checkCIF/PLATON report

Structure factors have been supplied for datablock(s) iaa065_0m_pl, mo, w

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

```
Bond precision:   C-C = 0.0646 A          Wavelength=0.71073

Cell:           a=17.8167(3)       b=17.9076(3)      c=19.7519(4)
                alpha=116.936(2)   beta=116.807(2)   gamma=90.012(1)
Temperature:    130 K
```

	Calculated	Reported
Volume	4846.0(2)	4846.01(19)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C48 H54 O40, C48 H56 O40, 3(Cl14 Mo6), 17(O)	?
Sum formula	C96 H110 Cl42 Mo18 O97	C96 H110 Cl42 Mo18 O97
Mr	6031.67	6031.65
Dx,g cm-3	2.067	2.067
Z	1	1
Mu (mm-1)	1.791	1.791
F000	2932.0	2932.0
F000'	2908.44	
h,k,lmax	24,24,27	24,24,26
Nref	54916[27458]	44790
Tmin,Tmax	0.657,0.699	0.977,1.000
Tmin'	0.633	

```
Correction method= # Reported T Limits: Tmin=0.977 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.63/0.82        Theta(max)= 29.676

R(reflections)= 0.1443( 42664)                    wR2(reflections)=
                                                  0.3202( 44790)
S = 1.091                  Npar= 1314
```

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

PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) ..... 175 Report
O42 O43 O44 O45 O46 etc.

Author Response: Complex disorder of the main structural part.

PLAT430_ALERT_2_A Short Inter D...A Contact O1 ..O9W . 2.44 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O1W ..O13 . 2.40 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O1W ..O6W . 2.42 Ang.
-1+x,y,z = 1_455 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O4W ..O5W . 2.46 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O6W ..O32 . 2.46 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O7W ..O16W . 2.45 Ang.
1+x,y,z = 1_655 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O9W ..O18W . 2.45 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O11W   ..O21   .   2.42 Ang.
                                                    x,y,z =   1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_A Short Inter D...A Contact O11W   ..O14W   .   2.48 Ang.
                                                  x,y,-1+z =   1_554 Check

Author Response: Hydrogen bonding or positional disordering

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.61Ang From Mo1A   4.48 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.81Ang From Mo2B   4.43 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.51Ang From Mo1B   3.71 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.50Ang From Cl1R   -3.78 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.43Ang From Cl3T   -3.69 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.93Ang From Cl1R   -3.58 eA-3

Author Response: Complex disorder of the main structural part.

Alert level B

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density   4.98 eA-3

Author Response: Complex disorder of the main structural part.

PLAT220_ALERT_2_B NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   6.7 Ratio

Author Response: Complex disorder of the main structural part.

```
PLAT221_ALERT_2_B Solv./Anion  Resd 3 Cl   Ueq(max)/Ueq(min) Range        8.6 Ratio
PLAT221_ALERT_2_B Solv./Anion  Resd 3 Mo   Ueq(max)/Ueq(min) Range       10.0 Ratio
PLAT221_ALERT_2_B Solv./Anion  Resd 5 Cl   Ueq(max)/Ueq(min) Range       10.0 Ratio
PLAT221_ALERT_2_B Solv./Anion  Resd 6 Cl   Ueq(max)/Ueq(min) Range       10.0 Ratio
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O1W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O2W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O3W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O4W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O5W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O6W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O7W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O8W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O9W Check
```

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O11W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O12W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O13W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O14W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O15W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O16W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O17W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O18W Check

Author Response: H-atoms of water molecules of crystallization were not refined.

```
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.06461 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact  H4A      ..H54A     .       1.80 Ang.
                                             x,y,z  =      1_555 Check
PLAT410_ALERT_2_B Short Intra H...H Contact  H18A     ..H47A     .       1.80 Ang.
                                             x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O1       ..O67      .       2.68 Ang.
                                        x,-1+y,-1+z  =      1_544 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O1W      ..O60      .       2.79 Ang.
                                            -1+x,-1+y,-1+z  =      1_444 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O2W      ..O4W      .       2.60 Ang.
                                              -1+x,y,z  =      1_455 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O2W      ..O18      .       2.66 Ang.
                                               x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3       ..O49      .       2.57 Ang.
                                            -1+x,-1+y,-1+z  =      1_444 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3W      ..O4W      .       2.63 Ang.
                                               x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3W      ..O29      .       2.69 Ang.
                                               x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O5W      ..O17      .       2.62 Ang.
                                             1+x,y,z  =      1_655 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O5W      ..O33      .       2.82 Ang.
                                               x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O6       ..O12W     .       2.83 Ang.
                                              x,-1+y,z  =      1_545 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O6W      ..O80      .       2.78 Ang.
                                                  x,y,-1+z  =      1_554 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O7       ..O24      .       2.68 Ang.
                                                  x,-1+y,z  =      1_545 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O7W      ..O38      .       2.60 Ang.
                                                  x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O7W      ..O11      .       2.79 Ang.
                                                  1+x,y,z  =      1_655 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O8       ..O74      .       2.81 Ang.
                                                  x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O8W      ..O16W     .       2.62 Ang.
                                                  1+x,y,z  =      1_655 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O8W      ..O39      .       2.65 Ang.
                                                  x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O9       ..O15W     .       2.68 Ang.
                                                  x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O9W      ..O69      .       2.62 Ang.
                                                  x,-1+y,-1+z  =      1_544 Check
```

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O11W ..O49 . 2.61 Ang.
-1+x,y,-1+z = 1_454 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O12W ..O28 . 2.72 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O13 ..O54 . 2.72 Ang.
-1+x,-1+y,-1+z = 1_444 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O13W ..O60 . 2.73 Ang.
x,-1+y,z = 1_545 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O13W ..O76 . 2.82 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O14W ..O69 . 2.82 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O15W ..O16W . 2.64 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O16 ..O42 . 2.66 Ang.
-1+x,y,-1+z = 1_454 Check

Author Response: Hydrogen bonding or positional disordering

PLAT430_ALERT_2_B Short Inter D...A Contact O17 ..O63 . 2.75 Ang.
x,y,z = 1_555 Check

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O17W     ..O80      .       2.72 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O18W     ..O49      .       2.83 Ang.
                                                 -1+x,-1+y,-1+z  =      1_444 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O21      ..O42      .       2.66 Ang.
                                                    -1+x,y,-1+z  =      1_454 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O26      ..O69      .       2.55 Ang.
                                                      x,y,-1+z  =      1_554 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O28      ..O55      .       2.82 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O32      ..O73      .       2.69 Ang.
                                                      x,y,-1+z  =      1_554 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O33      ..O48      .       2.83 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O37      ..O67      .       2.68 Ang.
                                                    x,-1+y,-1+z  =      1_544 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O38      ..O46      .       2.75 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 39 Note
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.61Ang From Mo2A 3.41 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.51Ang From Mo5B 3.11 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.97Ang From C130 2.86 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.32Ang From Mo16 2.85 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.48Ang From Mo3A 2.84 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.07Ang From C158 2.79 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.78Ang From Cl5F 2.78 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.91Ang From Cl3T 2.74 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.76Ang From Cl2D 2.72 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.40Ang From Cl1F 2.71 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.67Ang From Cl1I 2.67 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.43Ang From Mo1X 2.65 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.75Ang From Cl2B 2.62 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.42Ang From Cl1Y 2.61 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.65Ang From Mo1X 2.61 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.68Ang From Cl1J 2.60 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.25Ang From Cl20 2.58 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.01Ang From C117 2.56 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.66Ang From Cl5K 2.56 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.73Ang From Cl3Z 2.54 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.17Ang From Cl18 2.53 eA-3

Author Response: Complex disorder of the main structural part.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.35Ang From Mo2A 2.51 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.70Ang From Cl20 -3.44 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.76Ang From Cl18 -3.43 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.30Ang From Cl5F -3.33 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.76Ang From Mo1S -3.18 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.89Ang From Cl5K -3.12 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.92Ang From Cl3T -3.10 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.95Ang From Cl19 -3.05 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.98Ang From Cl3F -3.01 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.85Ang From Cl3T -2.90 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.85Ang From Cl1R -2.88 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.60Ang From Cl21 -2.82 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.74Ang From Cl5F -2.79 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.56Ang From Mo9A -2.77 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.85Ang From Cl5K -2.77 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.83Ang From Mo10 -2.75 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.53Ang From Mo5A -2.58 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.58Ang From Mo1A -2.58 eA-3

Author Response: Complex disorder of the main structural part.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.55Ang From Cl4T -2.54 eA-3

Author Response: Complex disorder of the main structural part.

```
PLAT972_ALERT_2_B Check Calcd Resid. Dens.  1.21Ang From Cl4T          -2.52 eA-3
```

Author Response: Complex disorder of the main structural part.

Alert level C

```
DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =     -3.690
           Test value =     -3.150
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.
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ........     Please Check
PLAT082_ALERT_2_C High R1 Value ..................................       0.14 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.32 Report
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density      -3.69 eA-3
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........         17 Check
             O1W     O2W     O3W     O4W     O5W     O6W                 etc.
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        3.7 Ratio
```

Author Response: Complex disorder of the main structural part.

```
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        3.4 Ratio
```

Author Response: Complex disorder of the main structural part.

```
PLAT221_ALERT_2_C Solv./Anion  Resd 5 Mo   Ueq(max)/Ueq(min) Range        4.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        6.5 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O45 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O56 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O64 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O77 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O81 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C56 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C95 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C125 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C13Y Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C122 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C136 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C138 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C150 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C10M Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C10O Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C10P Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C10R Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C10T Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C10W Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O68 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C31 Check
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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C47 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C54 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C73 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C94 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C117 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C124 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C145 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C147 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C151 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C158 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O42 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O45 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O46 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O47 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O48 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O49 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O53 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O54 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O55 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O58 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O59 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O60 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O63 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O64 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O67 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O69 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O70 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O71 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O73 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O74 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O75 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O78 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O79 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O80 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O1 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O3 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O6 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O7 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O8 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........         O9 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O11 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O12 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O13 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O16 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O17 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O18 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O21 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O23 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O24 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O26 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O28 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O29 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O32 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O33 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O34 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O37 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O38 Check
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PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O39 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C10      - C126     .       1.40 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C13      - C37      .       1.40 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C31      - C68      .       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C68      - C95      .       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C73      - C74      .       1.40 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C74      - C164     .       1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C79      - C80      .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C100     - C101     .       1.41 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C37      - C38      .       1.70 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C47      - C125     .       1.65 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C72      - C126     .       1.74 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H92A     ..H94A     .       1.93 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H12D     ..H122     .       1.97 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H13D     ..H28A     .       1.99 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O11      ..O71      .       2.85 Ang.
                                                     x,y,z  =      1_555 Check
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Author Response: Hydrogen bonding or positional disordering

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PLAT430_ALERT_2_C Short Inter D...A Contact  O17W     ..O57      .       2.85 Ang.
                                                   x,-1+y,z  =      1_545 Check
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Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O18      ..O59      .       2.87 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O39      ..O79      .       2.85 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Hydrogen bonding or positional disordering

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PLAT430_ALERT_2_C Short Inter D...A Contact  O53      ..O78      .       2.87 Ang.
                                                   x,1+y,z  =      1_565 Check
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Author Response: Hydrogen bonding or positional disordering

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PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         45 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.960 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.138 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         10 Note
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage         76 %
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          6 Check
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.56Ang From Cl1E          -2.48 eA-3
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Author Response: Complex disorder of the main structural part.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.98Ang From Mo13          -2.41 eA-3
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Author Response: Complex disorder of the main structural part.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.69Ang From Cl3U          -2.37 eA-3
```

Author Response: Complex disorder of the main structural part.

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PLAT977_ALERT_2_C Check Negative Difference Density on H6AA      .      -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3A       .      -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H4A       .      -0.85 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10A      .      -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10C      .      -1.03 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13A      .      -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13D      .      -0.92 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13I      .      -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13K      .      -0.89 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13Y      .      -0.56 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H14D      .      -0.48 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H14G      .      -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15D      .      -0.42 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15F      .      -0.56 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15G      .      -0.79 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H20B      .      -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H24A      .      -0.54 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H30A      .      -0.93 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H38A      .      -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H45A      .      -0.80 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H45B      .      -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H49A      .      -0.96 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H49B      .      -0.68 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H53A      .      -0.82 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H53B      .      -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H60A      .      -0.58 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H66A      .      -0.54 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H68A      .      -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H71A      .      -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H71B      .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H74A      .      -0.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H75A      .      -1.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H77A      .      -0.53 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H80A      .      -0.71 eA-3
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PLAT977_ALERT_2_C Check Negative Difference Density on H83A      .      -0.83 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H84A      .      -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H89A      .      -1.28 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H98A      .      -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H122      .      -0.55 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     478.89 Why ?
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         2         99 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New  Space Group         I2 Check
            Check Model Parameter Symmmetry for Reflection Data Support
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C6A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20B       Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20A       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6AA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B       Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20A       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo1S       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo1X       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo2S       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo2X       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo5X       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo6X       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo7X       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo8A       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo8B       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo8X       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo9A       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo9B       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1C       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1H       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1I       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1J       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1M       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1S       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2C       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2H       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2I       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2J       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2M       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2S       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2Z       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3Z       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1R       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2R       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3F       Constrained at        0.4 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of Cl3T       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4T       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5F       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5K       Constrained at       0.46 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl6K       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl18       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl19       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl20       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl21       Constrained at       0.14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of ClTS       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of ClTT       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo1B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo2B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo3B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo4A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo5A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo6B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1F       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1U       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1Y       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 Cl2K       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2N       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2T       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2X       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3H       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3U       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3Y       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl6Y       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of MoBA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo1A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo2A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo3A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo5B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo6A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1N       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1T       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1X       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1Z       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2F       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2U       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2Y       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3K       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4H       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4Y       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5Y       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        90% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        10% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C13Y Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C18      - C21      .       1.53 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O5       .      102.0 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O30      .      103.9 Degree
PLAT410_ALERT_2_G Short Intra H...H Contact  H1A      ..H6B      .       2.04 Ang.
                                                      x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H20B     ..H43A     .       2.05 Ang.
                                                      x,y,z  =      1_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl0P     ..O4W      .       3.08 Ang.
                                          -1+x,-1+y,-1+z  =      1_444 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl0R     ..O16W     .       3.09 Ang.
                                                x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl6Y     ..C90      .       3.25 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3F     ..C140     .       3.02 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3F     ..C13      .       3.13 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl4T     ..C58      .       3.25 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl6K     ..C128     .       3.05 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl6K     ..C10      .       3.12 Ang.
                                                      x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl0J     ..Cl1D     .       3.19 Ang.
                                                      x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl0J     ..Cl3D     .       3.39 Ang.
                                                      x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl0L     ..Cl3D     .       3.20 Ang.
                                                      x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........        14 Note
PLAT722_ALERT_1_G Angle   Calc      114.00, Rep      112.50 Dev...       1.50 Degree
             C5      -C6A     -H6AA       1_555  1_555  1_555     #   16 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      111.90 Dev...       1.10 Degree
             C11     -C9      -H9A        1_555  1_555  1_555     #   42 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      110.20 Dev...       1.20 Degree
             C21     -C20B    -H20B       1_555  1_555  1_555     #   96 Check
PLAT722_ALERT_1_G Angle   Calc      106.00, Rep      104.50 Dev...       1.50 Degree
             O19     -C29     -H29A       1_555  1_555  1_555     #  132 Check
PLAT722_ALERT_1_G Angle   Calc      103.00, Rep      104.50 Dev...       1.50 Degree
             C28     -C29     -H29A       1_555  1_555  1_555     #  133 Check
PLAT722_ALERT_1_G Angle   Calc      116.00, Rep      114.50 Dev...       1.50 Degree
             O48     -C37     -H37A       1_555  1_555  1_555     #  151 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.60 Dev...       1.60 Degree
             C19     -C45     -H45A       1_555  1_555  1_555     #  161 Check
PLAT722_ALERT_1_G Angle   Calc      107.00, Rep      108.70 Dev...       1.70 Degree
             H49A    -C49     -H49B       1_555  1_555  1_555     #  176 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      108.90 Dev...       1.10 Degree
             C29     -C66     -H66A       1_555  1_555  1_555     #  215 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      107.70 Dev...       1.30 Degree
             H66A    -C66     -H66B       1_555  1_555  1_555     #  218 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.10 Dev...       1.10 Degree
             C98     -C125    -H12E       1_555  1_555  1_555     #  415 Check
PLAT722_ALERT_1_G Angle   Calc      114.00, Rep      112.50 Dev...       1.50 Degree
             C150    -C147    -H14F       1_555  1_555  1_555     #  529 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      111.10 Dev...       1.10 Degree
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             C136    -C158    -H15F       1_555  1_555  1_555     #  562 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C6A      --C1              1.84 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C20A     --C43             1.88 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C72      --C126            1.73 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             Cl14 Mo6
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             Cl14 Mo6
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         15 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         21 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         23 Note
             O
PLAT791_ALERT_4_G Model has Chirality at C3          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C4          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C6B         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C9          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C10         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C11         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C13         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C13Y        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C14         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C16         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C18         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C19         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C20B        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C22         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C28         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C29         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C30         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C31         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C37         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C38         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C47         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C54         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C56         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C58         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C63         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C68         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C72         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C73         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C74         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C75         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C79         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C80         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C83         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C84         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C86         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C89         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C92         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C94         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C95         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C98         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C100        (Sohnke SpGr)          S Verify
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PLAT791_ALERT_4_G Model has Chirality at C101        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C104        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C105        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C106        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C107        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C113        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C117        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C119        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C122        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C124        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C125        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C126        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C127        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C128        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C129        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C130        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C131        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C132        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C134        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C135        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C136        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C137        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C138        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C139        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C140        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C141        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C150        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C151        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C156        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C158        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C159        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C162        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C163        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C164        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C166        (Sohnke SpGr)          R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          5 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       3510 Note
PLAT930_ALERT_2_G FCF-based   Twin Law ( 0 2-1)         Est.d BASF       0.33 Check
PLAT930_ALERT_2_G FCF-based   Twin Law ( 2 0-1)         Est.d BASF       0.33 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 2-1)         Est.d BASF       0.33 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 2 0-1)         Est.d BASF       0.33 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.6 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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16 **ALERT level A** = Most likely a serious problem - resolve or explain
105 **ALERT level B** = A potentially serious problem, consider carefully
161 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
234 **ALERT level G** = General information/check it is not something unexpected

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

```
 297 ALERT type 2 Indicator that the structure model may be wrong or deficient
  14 ALERT type 3 Indicator that the structure quality may be low
 185 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Datablock: iaa065_0m_pl

Bond precision: C-C = 0.0130 A Wavelength=0.71073

Cell: a=23.806(1) b=23.806(1) c=22.831(1)
alpha=90 beta=90 gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	12938.9(12)	12938.9(12)
Space group	P 4 21 2	P 4 21 2
Hall group	P 4ab 2ab	P 4ab 2ab
Moiety formula	C48 H56 O40, 0.05(Cl24 Mo8), 0.467(Cl5 Mo), 0.283(Cl4 Mo4), 6(O	Cl13.3 Mo6, 3(C48 H56 O40), 18(O), 0.7(Cl)
Sum formula	C48 H56 Cl4.67 Mo2 O46 [+ solvent]	C144 H168 Cl14 Mo6 O140
Mr	1726.24	5210.71
Dx,g cm-3	1.329	1.337
Z	6	2
Mu (mm-1)	0.521	0.522
F000	5252.0	5284.0
F000'	5238.93	
h,k,lmax	28,28,27	28,28,27
Nref	11518[6429]	11500
Tmin,Tmax	0.949,0.990	0.603,0.746
Tmin'	0.949	

Correction method= # Reported T Limits: Tmin=0.603 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.79/1.00 Theta(max)= 25.068

R(reflections)= 0.0749(10490) wR2(reflections)= 0.2199(11500)

S = 1.038 Npar= 740

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

DIFF005_ALERT_1_A _diffrn_measurement_method is missing
Mode of intensity measurement and scan.

PLAT430_ALERT_2_A Short Inter D...A Contact O1W ..O2W . 2.53 Ang.
x,y,z = 1_555 Check

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

Alert level B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O4W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O5W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O6W Check
PLAT430_ALERT_2_B Short Inter D...A Contact O1A ..O10B . 2.73 Ang.
-1/2-y,1/2+x,z = 2_455 Check

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

PLAT430_ALERT_2_B Short Inter D...A Contact O1C ..O2B . 2.72 Ang.
x,y,z = 1_555 Check

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

PLAT430_ALERT_2_B Short Inter D...A Contact O1W ..O4A . 2.83 Ang.
-1/2-y,1/2+x,-1+z = 2_454 Check

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

PLAT430_ALERT_2_B Short Inter D...A Contact O2B ..O10C . 2.76 Ang.
1/2+x,1/2-y,-1-z = 5_554 Check

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

PLAT430_ALERT_2_B Short Inter D...A Contact O2W ..O6C . 2.76 Ang.
x,y,z = 1_555 Check

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3A      ..O10C     .       2.79 Ang.
                                      -1/2+y,-1/2-x,1+z  =      4_446 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3C      ..O8B      .       2.74 Ang.
                                     -1/2-x,1/2+y,-1-z  =      7_454 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3W      ..O8C      .       2.71 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O4B      ..O6A      .       2.69 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O4W      ..O7B      .       2.68 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O4W      ..O5C      .       2.80 Ang.
                                    -1/2-x,-1/2+y,-1-z  =      7_444 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O5C      ..O9A      .       2.83 Ang.
                                     -1/2-y,1/2+x,-1+z  =      2_454 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O6A      ..O6W      .       2.71 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O6W      ..O6W      .       2.74 Ang.
                                                   y,x,-z  =      6_555 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O6W      ..O10B     .       2.80 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O7B      ..O8C      .       2.81 Ang.
                                               -1/2+y,-1/2-x,z  =      4_445 Check
```

Author Response: This alert is not relevant because it involves free water molecules with partial occupancy (50%).

```
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         11 Note
```

Alert level C

```
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.122
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.122 Report
PLAT220_ALERT_2_C NonSolvent   Resd 3  O   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C1C Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O4W      0.106 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O1A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O3A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O4A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O6A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O9A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O10A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O1B Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O2B Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O4B Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O7B Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O8B Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O10B Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O1C Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O3C Check
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PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O5C Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O6C Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O8C Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O10C Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01297 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H1B      ..H10B     .       1.98 Ang.
                                          -1/2-y,1/2+x,z  =      2_455 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
            C48 H56 O40
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.596          2 Report
PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on       Mo3      -1.09 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.44Ang From O1W     .       0.67 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.70Ang From O1W     .       0.63 eA-3
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C144 H168 Cl14 Mo6 O140
           Atom count from _chemical_formula_moiety:C144 H168 Cl14 Mo6 O138
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C144 H168 Cl14 Mo6 O140
           Atom count from the _atom_site data:  C144 H168 Cl14 Mo6 O138
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C144 H168 Cl14 Mo6 O140
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        288.00    288.00    0.00
          H        336.00    336.00    0.00
          Cl        28.00     28.00   -0.00
          Mo        12.00     12.00    0.00
          O        280.00    276.00    4.00
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          3 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      49.83 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Mo4        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo5        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl6        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl7        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl8        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl9        Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl10       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl11       Constrained at       0.15 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo2        Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2        Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4        Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo3        Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3        Constrained at        0.7 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of Cl5        Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mo1        Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1        Constrained at       0.85 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3W        Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )       4.80 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )       4.20 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )       4.20 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  7  )       6.80 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  8  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  9  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 10  )       0.50 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O1W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O2W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O3W Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         10 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.23 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      36.02 Deg.
              MO5  -CL4  -MO1     3_455   1_555   2_455 ......     #  562 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      35.90 Deg.
              MO5  -CL4  -MO1     2_455   1_555   1_555 ......     #  563 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.13 Deg.
              MO5  -CL4  -MO2     3_455   1_555   1_555 ......     #  566 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.08 Deg.
              MO5  -CL4  -MO2     2_455   1_555   1_555 ......     #  567 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      39.00 Deg.
              MO5  -CL4  -CL10    2_455   1_555   1_555 ......     #  570 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      38.90 Deg.
              MO5  -CL4  -CL10    3_455   1_555   2_455 ......     #  572 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      31.40 Deg.
              CL9  -CL4  -CL8     1_555   1_555   1_555 ......     #  594 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      32.88 Deg.
              MO4  -CL5  -MO1     4_445   1_555   1_555 ......     #  598 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.35 Deg.
              MO4  -CL5  -MO1     1_555   1_555   2_455 ......     #  600 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      34.68 Deg.
              MO4  -CL5  -MO3     4_445   1_555   1_555 ......     #  602 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      34.66 Deg.
              MO4  -CL5  -MO3     1_555   1_555   1_555 ......     #  603 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.30 Deg.
              MO4  -CL5  -CL7     4_445   1_555   4_445 ......     #  606 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.20 Deg.
              MO4  -CL5  -CL7     1_555   1_555   1_555 ......     #  608 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      30.20 Deg.
              CL7  -CL5  -CL6     4_445   1_555   4_445 ......     #  628 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      30.40 Deg.
              CL7  -CL5  -CL6     1_555   1_555   1_555 ......     #  629 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      31.60 Deg.
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              CL8  -CL5  -CL9     1_555   1_555   1_555 ......     #  634 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.30 Deg.
              MO2  -CL10 -MO5     1_555   1_555   1_555 ......     #  651 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.30 Deg.
              MO2  -CL10 -MO5     1_555   1_555   3_455 ......     #  652 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      24.40 Deg.
              MO5  -CL10 -MO1     2_455   1_555   1_555 ......     #  657 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      44.90 Deg.
              MO5  -CL10 -MO5     2_455   1_555   3_455 ......     #  659 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.90 Deg.
              MO3  -CL7  -MO4     1_555   1_555   2_455 ......     #  681 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.60 Deg.
              MO3  -CL7  -MO4     1_555   1_555   4_445 ......     #  682 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      23.40 Deg.
              MO4  -CL7  -MO1     1_555   1_555   2_455 ......     #  684 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      43.70 Deg.
              MO4  -CL7  -MO4     1_555   1_555   4_445 ......     #  686 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      44.30 Deg.
              MO4  -CL7  -MO4     1_555   1_555   2_455 ......     #  687 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      34.80 Deg.
              MO1  -CL8  -MO5     1_555   1_555   2_455 ......     #  708 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      28.75 Deg.
              MO1  -CL8  -MO4     2_455   1_555   1_555 ......     #  709 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.40 Deg.
              MO1  -CL8  -MO4     1_555   1_555   4_445 ......     #  710 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      39.40 Deg.
              MO4  -CL8  -MO4     4_445   1_555   1_555 ......     #  717 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      40.80 Deg.
              CL5  -CL8  -MO4     1_555   1_555   1_555 ......     #  724 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      43.10 Deg.
              CL9  -CL8  -MO1     1_555   1_555   2_455 ......     #  727 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      34.80 Deg.
              MO1  -CL9  -MO5     2_455   1_555   3_455 ......     #  736 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      29.00 Deg.
              MO1  -CL9  -MO4     1_555   1_555   4_445 ......     #  738 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      32.90 Deg.
              MO1  -CL9  -MO4     2_455   1_555   1_555 ......     #  740 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      39.50 Deg.
              MO4  -CL9  -MO4     1_555   1_555   4_445 ......     #  745 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.40 Deg.
              CL5  -CL9  -MO4     1_555   1_555   4_445 ......     #  753 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      43.50 Deg.
              CL8  -CL9  -MO1     1_555   1_555   1_555 ......     #  756 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      23.80 Deg.
              CL7  -CL6  -MO4     1_555   1_555   1_555 ......     #  765 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      16.70 Deg.
              CL10 -CL11 -MO5     1_555   1_555   2_455 ......     #  768 Check
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set     Please Do !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C48 H56 O40
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              C48 H56 O40
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
              Cl24 Mo8
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
              Cl5 Mo
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
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             Cl5 Mo
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
             Cl4 Mo4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          9 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         10 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         11 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         12 Note
             O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         13 Note
             O
PLAT791_ALERT_4_G Model has Chirality at C1B         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C2A         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C2B         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C2C         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C3A         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C3B         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C3C         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C4A         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C4B         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C4C         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C5A         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C5B         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C5C         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C6A         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C6C         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C7B         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C8A         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C8B         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C8C         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C9A         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C9B         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C9C         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C10A        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C10B        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C10C        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C11A        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C11B        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C11C        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C12A        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C12C        (Sohnke SpGr)          S Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        76% Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
20 **ALERT level B** = A potentially serious problem, consider carefully
32 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
133 **ALERT level G** = General information/check it is not something unexpected

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

```
  53 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
 119 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: w

Bond precision: C-C = 0.0513 A Wavelength=0.71073

Cell: a=35.7254(5) b=35.7254(5) c=34.3472(12)
alpha=90 beta=90 gamma=90
Temperature: 130 K

	Calculated	Reported
Volume	43838(2)	43837(2)
Space group	I 4 2 2	I 4 2 2
Hall group	I 4 2	I 4 2
Moiety formula	4(C48 H56 O40), 3(Cl14 W6), 29.6(O)	?
Sum formula	C192 H224 Cl42 O189.60 W18	C192 H224 Cl42 O189.60 W18
Mr	10363.35	10363.50
Dx,g cm-3	1.570	1.570
Z	4	4
Mu (mm-1)	5.035	5.035
F000	19755.2	19755.0
F000'	19732.13	
h,k,lmax	40,40,39	40,38,39
Nref	16872[9129]	16744
Tmin,Tmax	0.310,0.284	0.479,1.000
Tmin'	0.261	

Correction method= # Reported T Limits: Tmin=0.479 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.83/0.99 Theta(max)= 23.817

R(reflections)= 0.0657(10452) wR2(reflections)= 0.1922(16744)

S = 1.026 Npar= 958

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

PLAT430_ALERT_2_A Short Inter D...A Contact O3W ..O3W . 1.99 Ang.
1/2-y,1/2-x,3/2-z = 16_556 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_A Short Inter D...A Contact O3W ..O8W . 2.27 Ang.
x,y,z = 1_555 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_A Short Inter D...A Contact O8W ..O9W . 1.84 Ang.
y,1-x,z = 4_565 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in Structure ..... ! Check

Author Response: The full complex composition was found with elemental analysis

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on W6 2.61 eA-3

Author Response: Residual density without any sense

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on W3 2.47 eA-3

Author Response: Residual density without any sense

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on W1 2.17 eA-3

Author Response: Residual density without any sense

Alert level B

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5682
PLAT023_ALERT_3_B Resolution (too) Low [sin(theta)/Lambda < 0.6]..       0.57 Ang-1
PLAT035_ALERT_1_B _chemical_absolute_configuration Info  Not Given     Please Do !
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          5 Report
              O38A      O39B      C39A      C42B      C48
PLAT234_ALERT_4_B Large Hirshfeld Difference C14      --C15      .       0.26 Ang.
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.05128 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact  O1W      ..O2W      .       2.59 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O1W      ..O14      .       2.69 Ang.
                                                   y,1-x,z  =      4_565 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O2       ..O2       .       2.76 Ang.
                                         1/2+y,-1/2+x,3/2-z  =     15_546 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O2W      ..O7       .       2.62 Ang.
                                                   y,1-x,z  =      4_565 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O2W      ..O14      .       2.72 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3       ..O37      .       2.74 Ang.
                                         1/2-y,1/2-x,3/2-z  =     16_556 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3W      ..O22      .       2.60 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O4W ..O12 . 2.79 Ang.
x,y,z = 1_555 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O6W ..O16 . 2.73 Ang.
1-y,x,z = 3_655 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O6W ..O9 . 2.75 Ang.
x,y,z = 1_555 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O7 ..O17 . 2.76 Ang.
1-y,x,z = 3_655 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O7W ..O8 . 2.75 Ang.
x,y,z = 1_555 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O8W ..O33 . 2.76 Ang.
-y,x,z = 3_555 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O9 ..O36 . 2.84 Ang.
1/2-y,1/2-x,3/2-z = 16_556 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O13 ..O26 . 2.79 Ang.
1/2-y,1/2-x,3/2-z = 16_556 Check

Author Response: Disordered water molecules of crystallization with low occupancies

PLAT430_ALERT_2_B Short Inter D...A Contact O18 ..O23 . 2.79 Ang.
1/2-y,1/2-x,3/2-z = 16_556 Check

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O19      ..O14W     .       2.68 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O19      ..O15W     .       2.72 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O39B     ..O16W     .       2.84 Ang.
                                                     x,y,z  =      1_555 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         39 Note
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.31Ang From W4              3.01 eA-3
```

Author Response: Residual density without any sense

```
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on        W2       1.89 eA-3
```

Author Response: Residual density without any sense

```
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on        W4       1.73 eA-3
```

Author Response: Residual density without any sense

Alert level C

```
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ........     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.04 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          4 Check
             O5W     O6W     O10W    O11W
PLAT213_ALERT_2_C Atom O5              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C23             has ADP max/min Ratio .....        3.9 oblate
PLAT213_ALERT_2_C Atom C43             has ADP max/min Ratio .....        3.6 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.3 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range       5.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O27 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C42B Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C46 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C28 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C34 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C39A Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.3 Note
```

```
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........         O2 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........         O3 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........         O7 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........         O8 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........         O9 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O12 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O13 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O14 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O16 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O18 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O19 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O22 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O23 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O25 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O26 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O29 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O31 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O33 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O36 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........        O37 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........       O38A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........       O39B Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........       O40A Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........       O40B Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C17      - C18      .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C34      - C35      .       1.35 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C38      - C39      .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C39A     - C49      .       1.39 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H17A     ..H20A     .       1.96 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H29A     ..H32A     .       1.99 Ang.
                                                     x,y,z  =      1_555 Check
PLAT430_ALERT_2_C Short Inter D...A Contact  O2       ..O2       .       2.85 Ang.
                                    1/2-y,1/2-x,3/2-z  =     16_556 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O3       ..O13W     .       2.85 Ang.
                                    1/2+x,1/2-y,3/2-z  =     14_556 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O4       ..O14W     .       2.89 Ang.
                                                  1-y,x,z  =      3_655 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O5W      ..O25      .       2.88 Ang.
                                    1/2+x,1/2-y,3/2-z  =     14_556 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT430_ALERT_2_C Short Inter D...A Contact  O7W      ..O23      .       2.89 Ang.
                                    1/2+x,1/2-y,3/2-z  =     14_556 Check
```

Author Response: Disordered water molecules of crystallization with low occupancies

```
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -1.238 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.568         20 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.26Ang From Cl3              1.87 eA-3
```

Author Response: Residual density without any sense

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.12Ang From W4               1.78 eA-3
```

Author Response: Residual density without any sense

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.37Ang From W4               1.76 eA-3
```

Author Response: Residual density without any sense

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.27Ang From W5               1.72 eA-3
```

Author Response: Residual density without any sense

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.32Ang From W5               1.69 eA-3
```

Author Response: Residual density without any sense

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.14Ang From W1               1.65 eA-3
```

Author Response: Residual density without any sense

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.16Ang From W5               1.56 eA-3
```

Author Response: Residual density without any sense

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.28Ang From W4               1.52 eA-3
```

Author Response: Residual density without any sense

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         12 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
```

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     957.94 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O40A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O40B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A1       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A2       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1BA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1BB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5W        Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6W        Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O9W        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10W       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O11W       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O13W       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O14W       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O15W       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O16W       Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O17W       Constrained at        0.4 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 14  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 16  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 17  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 18  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 19  )        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  7  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  8  )       0.60 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  9  )       0.70 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 10  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 11  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 12  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 13  )       0.40 Check
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```
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 14  )       0.70 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 15  )       0.40 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 16  )       0.40 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 17  )       0.30 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 18  )       0.20 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 19  )       0.20 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O1W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O2W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O3W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O4W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O5W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O6W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O7W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O8W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O9W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O10W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O11W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O13W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O14W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O15W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O16W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O17W Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         4 Note
PLAT791_ALERT_4_G Model has Chirality at C1          (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C2          (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C3          (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C4          (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C5          (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C8          (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C9          (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C10         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C12         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C13         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C14         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C15         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C16         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C17         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C18         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C20         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C21         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C23         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C24         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C25         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C30         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C31         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C32         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C34         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C35         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C36         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C37         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C38         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C39         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C40         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C41         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C43         (Sohnke SpGr)         R Verify
PLAT791_ALERT_4_G Model has Chirality at C45         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C46         (Sohnke SpGr)         R Verify
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PLAT791_ALERT_4_G Model has Chirality at C47         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C48         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C49         (Sohnke SpGr)          R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        55 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        69 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ         2 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
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```
  7 ALERT level A = Most likely a serious problem - resolve or explain
 29 ALERT level B = A potentially serious problem, consider carefully
 62 ALERT level C = Check. Ensure it is not caused by an omission or oversight
127 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
110 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
100 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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checkCIF publication errors

Alert level A

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PUBL004_ALERT_1_A  The contact author's name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
           e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
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).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
```

```
  7 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.

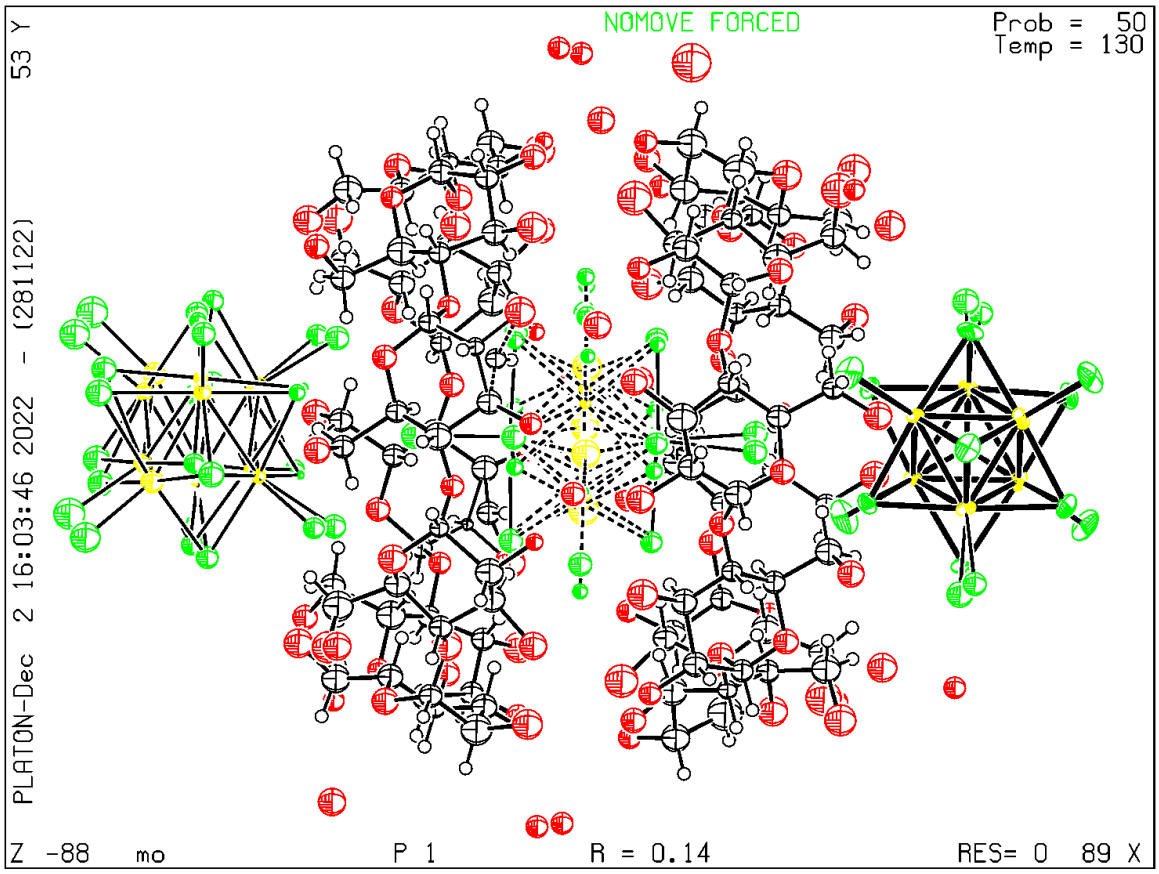
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_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: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_DIFF005_iaa065_0m_pl
;
PROBLEM: _diffrn_measurement_method is missing
RESPONSE: ...
;
# end Validation Reply Form
```

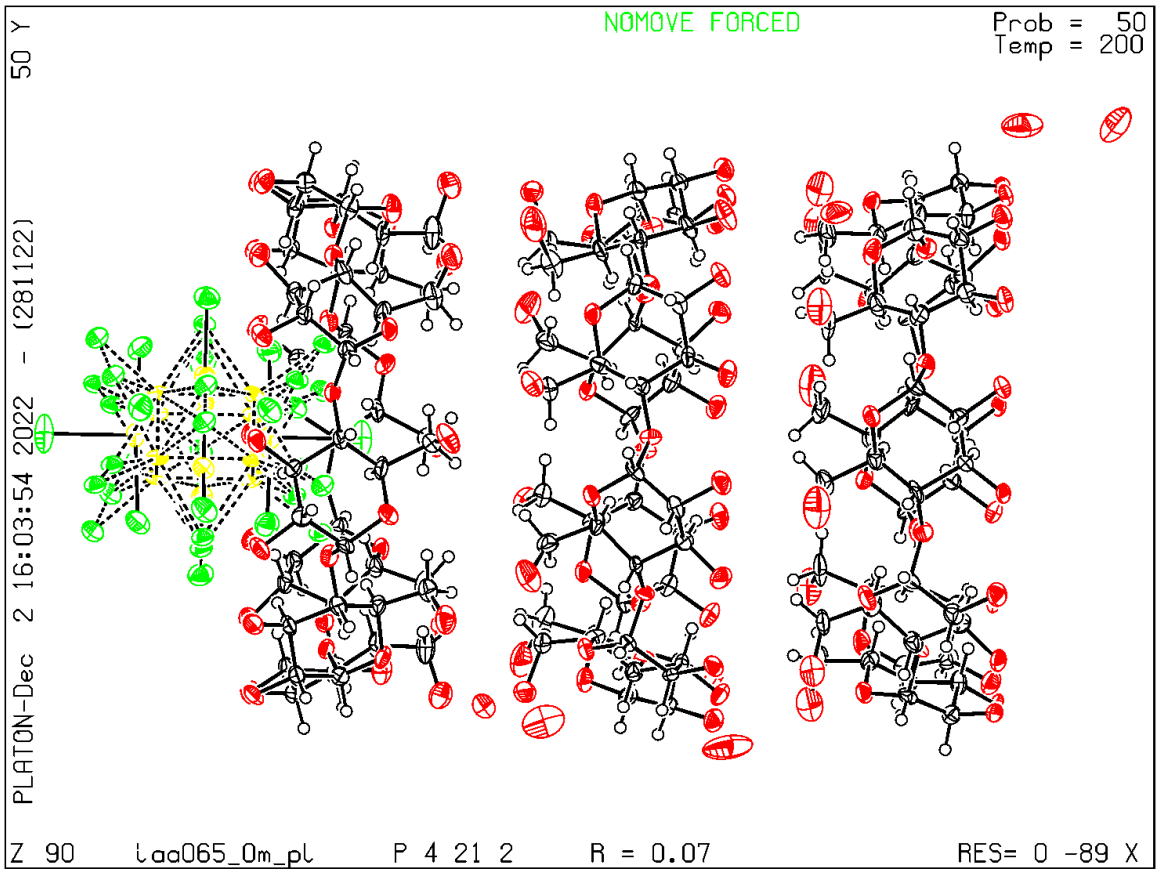
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you 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 28/11/2022; check.def file version of 09/08/2022

Datablock mo - ellipsoid plot



Datablock iaa065_0m_pl - ellipsoid plot



Datablock w - ellipsoid plot

