checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1

Bond precision: C-C = 0.0078 A Wavelength=0.71073

Cell: a=11.2652(15) b=12.2246(15) c=12.2787(18)
alpha=94.758(11) beta=115.462(14) gamma=111.252(12)
Temperature: 293 K

	Calculated	Reported
Volume	1364.4(4)	1364.4(3)
Space group	P -1	P-1
Hall group	-P 1	-P1
Moiety formula	C26 H18 N12 O Zn, 0.5(H4 O2), 2(H2 O)	C26 H18 N12 O Zn, 3(H2 O)
Sum formula	C26 H24 N12 O4 Zn	C26 H24 N12 O4 Zn
Mr	633.96	633.94
Dx,g cm-3	1.543	1.543
Z	2	2
Mu (mm-1)	0.959	0.959
F000	652.0	652.0
F000’	652.77	
h,k,lmax	13,14,14	13,14,14
Nref	4815	4793
Tmin,Tmax	0.813,0.891	0.983,1.000
Tmin’	0.810	

Correction method= # Reported T Limits: Tmin=0.983 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.000

R(reflections)= 0.0575(3537) wR2(reflections)= 0.1616(4793)

S = 1.031 Npar= 388

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	Large Non-Solvent N Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N5 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N6 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N7 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C14 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.3 Note
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00777 Ang.
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O2 - H2B ..	1.01 Ang.

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

---

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

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

Datablock: 2

Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=8.2082(6) b=10.6317(8) c=12.4526(10)
alpha=79.480(7) beta=74.303(7) gamma=69.897(7)
Temperature: 293 K

	Calculated	Reported
Volume	977.60(14)	977.60(13)
Space group	P -1	P-1
Hall group	-P 1	-P1
Moiety formula	C20 H13 Cd N10 O	C20 H13 Cd N10 O
Sum formula	C20 H13 Cd N10 O	C20 H13 Cd N10 O
Mr	521.81	521.80
Dx,g cm-3	1.773	1.773
Z	2	2
Mu (mm-1)	1.155	1.155
F000	518.0	518.0
F000’	516.52	
h,k,lmax	9,12,14	9,12,14
Nref	3446	3432
Tmin,Tmax	0.812,0.871	0.958,1.000
Tmin’	0.812	

Correction method= # Reported T Limits: Tmin=0.958 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.000

R(reflections)= 0.0256(3126) wR2(reflections)= 0.0550(3432)

S = 1.053 Npar= 289

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

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note

---

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT093_ALERT_1_G No s.u.’s on H-positions, Refinement Reported as mixed Check
PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.007 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 13 Info

---

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

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

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

Datablock: 3

Bond precision: C-C = 0.0070 A Wavelength=0.71073

Cell: a=28.6376(15) b=10.5812(4) c=22.7685(10)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	6899.3(5)	6899.3(5)
Space group	P c c a	P c c a
Hall group	-P 2a 2ac	-P 2a 2ac
Moiety formula	C26 H20 Cd N12 O2, C4 H9 N O	C26 H20 Cd N12 O2, C4 H9 N O
Sum formula	C30 H29 Cd N13 O3	C30 H29 Cd N13 O3
Mr	732.07	732.06
Dx,g cm-3	1.410	1.410
Z	8	8
Mu (mm-1)	0.684	0.684
F000	2976.0	2976.0
F000’	2970.45	
h,k,lmax	34,12,27	34,12,26
Nref	6093	6076
Tmin,Tmax	0.884,0.921	0.934,1.000
Tmin’	0.884	

Correction method= # Reported T Limits: Tmin=0.934 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.000

R(reflections)= 0.0517(4213) wR2(reflections)= 0.1458(6076)

S = 1.047 Npar= 518

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
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.6 Note
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O3 Check

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         20 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         56 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.76 Why ?
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............. Percentage =         24 Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in Structure ...        199 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          9 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         99 Check
              N10A -C18  -N10     1.555   1.555   1.555             18.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        109 Check
              N11  -C21  -N11A    1.555   1.555   1.555             14.80 Deg.
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          14 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1702 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
```

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

   3 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

Datablock: btzb

```
Bond precision:  C-C = 0.0018 A          Wavelength=0.71073

Cell:            a=5.9576(7)    b=16.0500(18)       c=16.1222(18)
                 alpha=90       beta=100.028(2)     gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1518.1(3)	1518.0(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C14 H10 N8 O, H2 O	C14 H10 N8 O, H2 O
Sum formula	C14 H12 N8 O2	C14 H12 N8 O2
Mr	324.32	324.32
Dx,g cm-3	1.419	1.419
Z	4	4
Mu (mm-1)	0.103	0.103
F000	672.0	672.0
F000’	672.24	
h,k,lmax	7,19,19	7,19,19
Nref	2663	2661
Tmin,Tmax	0.980,0.992	0.947,1.000
Tmin’	0.980	

Correction method= # Reported T Limits: Tmin=0.947 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0332(2255) wR2(reflections)= 0.0886(2661)

S = 1.078 Npar= 217

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 G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT093_ALERT_1_G	No s.u.’s on H-positions, Refinement Reported as	mixed Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	3 Info

---

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

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

---

checkCIF publication errors

Alert level A

```
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.
```

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

2 **ALERT level A** = Data missing that is essential or data in wrong format
1 **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

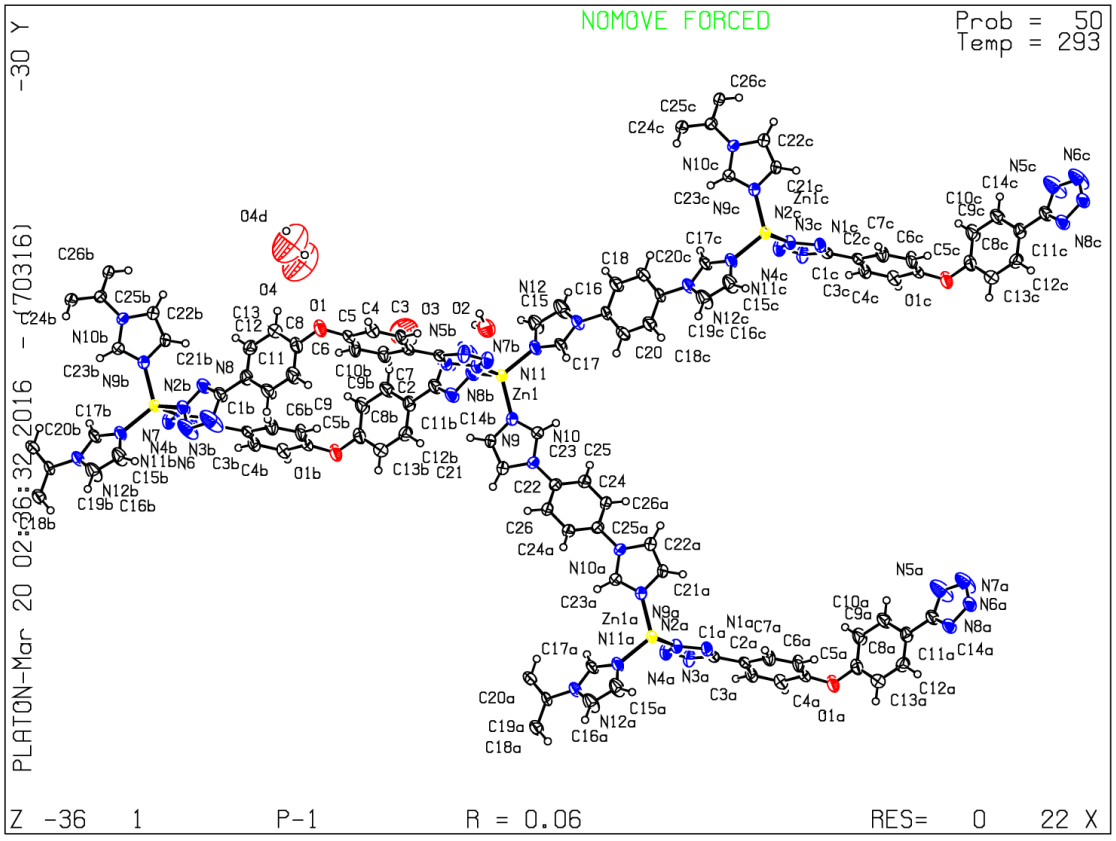
Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

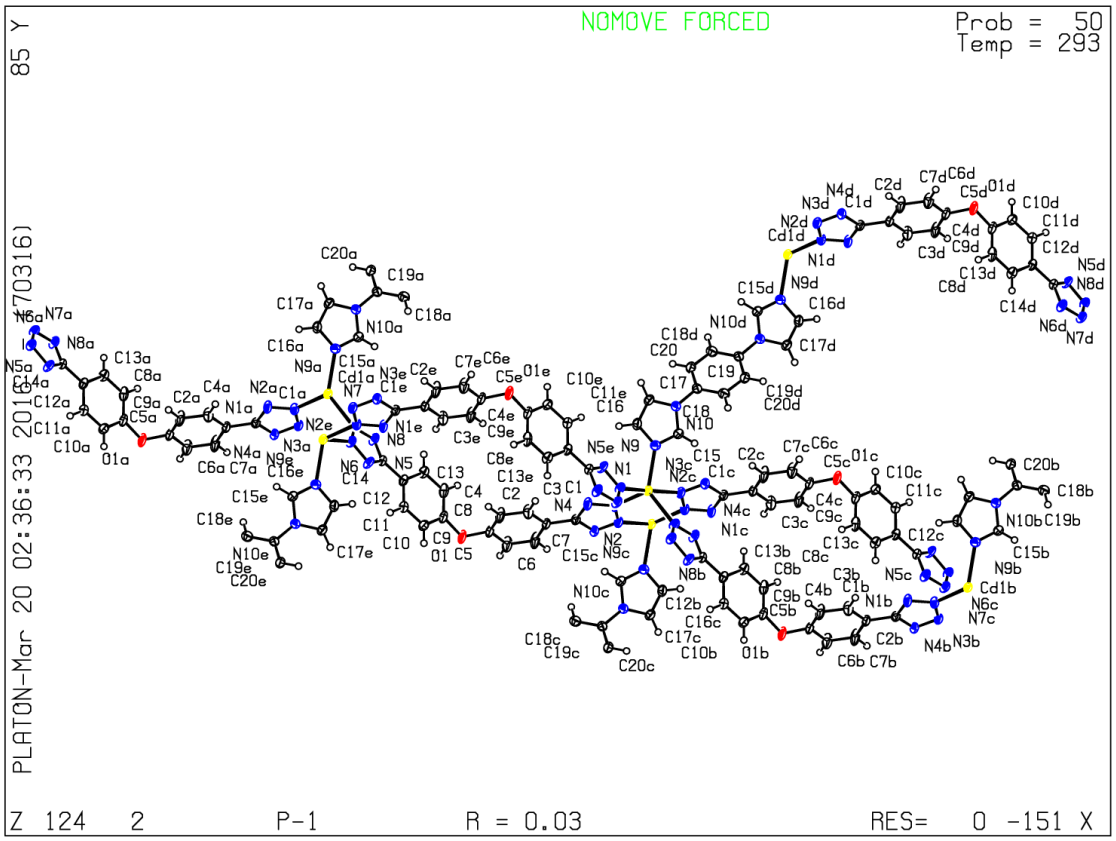
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you 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 07/03/2016; check.def file version of 02/03/2016

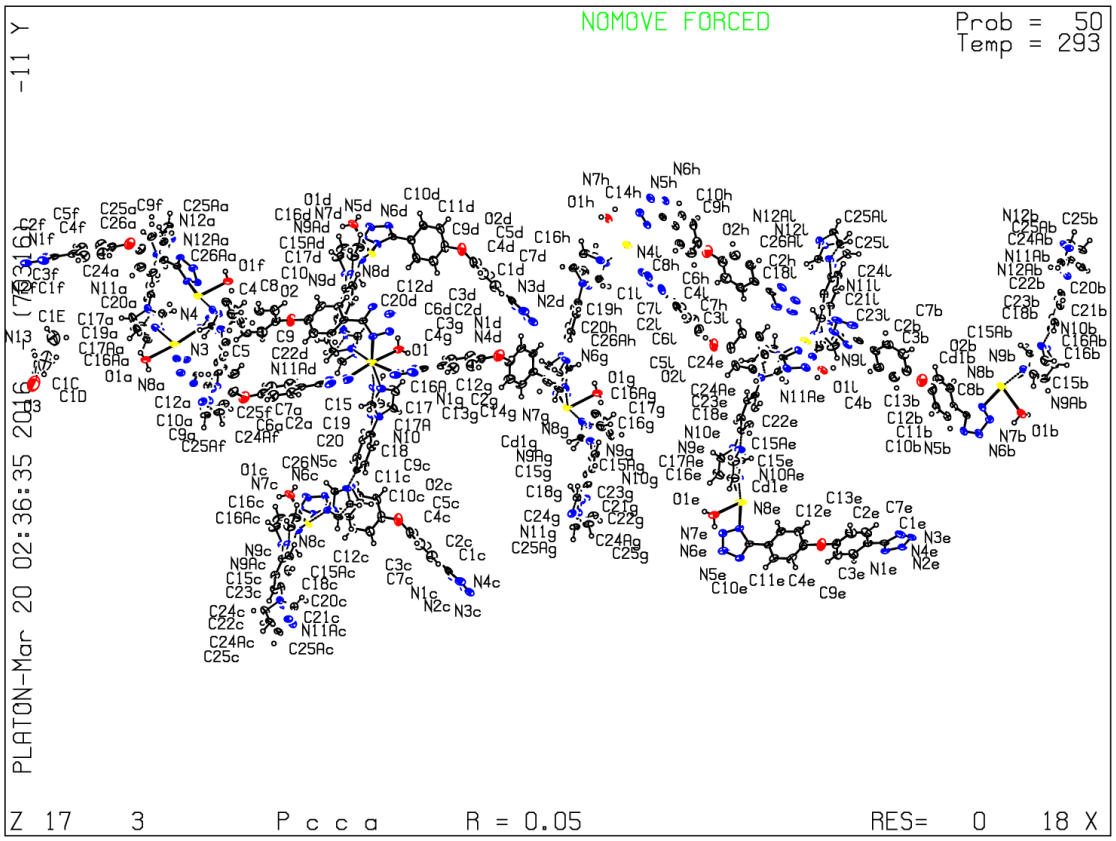
Datablock 1 - ellipsoid plot



Datablock 2 - ellipsoid plot



Datablock 3 - ellipsoid plot



Datablock btzb - ellipsoid plot