checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ZL321F4REDO2, ZL359F3F, cu_zl359f4clean_0m_a, mo_PM012F3_0m_L, mo_PM012F7_0m_a, mo_ZL313F4_0m_a, mo_ZL321F4_1_0m_a

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_PM012F3_0m_L

```
Bond precision:  C-C = 0.0036 A          Wavelength=0.71073

Cell:           a=52.4504(19)    b=7.4685(3)         c=25.3205(9)
                alpha=90         beta=114.770(1)     gamma=90
Temperature:    150 K

                Calculated                Reported
Volume          9006.2(6)                 9006.1(6)
Space group     C 2/c                     C 2/c
Hall group      -C 2yc                    -C 2yc
Moiety formula  C20 H18 Cr O6 S3          ?
Sum formula     C20 H18 Cr O6 S3          C20 H18 Cr O6 S3
Mr              502.52                    502.52
Dx,g cm-3       1.482                     1.482
Z               16                        16
Mu (mm-1)       0.819                     0.819
F000            4128.0                    4128.0
F000'           4140.79
h,k,lmax        61,8,29                   61,8,29
Nref            7679                      7672
Tmin,Tmax       0.734,0.912               0.634,0.714
Tmin'           0.717

Correction method= # Reported T Limits: Tmin=0.634 Tmax=0.714
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 24.713

R(reflections)= 0.0321( 6651)     wR2(reflections)= 0.0994( 7672)

S = 1.039                 Npar= 555
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5882
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem       c/2         91 %Fit
```

Author Response: See detailed response below under _refine_special_details.

```
PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range        3.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    S22      --C35      .        6.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    S22      --C36      .        6.6 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cr21     --C26      .        5.7 s.u.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588          3 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          6 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      15.88 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/c       I2/a Note
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          4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O21      --C21      .        6.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C37      --C38      .       10.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C38      --C39      .       13.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C39      --C40      .       21.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O2       --C2       .        5.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O5       --C5       .        5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr21     --C21      .        8.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr21     --C22      .        7.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr21     --C23      .        6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr21     --C24      .        7.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr21     --C25      .        7.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C1       .        6.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C2       .        9.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C3       .        8.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C4       .        7.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C5       .        8.7 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        13% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         41 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         78% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          9 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  30 ALERT level G = General information/check it is not something unexpected

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

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

Datablock: mo_PM012F7_0m_a

```
Bond precision:  C-C = 0.0040 A          Wavelength=0.71073

Cell:          a=7.7699(7)         b=10.8891(11)    c=17.2416(17)
               alpha=104.632(4)    beta=94.044(4)   gamma=96.766(4)
Temperature:   150 K
```

	Calculated	Reported
Volume	1394.0(2)	1394.0(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H12 Cr2 O12 S3	?
Sum formula	C24 H12 Cr2 O12 S3	C24 H12 Cr2 O12 S3
Mr	692.52	692.52
Dx,g cm-3	1.650	1.650
Z	2	2
Mu (mm-1)	1.066	1.066
F000	696.0	696.0
F000’	698.37	
h,k,lmax	9,12,20	9,12,20
Nref	4754	4749
Tmin,Tmax	0.747,0.887	0.760,1.000
Tmin’	0.724	

```
Correction method= # Reported T Limits: Tmin=0.760 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 24.712

R(reflections)= 0.0309( 3603)     wR2(reflections)= 0.0830( 4749)

S = 1.001                 Npar= 372
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range       4.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       4.8 Ratio
```

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.195 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588          2 Report
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.004 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C1       .        5.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C2       .        6.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C3       .        7.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C4       .        8.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C5       .        6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr2      --C18      .        7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr2      --C19      .        6.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr2      --C20      .        5.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr2      --C21      .        7.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr2      --C22      .        6.2 s.u.
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        53% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: mo_ZL313F4_0m_a

```
Bond precision:  C-C = 0.0031 A          Wavelength=0.71073

Cell:          a=7.4794(7)        b=11.9763(11)    c=12.1963(12)
               alpha=110.742(3)   beta=91.017(3)   gamma=103.342(3)
Temperature:   150 K
```

	Calculated	Reported
Volume	988.15(16)	988.15(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H13 Cr N O5 S3	?
Sum formula	C18 H13 Cr N O5 S3	C9 H6.50 Cr0.50 N0.50 O2.50 S1.50
Mr	471.47	235.74
Dx,g cm-3	1.585	1.585
Z	2	4
Mu (mm-1)	0.926	0.926
F000	480.0	480.0
F000’	481.57	
h,k,lmax	9,14,15	9,14,15
Nref	3885	3883
Tmin,Tmax	0.875,0.973	0.665,1.000
Tmin’	0.744	

Correction method= # Reported T Limits: Tmin=0.665 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.022

R(reflections)= 0.0285(3429) wR2(reflections)= 0.0722(3883)

S = 1.025 Npar= 244

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT220_ALERT_2_C	NonSolvent Resd 1	C	Ueq(max) / Ueq(min) Range		3.9	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1	H	Uiso(max)/Uiso(min) Range		4.8	Ratio

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Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				2	Note
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...				0.50	Check
PLAT154_ALERT_1_G	The s.u.’s on the Cell Angles are Equal ..(Note)				0.003	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				1	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	S3B	--C13	.	8.9	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	S3B	--C15	.	6.6	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O2	--C2	.	5.4	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O3	--C3	.	5.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C1	.	9.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C2	.	10.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C3	.	9.8	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C4	.	8.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C5	.	7.9	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C16	.	8.9	s.u.

```
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         7% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          1 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15      --C14B           1.84 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         1 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         5 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         2 Check
```

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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  24 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: mo_ZL321F4_1_0m_a

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=6.8382(7) b=9.8055(10) c=14.0893(13)
       alpha=104.167(3) beta=97.269(3) gamma=104.205(3)
Temperature: 150 K

	Calculated	Reported
Volume	870.30(15)	870.30(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H8 Cr O6 S3	?
Sum formula	C16 H8 Cr O6 S3	C16 H8 Cr O6 S3
Mr	444.40	444.40
Dx,g cm-3	1.696	1.696
Z	2	2
Mu (mm-1)	1.048	1.048
F000	448.0	448.0
F000′	449.58	
h,k,lmax	8,11,16	8,11,16
Nref	2975	2957
Tmin,Tmax	0.675,0.778	0.442,1.000
Tmin′	0.617	

Correction method= # Reported T Limits: Tmin=0.442 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 24.712

R(reflections)= 0.0280(2696) wR2(reflections)= 0.0692(2957)

S = 1.047 Npar= 237

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cr1      --C6       .        6.2 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         17 Report
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C1       .        7.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C2       .        7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C3       .        6.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C4       .        8.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cr1      --C5       .        7.4 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C15      ..C15             3.19 Ang.
                                          1-x,2-y,1-z  =      2_676 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        82% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          5 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

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

Datablock: ZL321F4REDO2

Bond precision: C-C = 0.0102 A Wavelength=1.54184

Cell: a=7.6425(1) b=9.4015(2) c=16.0890(3)
alpha=94.709(1) beta=99.669(1) gamma=90.360(1)
Temperature: 150 K

	Calculated	Reported
Volume	1135.51(4)	1135.50(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C16 H8 O6 S3 W), C6 O6 W?	
Sum formula	C38 H16 O18 S6 W3	C19 H8 O9 S3 W1.50
Mr	1504.39	752.21
Dx,g cm-3	2.200	2.200
Z	1	2
Mu (mm-1)	16.963	16.963
F000	706.0	706.0
F000'	693.28	
h,k,lmax	9,11,19	9,11,19
Nref	4478	4461
Tmin,Tmax	0.002,0.009	0.173,1.000
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.173 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 72.119

R(reflections)= 0.0491(3867) wR2(reflections)= 0.1235(4461)

S = 1.045 Npar= 297

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.01A From W2 2.66 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.07A From W1 2.62 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.04A From W1 2.55 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

Alert level C

```
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01022 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.032 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          7 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  2.29A   From O3              2.24 eA-3
```

Author Response: The residual density peak could not be modelled as any chemically sens

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  2.20A   From C5              2.11 eA-3
```

Author Response: The residual density peak could not be modelled as any chemically sens

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  2.34A   From O9              2.06 eA-3
```

Author Response: The residual density peak could not be modelled as any chemically sens

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.80A   From W1             -2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.90A   From W2             -1.89 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.07A   From W1             -1.72 eA-3
```

Alert level G

```
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         1 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
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        10 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

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

Datablock: ZL359F3F

Bond precision: C-C = 0.0145 A Wavelength=0.71073

Cell:	a=19.5378(6)	b=6.4155(2)	c=15.0044(4)
	alpha=90	beta=99.372(3)	gamma=90
Temperature:	150 K		

	Calculated	Reported
Volume	1855.62(10)	1855.62(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H9 N O5 S3 W	?
Sum formula	C16 H9 N O5 S3 W	C16 H9 N O5 S3 W
Mr	575.26	572.25
Dx,g cm-3	2.059	2.048
Z	4	4
Mu (mm-1)	6.589	6.589
F000	1096.0	1084.0
F000’	1094.66	
h,k,lmax	24,8,18	24,8,18
Nref	3790	3788
Tmin,Tmax	0.115,0.249	0.642,1.000
Tmin’	0.069	

Correction method= # Reported T Limits: Tmin=0.642 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.370

R(reflections)= 0.0528(3529) wR2(reflections)= 0.1438(3788)

S = 1.150 Npar= 237

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.58A From O5 3.03 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.82A From W1 -2.68 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.85A   From W1   -2.58 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

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Alert level C

CHEMW01_ALERT_1_C The difference between the given and expected weight for
compound is greater 1 mass unit. Check that all hydrogen
atoms have been taken into account.
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given   0.142
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   3.01 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   S2 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0145 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   4.141 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.94A   From W1   2.13 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.26A   From C6   2.07 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.96A   From W1   2.03 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.01A   From C3   2.01 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.99A   From W1   1.84 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.08A   From C5   1.74 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 2.02A   From C15   -1.67 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

PLAT977_ALERT_2_C Check Negative Difference Density on H8B   -0.34 eA-3

Alert level G

PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.142 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	17.32 Why ?
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	2 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note
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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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: cu_zl359f4clean_0m_a

Bond precision: C-C = 0.0164 A Wavelength=1.54178

Cell: a=6.5741(5) b=15.1714(10) c=32.440(2)
       alpha=90 beta=95.543(3) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3220.4(4)	3220.4(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C24 H14 N2 O10 S3 W2	C24 H14 N2 O10 S3 W2
Sum formula	C24 H14 N2 O10 S3 W2	C24 H14 N2 O10 S3 W2
Mr	954.23	954.25
Dx,g cm-3	1.968	1.968
Z	4	4
Mu (mm-1)	15.285	15.285
F000	1792.0	1792.0
F000'	1756.45	
h,k,lmax	8,18,40	8,18,40
Nref	6342	6328
Tmin,Tmax	0.196,0.290	0.457,0.754
Tmin'	0.004	

Correction method= # Reported T Limits: Tmin=0.457 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 72.118

R(reflections)= 0.0582(4414) wR2(reflections)= 0.2062(6328)

S = 1.196 Npar= 374

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
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Author Response: No mentionable electron density in the final Fourier difference map is

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Alert level B
PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.83A From W2 -2.74 eA-3

Author Response: The residual density peak could not be modelled as any chemically sens

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Alert level C
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.130
PLAT234_ALERT_4_C Large Hirshfeld Difference W1 --C1 . 0.22 Ang.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference W2       --C24      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1       --C1       .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1       --C8       .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11      --C14      .       0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         S1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         S2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         S3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         W1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         W2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01644 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     14.670 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.638 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          4 Report
PLAT924_ALERT_1_C The Reported and Calculated Rho(min) Differ by .       1.05 eA-3
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by .       1.37 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.87A   From W1            -2.27 eA-3
```

Author Response: The residual density peak could not be modelled as any chemically sens

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.86A   From W2            -2.10 eA-3
```

Author Response: The residual density peak could not be modelled as any chemically sens

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.94A   From W1            -1.93 eA-3
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Author Response: The residual density peak could not be modelled as any chemically sens

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.51A   From C3            -1.69 eA-3
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Author Response: The residual density peak could not be modelled as any chemically sens

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.96A   From C22           -1.63 eA-3
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Author Response: The residual density peak could not be modelled as any chemically sens

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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        10 Note
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......    Please Check
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........     0.130 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     38.71 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         4 Report
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         2 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        8 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        11 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         2 Note
```

```
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

```
   1 ALERT level A = Most likely a serious problem - resolve or explain
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  23 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
   8 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

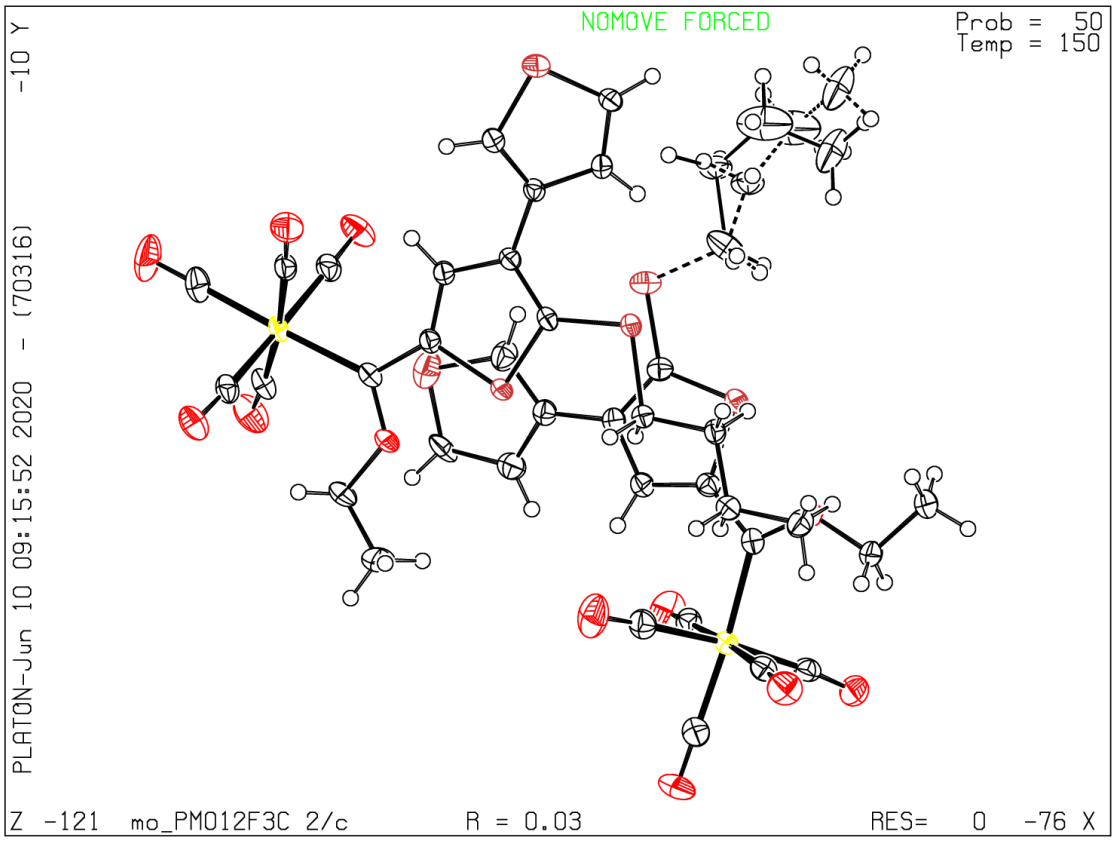
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

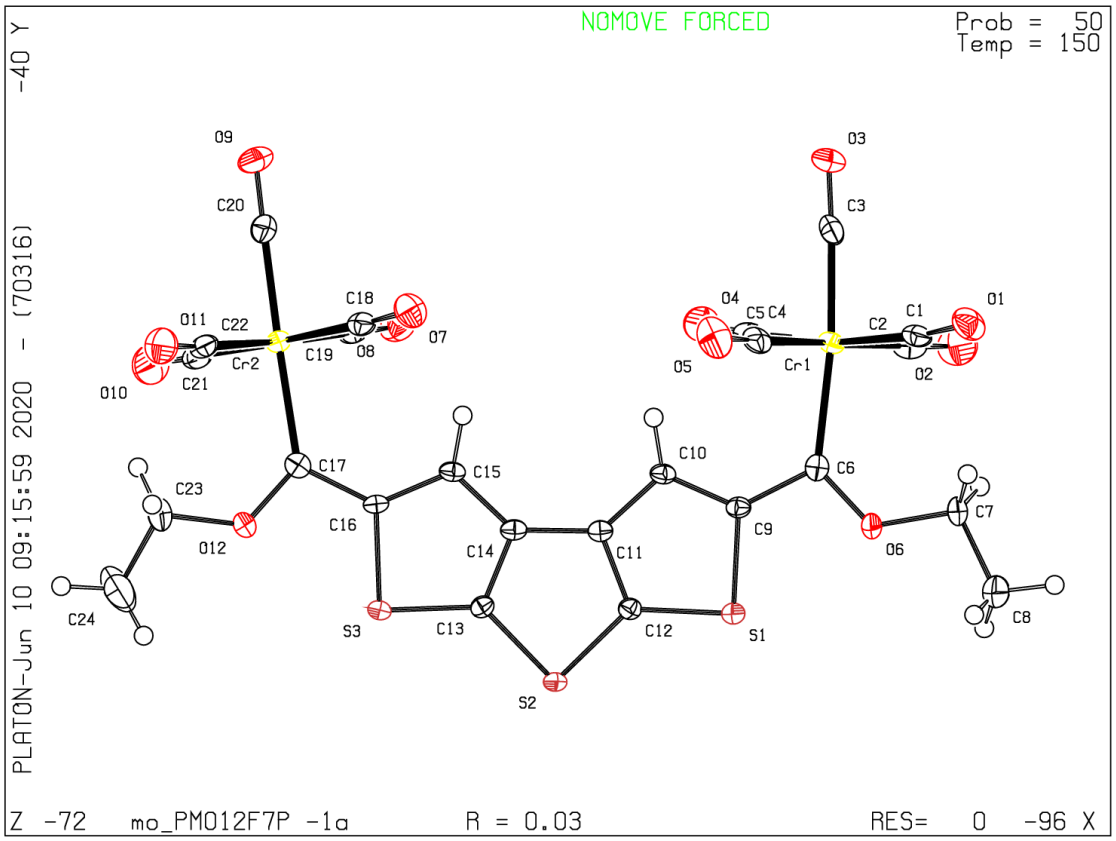
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 04/06/2020; check.def file version of 02/06/2020

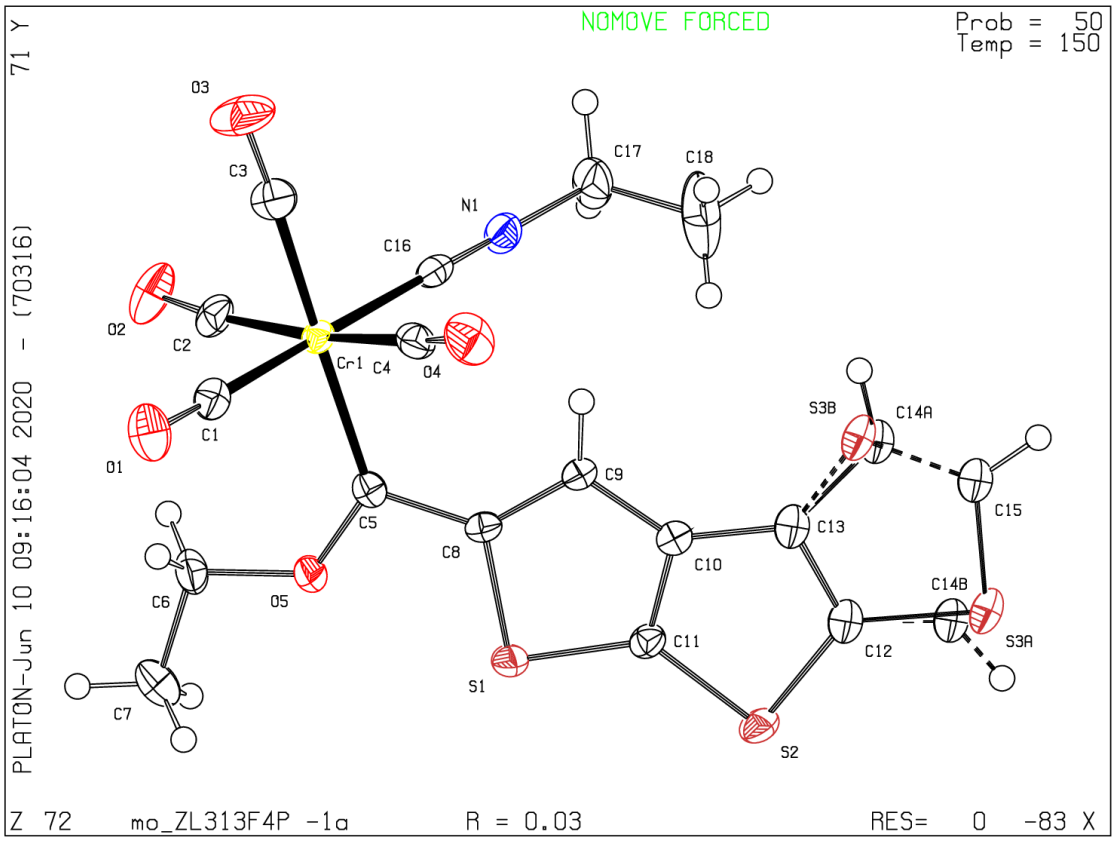
Datablock mo_PM012F3_0m_L - ellipsoid plot



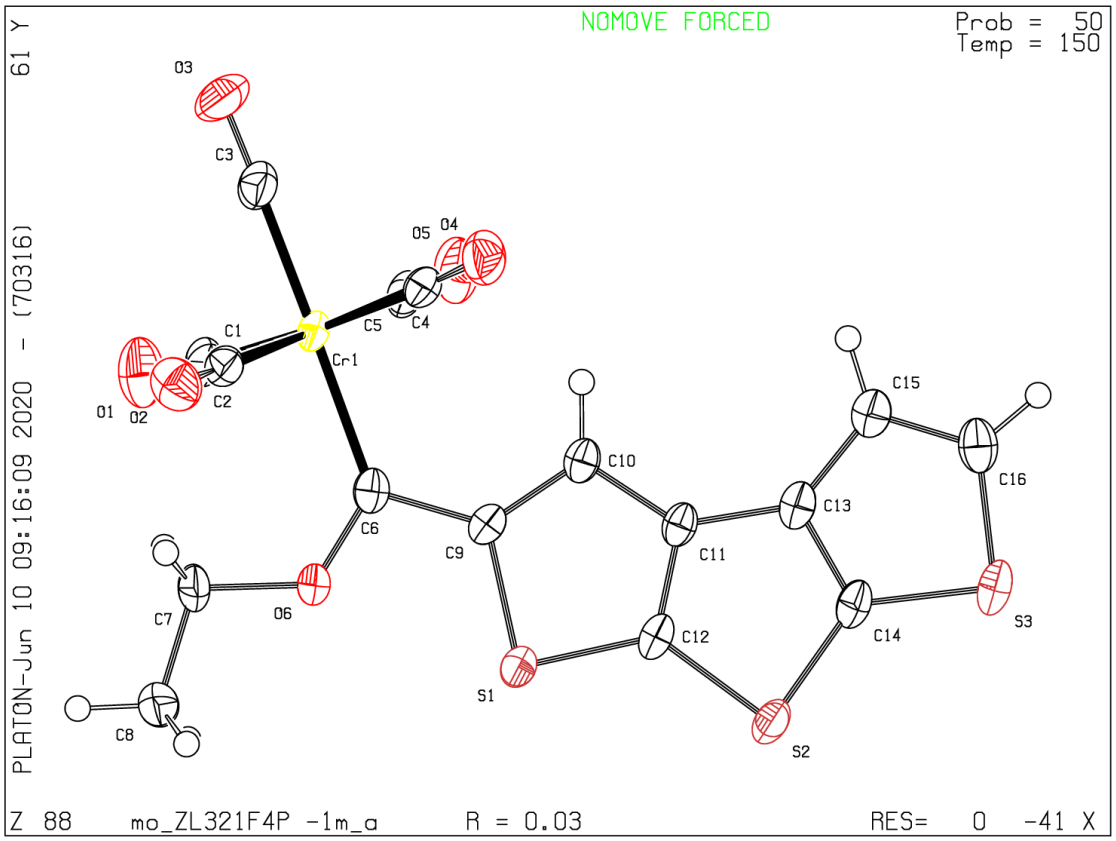
Datablock mo_PM012F7_0m_a - ellipsoid plot



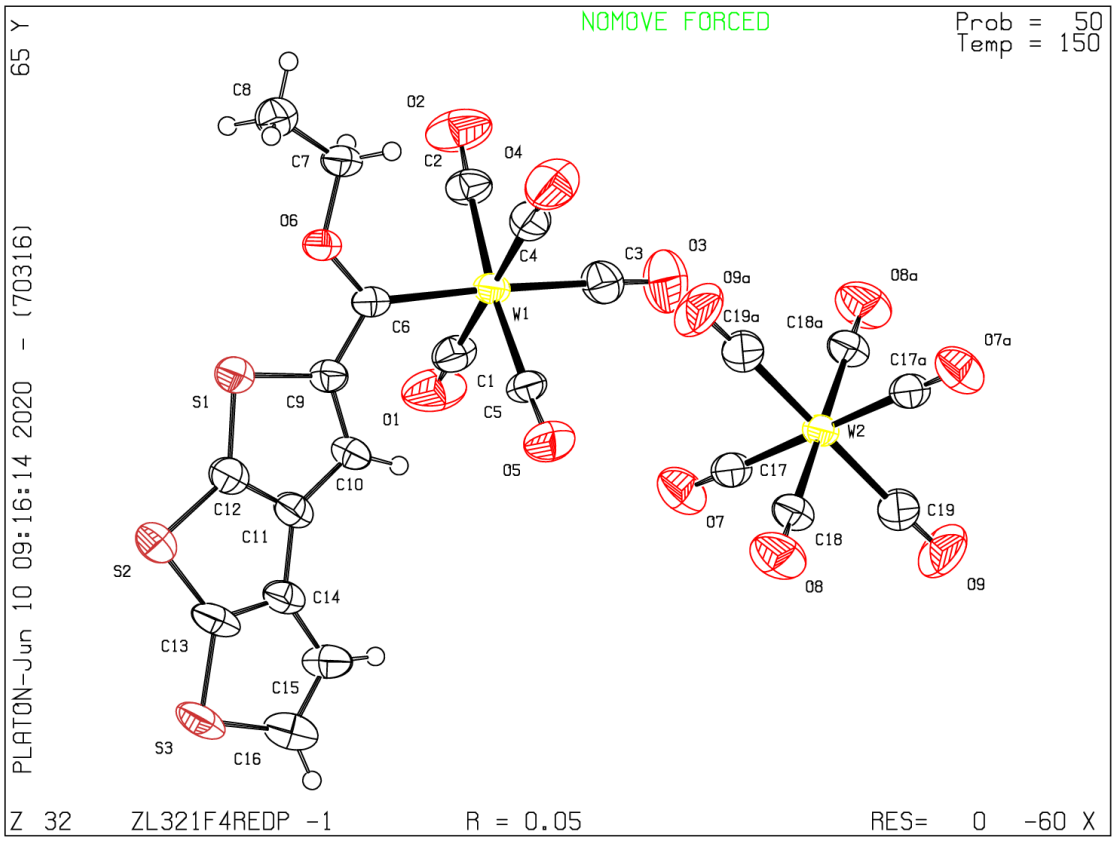
Datablock mo_ZL313F4_0m_a - ellipsoid plot



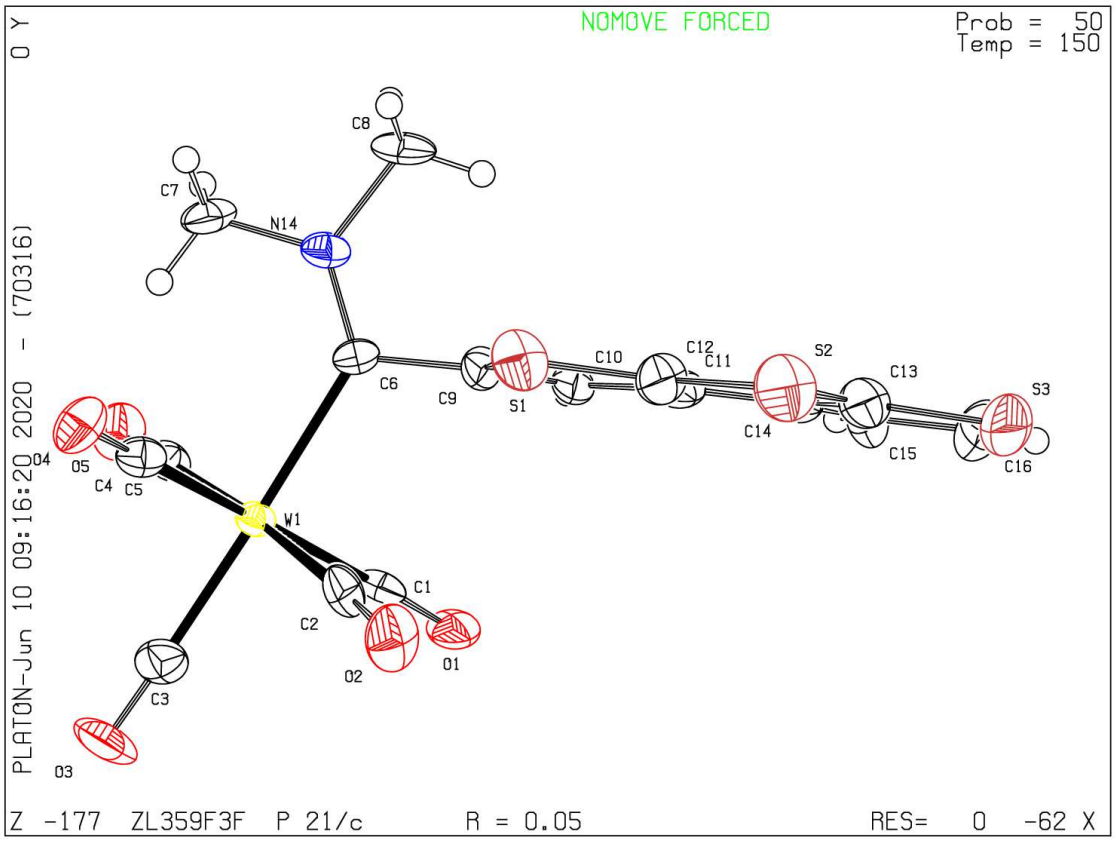
Datablock mo_ZL321F4_1_0m_a - ellipsoid plot



Datablock ZL321F4REDO2 - ellipsoid plot



Datablock ZL359F3F - ellipsoid plot



Datablock cu_zl359f4clean_0m_a - ellipsoid plot