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1B
                                                                      107.6 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2B
                                                                      103.4 Degree
PLAT395_ALERT_2_G Deviating X-O-Y
                                    Angle From 120 for O3B
                                                                      102.5 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4B
                                                                       103.2 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact C13 ...C5B
                                                                       3.04 Ang.
                                            x, 3/2-y, -1/2+z =
                                                                   4_575 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact
                                           C14 ..C5B
                                                                        3.18 Ang.
                                            x,3/2-y,-1/2+z =
                                                                   4_575 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C55
                                                   ..C55
                                                                       3.06 Ang.
                                                -x, 2-y, 1-z =
                                                                   3_576 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....
                                                                           ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ......
                                                                         552 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .
                                                                      Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still
                                                                         68% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).
                                                                           1 Note
                1 0 0,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....
                                                                           1 Note
                0 4 3,
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.
                                                                          12 Info
```

```
1 ALERT level B = A potentially serious problem, consider carefully
17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
82 ALERT level G = General information/check it is not something unexpected

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

checkCIF publication errors

```
Alert level A

PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).

PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).

2 ALERT level A = Data missing that is essential or data in wrong format 0 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
```

```
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 14/11/2023; check.def file version of 14/09/2023

Datablock mcg2267 - ellipsoid plot







