checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2, 3

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 = 0.0107 A Wavelength=0.71069

Cell: a=9.685(5) b=10.309(5) c=16.725(5)
alpha=92.107(5) beta=103.546(5) gamma=102.952(5)
Temperature: 293 K

	Calculated	Reported
Volume	1575.1(12)	1575.1(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H42 Cd3 N8 O18, 8(H2 O)	C62 H42 Cd3 N8 O18, 4(H4 O2)
Sum formula	C62 H58 Cd3 N8 O26	C62 H58 Cd3 N8 O26
Mr	1668.39	1668.36
Dx,g cm-3	1.759	1.759
Z	1	1
Mu (mm-1)	1.098	1.098
F000	838.0	838.0
F000’	836.00	
h,k,lmax	12,12,20	12,12,20
Nref	6492	6492
Tmin,Tmax	0.768,0.803	0.768,0.803
Tmin’	0.768	

Correction method= # Reported T Limits: Tmin=0.768 Tmax=0.803
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 26.454

R(reflections)= 0.0515(4333) wR2(reflections)= 0.1507(6463)

S = 1.033 Npar= 449

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H2WA ..H5WB . 1.98 Ang.
x,y,z = 1_555 Check
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

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Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
clourless
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT213_ALERT_2_C Atom O8 has ADP max/min Ratio ..... 3.1 prolat
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 5.9 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C12 --C13 . 0.17 Ang.
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of O2 Check
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of O3 Check
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of O4 Check
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of Cd2 Check
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of C23 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O3W 0.131 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O4W 0.147 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O5W 0.131 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01073 Ang.
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 62.84 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.27A From O8 2.14 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.64A From O5W -0.63 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.64A From O3W -0.61 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.65A From O5W -0.59 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.54A From O5W -0.56 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.72A From O3W -0.54 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.81A From O5W -0.45 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.97A From O5W -0.44 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.69A From O4W -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2WB -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3WB -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5WA -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5WB -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1WA -0.40 eA-3

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 ... 13 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 12 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT153_ALERT_1_G The s.u.’s on the Cell Axes are Equal ..(Note) 0.005 Ang.
PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.005 Degree
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

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PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd2      --O4       .        8.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd2      --O5_c     .        5.3 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         10 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1       (II)      .      2.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2       (II)      .      2.03 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        80 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        30 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         1 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  32 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

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  31 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   5 ALERT type 5 Informative message, check
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Datablock: 2

Bond precision: C-C = 0.0068 A Wavelength=0.71073

Cell: a=9.4403(5) b=10.1765(6) c=16.5532(9)
       alpha=91.772(1) beta=102.093(1) gamma=101.501(1)
Temperature: 296 K

	Calculated	Reported
Volume	1519.35(15)	1519.35(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H42 N8 O18 Zn3, 2(H2 O) [+ solvent]	C62 H42 N8 O18 Zn3, H4 O2
Sum formula	C62 H46 N8 O20 Zn3 [+ solvent]	C62 H46 N8 O20 Zn3
Mr	1419.24	1419.18
Dx,g cm-3	1.551	1.551
Z	1	1
Mu (mm-1)	1.259	1.259
F000	724.0	724.0
F000’	725.18	
h,k,lmax	12,13,22	12,13,22
Nref	7605	7605
Tmin,Tmax	0.747,0.777	0.747,0.777
Tmin’	0.732	

Correction method= # Reported T Limits: Tmin=0.747 Tmax=0.777
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 28.355

R(reflections)= 0.0543(4956) wR2(reflections)= 0.1556(7538)

S = 1.014 Npar= 425

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

PLAT420_ALERT_2_B	D-H Without Acceptor O2W --H2WB .	Please Check
PLAT919_ALERT_3_B	Reflection # Likely Affected by the Beamstop ...	1 Check

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Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.32 Report
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range	3.2 Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max) / Ueq(min) Range	4.6 Ratio
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O2W	0.102 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00677 Ang.
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1 Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.88A From O7	-0.45 eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT154_ALERT_1_G	The s.u.’s on the Cell Angles are Equal ..(Note)	0.001 Degree
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	52 A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	4 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .	1.91 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn2 (II) .	1.92 Info
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	! Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	66 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	1 Check

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5 ALERT type 5 Informative message, check

Datablock: 3

Bond precision: C-C = 0.0086 A Wavelength=0.71073

Cell: a=9.4573(6) b=10.1544(6) c=16.5808(10)
alpha=92.219(2) beta=101.862(1) gamma=101.043(1)
Temperature: 296 K

	Calculated	Reported
Volume	1524.39(16)	1524.39(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H42 Co3 N8 O18, 4(H2 O)	C62 H42 Co3 N8 O18, 2(H4 O2)
Sum formula	C62 H50 Co3 N8 O22	C62 H50 Co3 N8 O22
Mr	1435.89	1435.89
Dx,g cm-3	1.564	1.564
Z	1	1
Mu (mm-1)	0.895	0.895
F000	735.0	735.0
F000’	736.40	
h,k,lmax	11,12,19	11,12,19
Nref	5445	5445
Tmin,Tmax	0.807,0.836	0.807,0.836
Tmin’	0.807	

Correction method= # Reported T Limits: Tmin=0.807 Tmax=0.836
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.135

R(reflections)= 0.0612(3981) wR2(reflections)= 0.1838(5431)

S = 1.032 Npar= 437

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

PLAT094_ALERT_2_B	Ratio of Maximum / Minimum Residual Density				4.28 Report
PLAT420_ALERT_2_B	D-H Without Acceptor	O3W	--H3WB	.	Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	O2W	--H2WA	.	Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	O2W	--H2WB	.	Please Check

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Alert level C

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

The relevant atom site should be identified.

PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	2.43	eA-3
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	4.5	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C23 --C24 .	0.16	Ang.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O2W	0.176	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O3W	0.108	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00863	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.598	13	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.44A From O3W	2.32	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.86A From O7	-0.44	eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II) .	1.92	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Co2 (II) .	1.86	Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	56%	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.	1	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2	Check

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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

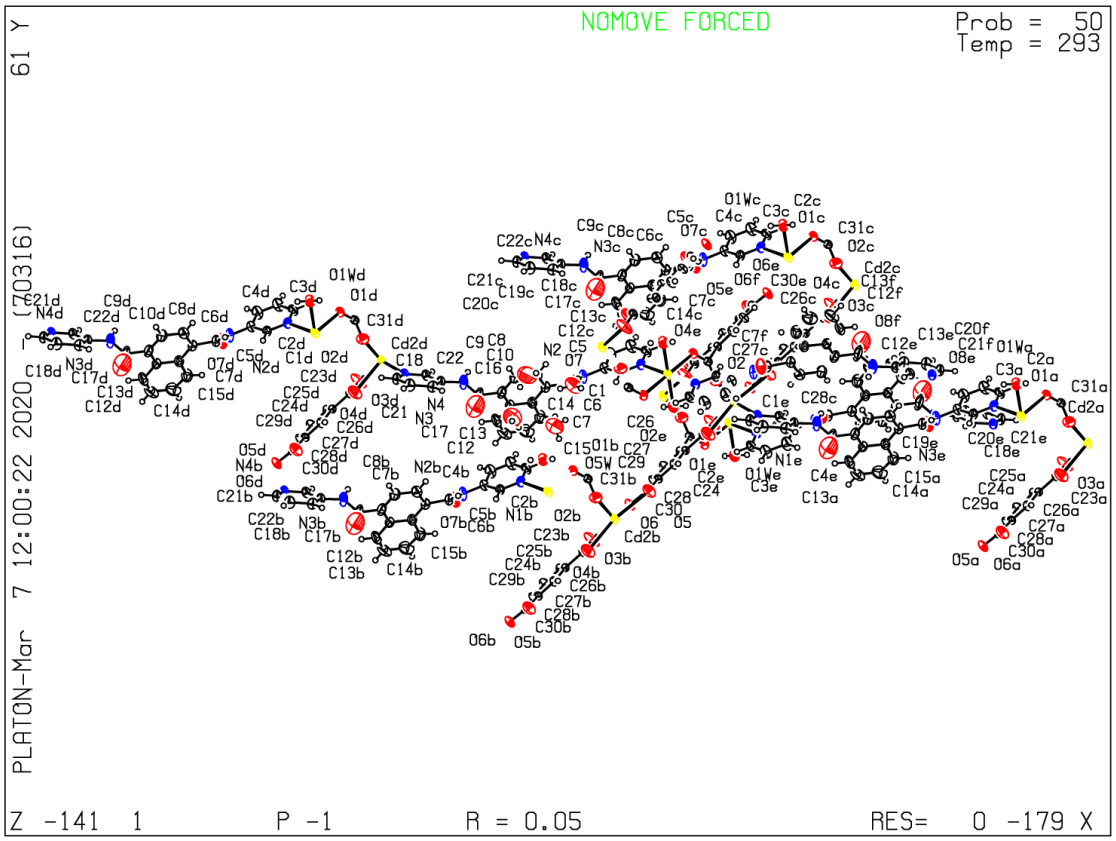
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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

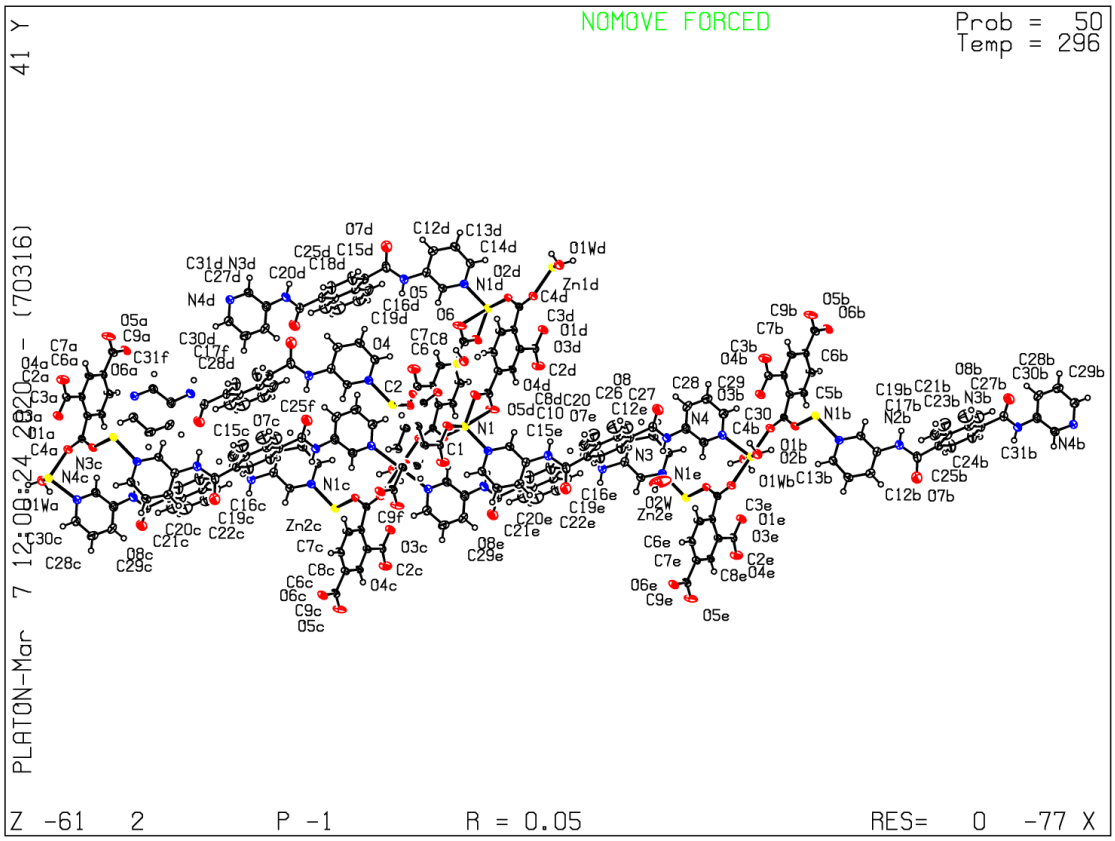
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock 1 - ellipsoid plot



Datablock 2 - ellipsoid plot



Datablock 3 - ellipsoid plot