checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mw_173_8m, mw_175_1m, mw_175_6m, mw_175_7film, mw_175filfilm

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: mw_175_7film

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Bond precision:   C-C = 0.0021 A          Wavelength=0.71073

Cell:             a=13.5750(8)     b=15.5145(9)     c=19.4970(11)
                  alpha=90         beta=90          gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           4106.3(4)                 4106.2(4)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C45 H54 In N3 O2          ?
Sum formula      C45 H54 In N3 O2          C45 H54 In N3 O2
Mr               783.73                    783.73
Dx,g cm-3        1.268                     1.268
Z                4                         4
Mu (mm-1)        0.614                     0.614
F000             1640.0                    1640.0
F000'            1637.61
h,k,lmax         22,25,32                  22,25,32
Nref             20021[ 10841]             19997
Tmin,Tmax        0.854,0.935               0.710,0.750
Tmin'            0.854

Correction method= # Reported T Limits: Tmin=0.710 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 1.84/1.00        Theta(max)= 36.386

R(reflections)= 0.0210( 18961)                wR2(reflections)=
                                              0.0512( 19997)
S = 1.049                  Npar= 471
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.19 Report
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        4.5 Ratio
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Alert level G

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  In1      --N3       .        8.4 s.u.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          7 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         17 Info
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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: mw_175_6m

Bond precision: C-C = 0.0034 A Wavelength=0.71073

Cell:	a=16.620(5)	b=18.867(6)	c=19.008(6)
	alpha=90	beta=99.398(5)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	5880(3)	5880(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C114 H122 Al2 N4 O8, 4(C7 H8)	?
Sum formula	C142 H154 Al2 N4 O8	C142 H154 Al2 N4 O8
Mr	2098.65	2098.64
Dx,g cm-3	1.185	1.185
Z	2	2
Mu (mm-1)	0.086	0.086
F000	2248.0	2248.0
F000'	2249.09	
h,k,lmax	22,25,25	22,25,25
Nref	14720	14551
Tmin,Tmax	0.982,0.986	0.630,0.750
Tmin'	0.982	

Correction method= # Reported T Limits: Tmin=0.630 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 28.368

R(reflections)= 0.0689(9783) wR2(reflections)= 0.1546(14551)

S = 1.126 Npar= 719

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 10.902 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.034 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note

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Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.80 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1 --O3 . 5.6 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 30 Note
PLAT793_ALERT_4_G Model has Chirality at C30 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C31 (Centro SPGR) S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Al1 (III) . 2.84 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 165 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 13 Info

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1 ALERT type 5 Informative message, check

Datablock: mw_175_1m

Bond precision: C-C = 0.0018 A Wavelength=1.54178

Cell: a=12.3771(5) b=12.9748(5) c=24.5551(10)
alpha=97.796(2) beta=96.978(2) gamma=106.7538(19)
Temperature: 100 K

	Calculated	Reported
Volume	3687.0(3)	3687.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C72 H92 Al2 N4 O2, 2(C6 H6)	?
Sum formula	C84 H104 Al2 N4 O2	C84 H104 Al2 N4 O2
Mr	1255.68	1255.67
Dx,g cm-3	1.131	1.131
Z	2	2
Mu (mm-1)	0.725	0.725
F000	1356.0	1356.0
F000'	1360.13	
h,k,lmax	15,16,31	15,16,31
Nref	16176	15992
Tmin,Tmax	0.845,0.957	0.680,0.750
Tmin'	0.845	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 80.424

R(reflections)= 0.0342(13579)

wR2(reflections)= 0.0889(15992)

S = 1.028 Npar= 904

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 4.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.7 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report

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Alert level G

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 3) 6.41 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4) 5.59 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 36 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 108 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 178 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 16 Info

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

Datablock: mw_175filfilm

Bond precision: C-C = 0.0024 A Wavelength=0.71073

Cell: a=12.902(2) b=23.139(4) c=25.361(4)
alpha=95.653(9) beta=104.445(8) gamma=91.410(8)
Temperature: 100 K

	Calculated	Reported
Volume	7287(2)	7287(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C72 H92 Al2 N4 O2), 3(C6 H14)	?
Sum formula	C162 H226 Al4 N8 O4	C81 H113 Al2 N4 O2
Mr	2457.44	1228.71
Dx,g cm-3	1.120	1.120
Z	2	4
Mu (mm-1)	0.088	0.088
F000	2676.0	2676.0
F000'	2677.34	
h,k,lmax	18,33,36	18,33,36
Nref	44512	44487
Tmin,Tmax	0.965,0.985	0.680,0.750
Tmin'	0.965	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 30.508

R(reflections)= 0.0531(29407) wR2(reflections)= 0.1385(44487)

S = 1.006 Npar= 1677

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

PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor .... 5.2 Note

Author Response: Diffuse disorder of a solvent molecule that cannot be resolved any further.

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.8 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 5.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 4.7 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C44_1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C1_6 0.103 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         26 Report
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         21 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          6 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C1_6       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5_6       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2_6       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3_6       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4_6       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6_6       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1C_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5AB_6     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2AB_6     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AB_6     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4AB_6     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B_6      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6C_6      Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )        100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        414 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         20 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        334 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          9 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
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   5 ALERT type 3 Indicator that the structure quality may be low
  28 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Datablock: mw_173_8m

Bond precision: C-C = 0.0016 A Wavelength=1.54178

Cell: a=9.5575(5) b=9.9812(5) c=15.3139(7)
alpha=98.5868(15) beta=91.1274(14) gamma=106.0286(13)
Temperature: 100 K

	Calculated	Reported
Volume	1385.49(12)	1385.49(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C31 H17 B F10 N2 O2	?
Sum formula	C31 H17 B F10 N2 O2	C31 H17 B F10 N2 O2
Mr	650.28	650.27
Dx,g cm-3	1.559	1.559
Z	2	2
Mu (mm-1)	1.266	1.266
F000	656.0	656.0
F000'	658.83	
h,k,lmax	12,12,19	12,12,19
Nref	6051	6000
Tmin,Tmax	0.817,0.901	0.640,0.750
Tmin'	0.626	

Correction method= # Reported T Limits: Tmin=0.640 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 80.165

R(reflections)= 0.0310(5746) wR2(reflections)= 0.0824(6000)

S = 1.040 Npar= 417

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

PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 32 Ang**3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

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Alert level G

PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C5 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 . 106.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 . 107.1 Degree

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PLAT432_ALERT_2_G Short Inter X...Y Contact  F5       ..C1       .       2.91 Ang.
                                                 1-x,-y,-z  =      2_655 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5       ..F5       .       2.82 Ang.
                                                 1-x,-y,-z  =      2_655 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         48 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         17 Info
```

```
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```

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

Publication of your CIF in IUCr journals

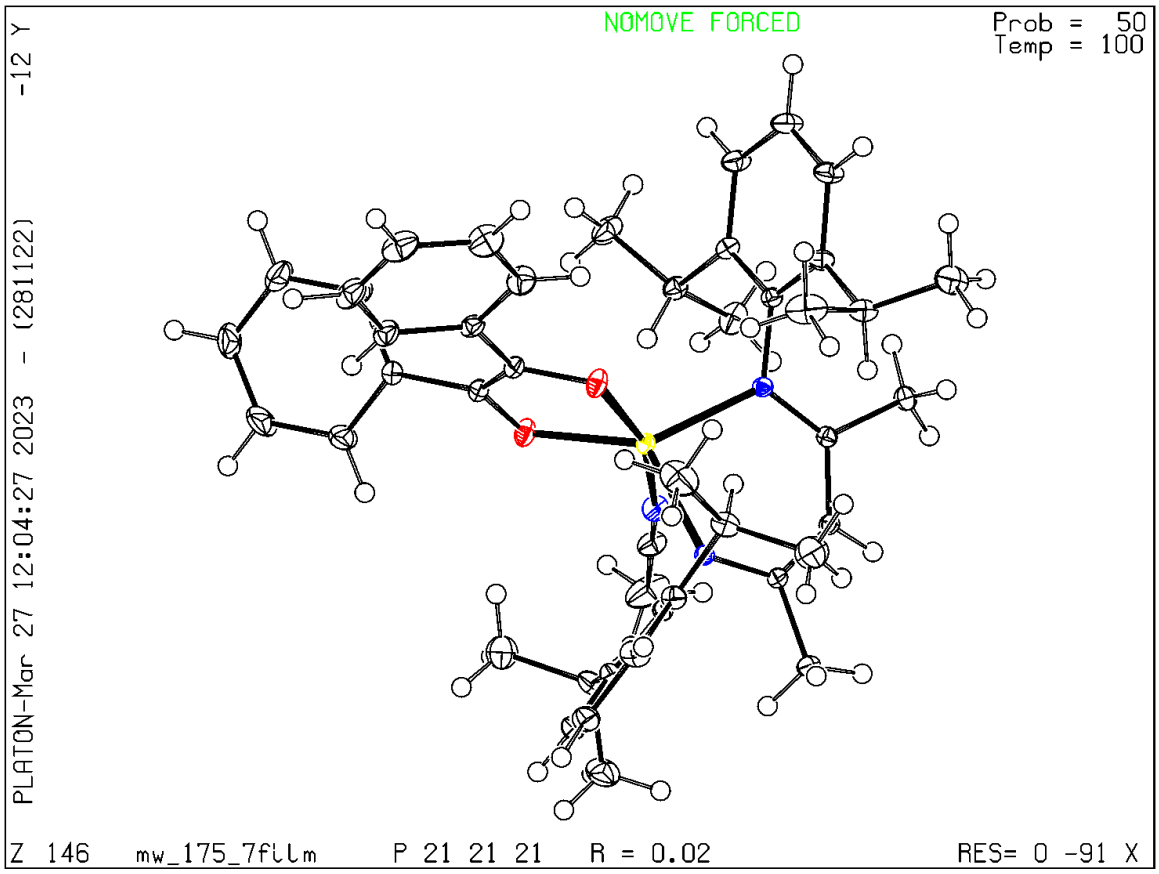
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

Publication of your CIF in other journals

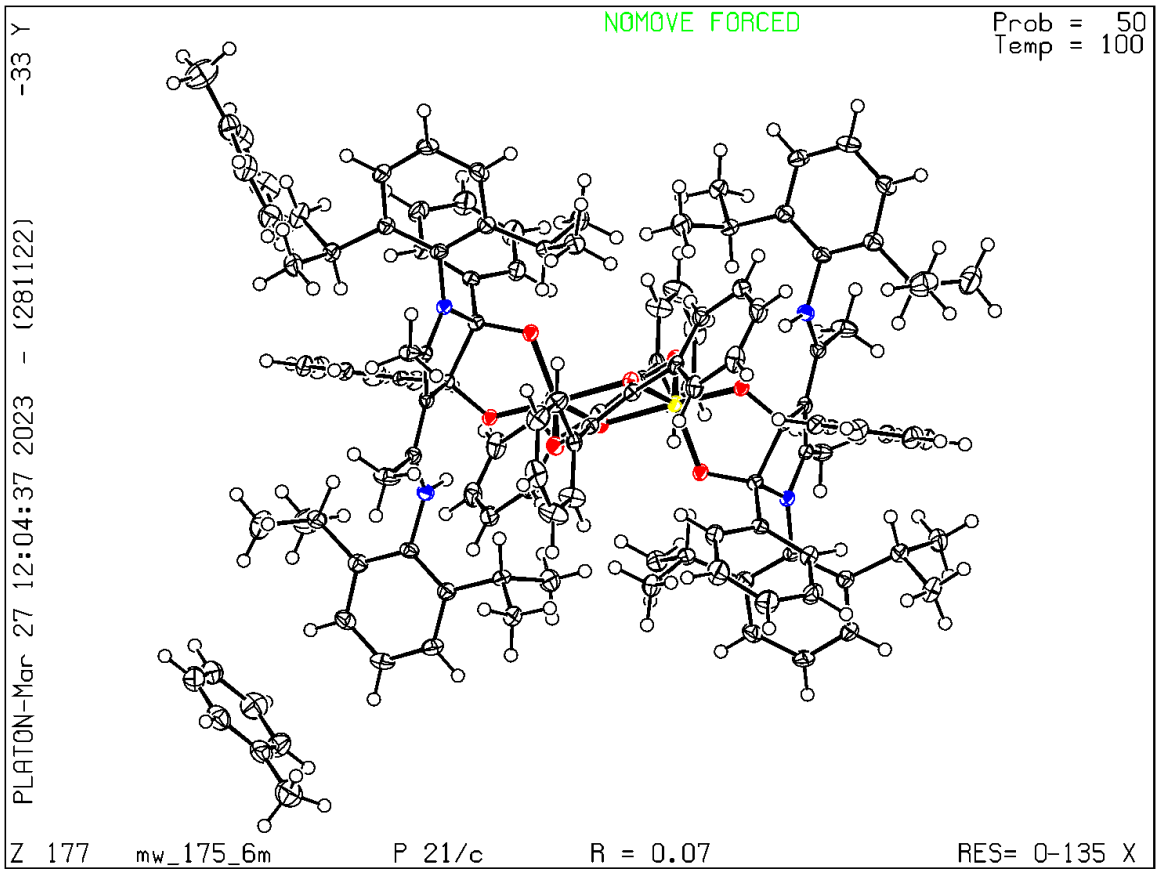
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

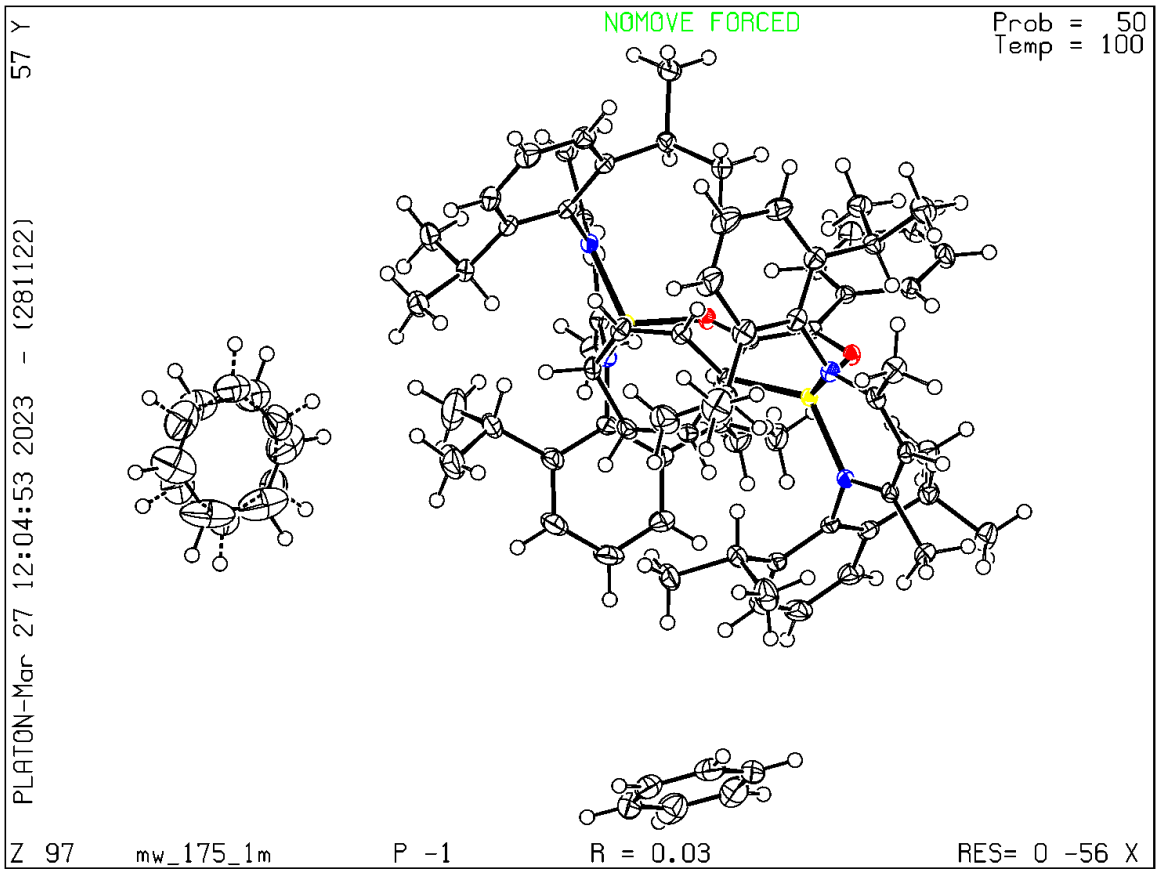
Datablock mw_175_7film - ellipsoid plot



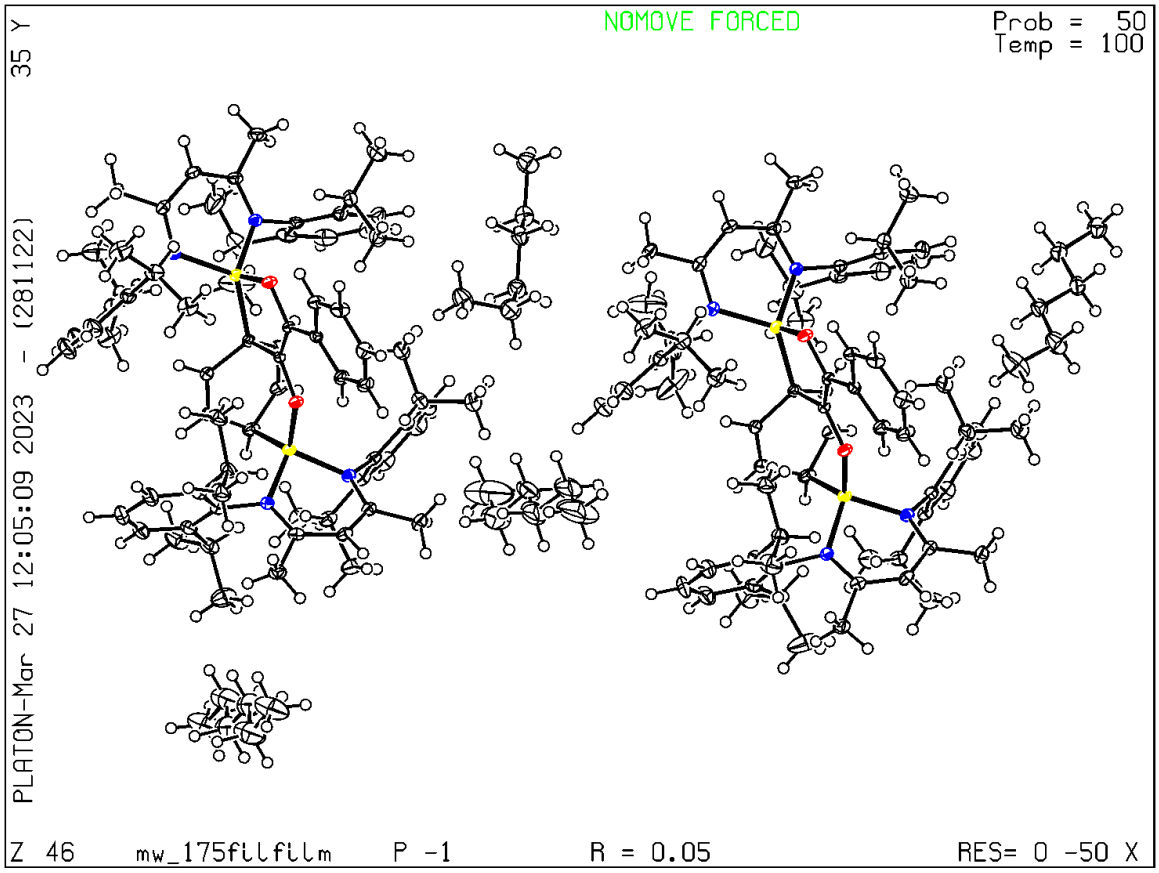
Datablock mw_175_6m - ellipsoid plot



Datablock mw_175_1m - ellipsoid plot



Datablock mw_175filfilm - ellipsoid plot



Datablock mw_173_8m - ellipsoid plot