

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UAD_-173_uracdih_100k

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: UAD_-173_uracdih_100k

Bond precision: = 0.0000 A Wavelength=1.54184

Cell: a=7.2559(4) b=6.3669(4) c=17.4739(13)
 alpha=90 beta=90.036(6) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	807.25(9)	807.25(9)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C5 H4 N4 O3, 2(H2 O)	C5 H4 N4 O3, 2(H2 O)
Sum formula	C5 H8 N4 O5	C5 H8 N4 O5
Mr	204.15	204.15
Dx,g cm-3	1.680	1.680
Z	4	4
Mu (mm-1)	1.321	1.321
F000	424.0	424.0
F000'	425.73	
h,k,lmax	8,7,21	8,7,21
Nref	1531	1518
Tmin,Tmax	0.912,0.971	0.729,1.000
Tmin'	0.903	

Correction method= # Reported T Limits: Tmin=0.729 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 69.983

R(reflections)= 0.0475(1265) wR2(reflections)= 0.1304(1518)

S = 1.059 Npar= 166

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**

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.14	Note
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) Ow2 - Hw2A .	1.01	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # C5 H4 N4 O3	1	Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.076	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	8	Report

● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	10	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 1	9.41	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	6.59	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C5 H4 N4 O3	2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	3	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	4	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	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	4	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.54	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note

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

1 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
6 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

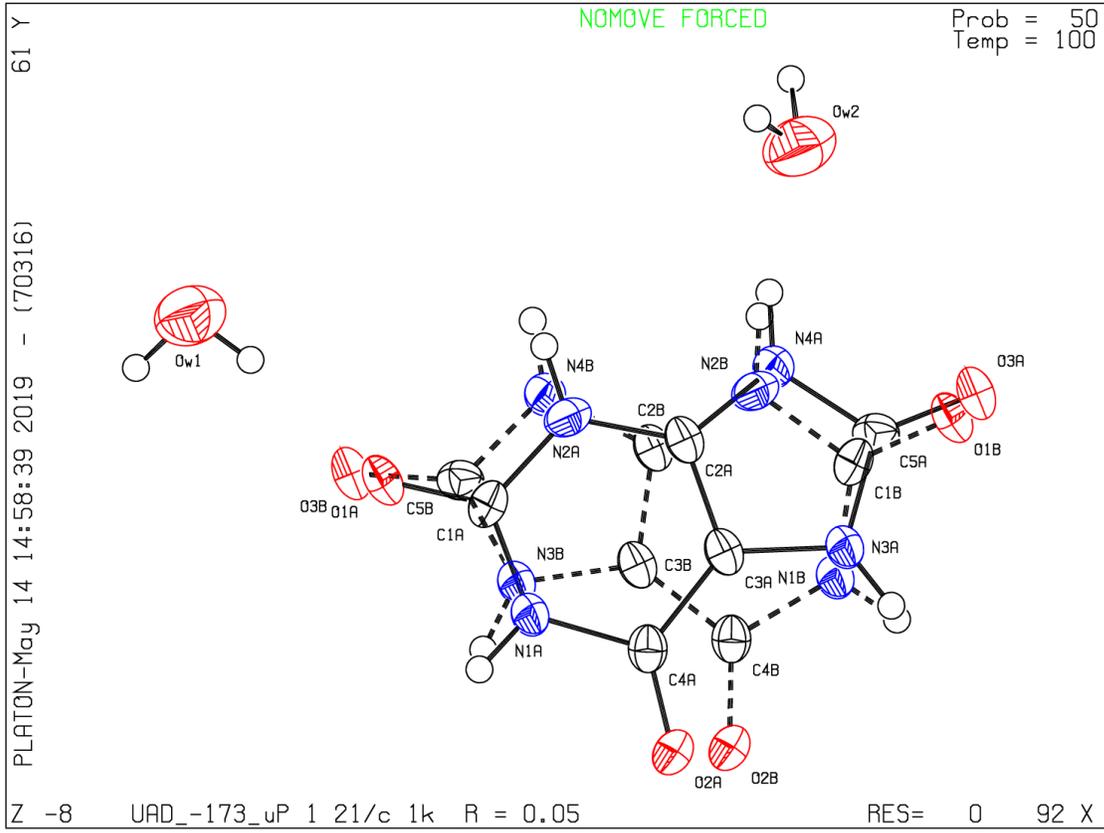
Publication of your CIF in IUCr journals

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Publication of your CIF in other journals

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PLATON version of 03/05/2019; check.def file version of 29/04/2019



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UAD_-130_uracdih_143k

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: UAD_-130_uracdih_143k

Bond precision: = 0.0000 A Wavelength=1.54184

Cell: a=7.2830(3) b=6.3616(3) c=17.4781(9)
 alpha=90 beta=90.020(4) gamma=90

Temperature: 143 K

	Calculated	Reported
Volume	809.79(7)	809.79(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	0.5(C5 H4 N4 O3), H2 O	C5 H4 N4 O3, 2(H2 O)
Sum formula	C2.50 H4 N2 O2.50	C5 H8 N4 O5
Mr	102.07	204.15
Dx,g cm-3	1.674	1.675
Z	8	4
Mu (mm-1)	1.317	1.317
F000	424.0	424.0
F000'	425.69	
h,k,lmax	8,7,21	8,7,21
Nref	1536	1524
Tmin,Tmax	0.912,0.971	0.609,1.000
Tmin'	0.904	

Correction method= # Reported T Limits: Tmin=0.609 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 69.984

R(reflections)= 0.0456(1241) wR2(reflections)= 0.1260(1524)

S = 1.058 Npar= 165

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

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio		9.24	Note
PLAT417_ALERT_2_C	Short Inter D-H..H-D	Hw1B ..H4B .	2.10	Ang.
		-x,1/2+y,-1/2-z =	2_554	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	Hw2B ..H4A .	2.14	Ang.
		x,y,z =	1_555	Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1	Note
	C5 H4 N4 O3			
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.008	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	5	Report

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		7	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		8	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		2.00	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		10	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		4	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C3A --C4A .	5.7	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O1A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N3A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N4A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4A	Constrained at	0.5849	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N3B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N4B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3B	Constrained at	0.415	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4B	Constrained at	0.415	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	Resd 1	9.36	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	Resd 2	6.64	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		6	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C5 H4 N4 O3			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	H2 O			

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # H2 O	4 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	5 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..	! 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	7 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.55 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	4 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
54 **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
6 ALERT type 3 Indicator that the structure quality may be low
43 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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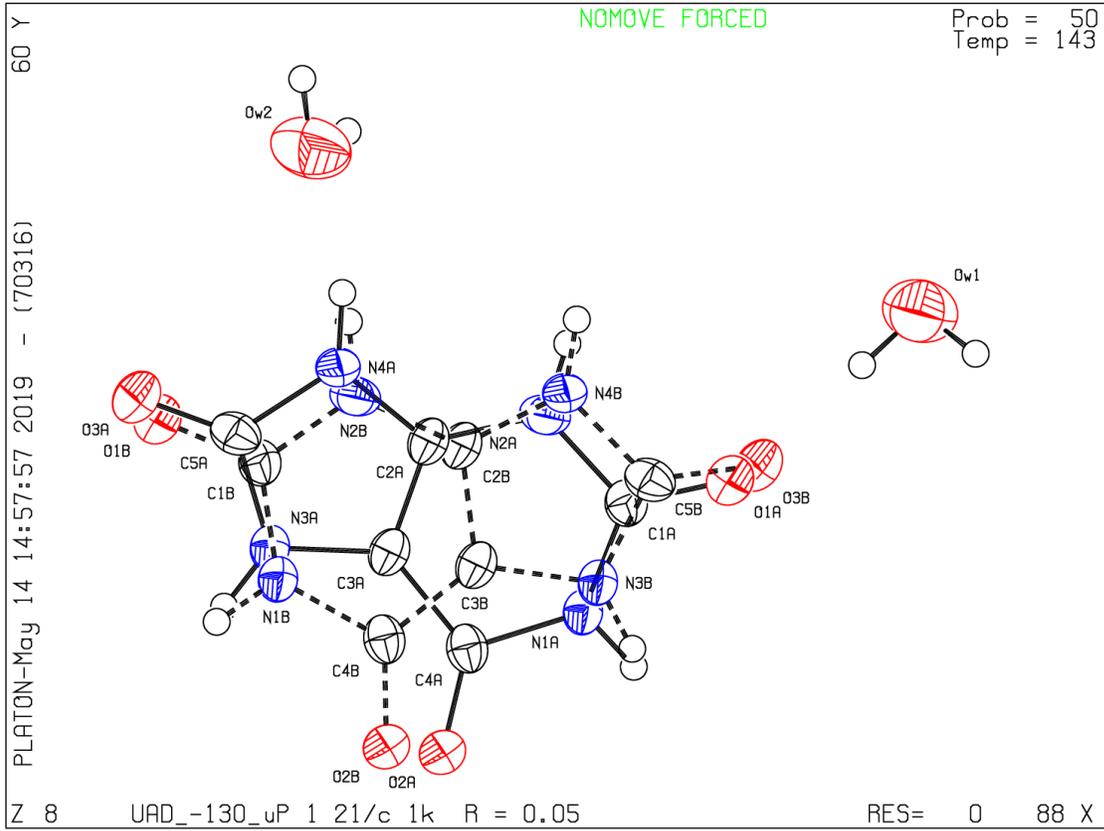
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PLATON version of 03/05/2019; check.def file version of 29/04/2019



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UAD_-90_uracdih_183k

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: UAD_-90_uracdih_183k

Bond precision: = 0.0000 A Wavelength=1.54184

Cell: a=7.3175(3) b=6.3565(3) c=17.4962(8)
 alpha=90 beta=90.010(4) gamma=90

Temperature: 183 K

	Calculated	Reported
Volume	813.81(6)	813.82(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C5 H4 N4 O3, 2(H2 O)	C5 H4 N4 O3, 2(H2 O)
Sum formula	C5 H8 N4 O5	C5 H8 N4 O5
Mr	204.15	204.15
Dx,g cm-3	1.666	1.666
Z	4	4
Mu (mm-1)	1.311	1.311
F000	424.0	424.0
F000'	425.73	
h,k,lmax	8,7,21	8,7,21
Nref	1541	1529
Tmin,Tmax	0.913,0.972	0.508,1.000
Tmin'	0.904	

Correction method= # Reported T Limits: Tmin=0.508 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 69.947

R(reflections)= 0.0470(1225) wR2(reflections)= 0.1326(1529)

S = 1.032 Npar= 166

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**

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.21	Note
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # C5 H4 N4 O3	1	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	7	Report

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	10	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for N2A --C2A .	7.5	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 1	9.36	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	6.64	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C5 H4 N4 O3	2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	3	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	4	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	5	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	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	6	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.55	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note

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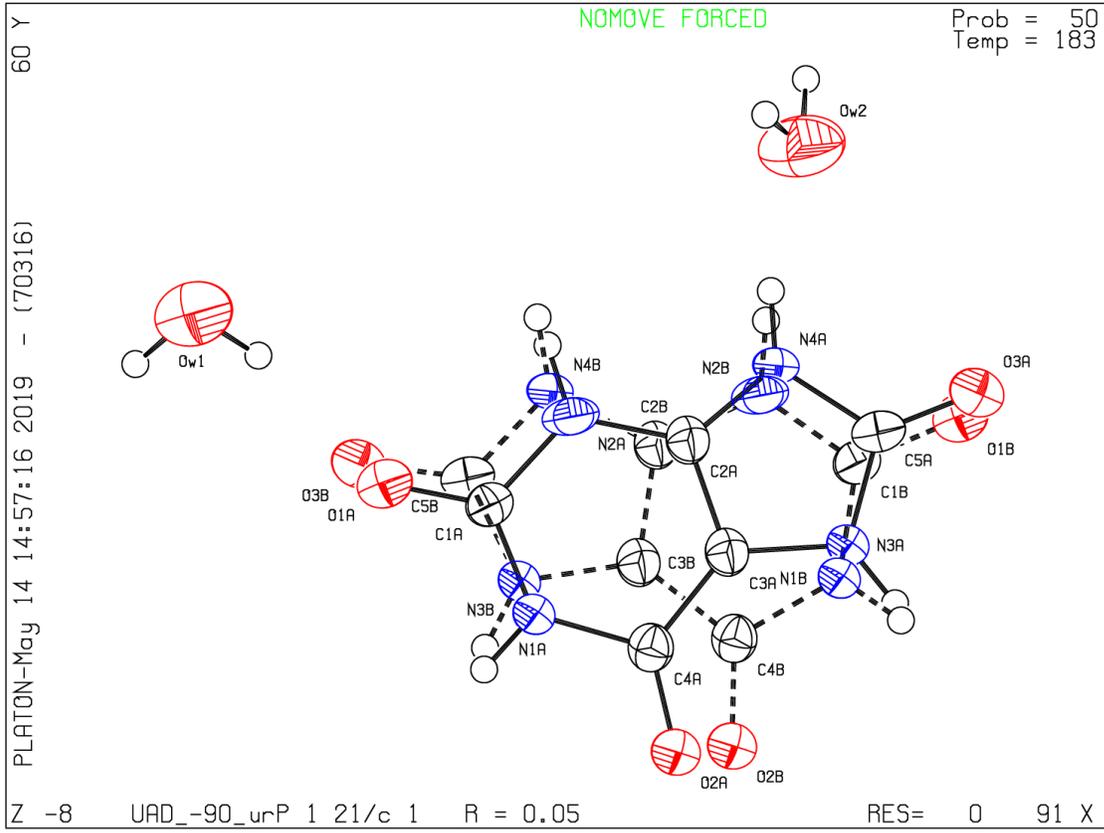
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No syntax errors found. CIF dictionary Interpreting this report

Datablock: UAD_-50_uracdih_223k

Bond precision: = 0.0000 A Wavelength=1.54184

Cell: a=7.3553(4) b=6.3485(3) c=17.5125(9)
 alpha=90 beta=90.005(5) gamma=90

Temperature: 223 K

	Calculated	Reported
Volume	817.75(7)	817.75(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C5 H4 N4 O3, 2(H2 O)	C5 H4 N4 O3, 2(H2 O)
Sum formula	C5 H8 N4 O5	C5 H8 N4 O5
Mr	204.15	204.15
Dx,g cm-3	1.658	1.658
Z	4	4
Mu (mm-1)	1.304	1.304
F000	424.0	424.0
F000'	425.73	
h,k,lmax	8,7,21	8,7,21
Nref	1544	1533
Tmin,Tmax	0.913,0.972	0.463,1.000
Tmin'	0.904	

Correction method= # Reported T Limits: Tmin=0.463 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 69.786

R(reflections)= 0.0500(1214) wR2(reflections)= 0.1441(1533)

S = 1.044 Npar= 166

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**

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.23	Note
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # C5 H4 N4 O3	1	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	7	Report

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	10	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 1	9.55	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	6.45	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C5 H4 N4 O3	2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	3	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	4	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	5	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	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	4	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.44	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note

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PLATON version of 03/05/2019; check.def file version of 29/04/2019

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UAD_-10_uracdih_263k

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: UAD_-10_uracdih_263k

Bond precision: = 0.0000 A Wavelength=1.54184

Cell: a=7.3872(4) b=6.3397(3) c=17.5312(9)
 alpha=90 beta=90.004(5) gamma=90

Temperature: 263 K

	Calculated	Reported
Volume	821.03(7)	821.03(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C5 H4 N4 O3, 2(H2 O)	C5 H4 N4 O3, 2(H2 O)
Sum formula	C5 H8 N4 O5	C5 H8 N4 O5
Mr	204.15	204.15
Dx,g cm-3	1.652	1.652
Z	4	4
Mu (mm-1)	1.299	1.299
F000	424.0	424.0
F000'	425.73	
h,k,lmax	9,7,21	9,7,21
Nref	1549	1538
Tmin,Tmax	0.914,0.972	0.423,1.000
Tmin'	0.905	

Correction method= # Reported T Limits: Tmin=0.423 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 69.923

R(reflections)= 0.0476(1167) wR2(reflections)= 0.1366(1538)

S = 1.051 Npar= 165

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**

PLAT088_ALERT_3_C Poor Data / Parameter Ratio 9.32 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ow2 0.106 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D Hw1B ..H4B . 2.12 Ang.
-x,1/2+y,-1/2-z = 2_554 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C5 H4 N4 O3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

● **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 8 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 10 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N4A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A Constrained at 0.5852 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N4B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3B Constrained at 0.4148 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B Constrained at 0.4148 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 100% Note
PLAT301_ALERT_3_G Main Residue Disorder(Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 1 9.36 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 2 6.64 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C5 H4 N4 O3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note
H2 O
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 5 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! 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	4 Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.44 Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4 Note

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5 ALERT type 3 Indicator that the structure quality may be low
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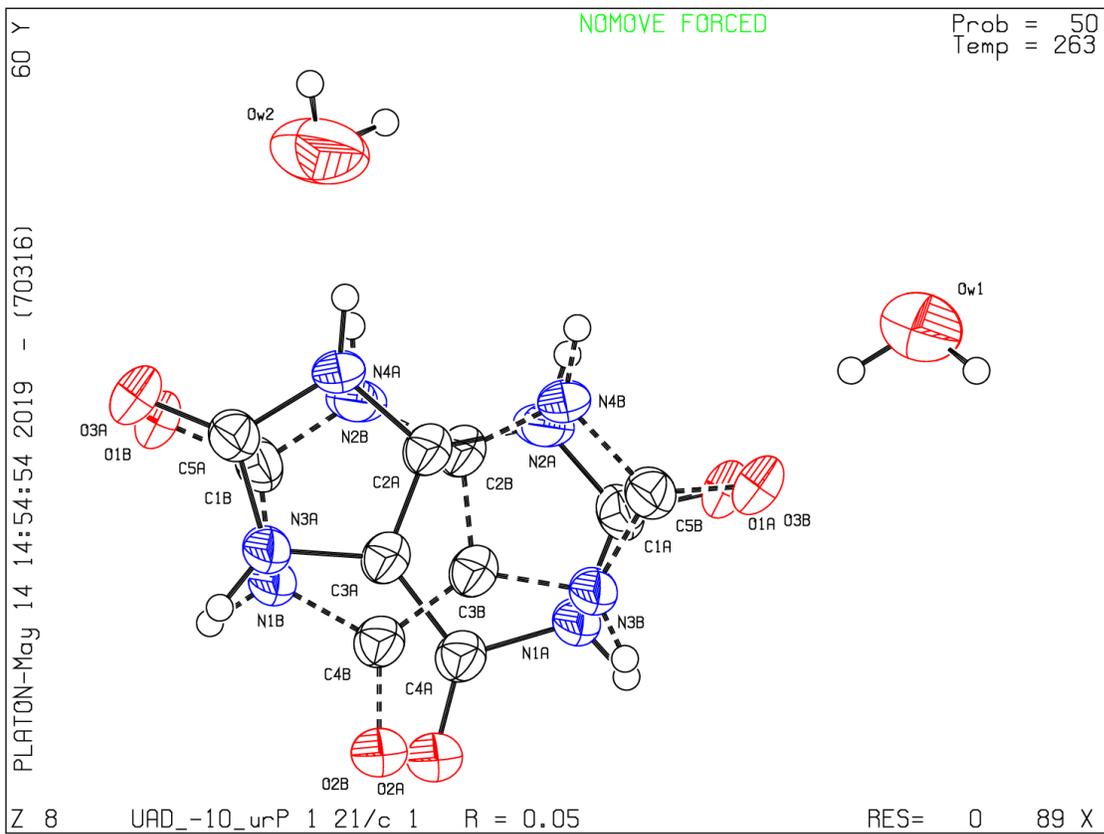
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PLATON version of 03/05/2019; check.def file version of 29/04/2019



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) UAD_30_uracdih_303k

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: UAD_30_uracdih_303k

Bond precision:	= 0.0000 A	Wavelength=1.54184	
Cell:	a=7.4283(8)	b=6.3266(5)	c=17.5627(16)
	alpha=90	beta=90.044(10)	gamma=90
Temperature:	303 K		
	Calculated	Reported	
Volume	825.37(13)	825.37(13)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C5 H4 N4 O3, 2(H2 O)	C5 H4 N4 O3, 2(H2 O)	
Sum formula	C5 H8 N4 O5	C5 H8 N4 O5	
Mr	204.15	204.15	
Dx,g cm-3	1.643	1.643	
Z	4	4	
Mu (mm-1)	1.292	1.292	
F000	424.0	424.0	
F000'	425.73		
h,k,lmax	9,7,21	9,7,21	
Nref	1559	1415	
Tmin,Tmax	0.914,0.972	0.318,1.000	
Tmin'	0.905		

Correction method= # Reported T Limits: Tmin=0.318 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.908 Theta(max)= 69.959

R(reflections)= 0.0941(510) wR2(reflections)= 0.3462(1415)

S = 0.969 Npar= 165

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**

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.916 Why?

Author Response: Due to the distruction of the crystal caused by dehydration.

 **Alert level B**

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 36% Check

Author Response: Due to the distruction of the crystal caused by dehydration.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 125 Report

Author Response: Due to the distruction of the crystal caused by dehydration.

 **Alert level C**

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.35 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.58 Note
PLAT234_ALERT_4_C Large Hirshfeld Difference O1A --C1A . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1A --C4A . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4A --C5A . 0.18 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ow1 0.138 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ow2 0.138 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) 01B Check
PLAT417_ALERT_2_C Short Inter D-H..H-D Hw2B ..H4A . 2.11 Ang.
x,y,z = 1_555 Check
PLAT728_ALERT_1_C D-H..A Calc 177.00, Rep 175(19) Dev... 2.00 Degree
Ow1 -Hw1A -O3B 1.555 1.555 1.555 # 44 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C5 H4 N4 O3

 **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 8 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.19 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 10 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 100% Note
PLAT301_ALERT_3_G Main Residue Disorder(Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 1 8.96 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 2 7.04 Check
PLAT309_ALERT_2_G Single Bonded Oxygen (C-O > 1.3 Ang) 03B Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2B --C5B 2.01 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 28 Check
N4B -C2B -C5B 1.555 1.555 1.555 43.00 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	38	Check
N4B -C5B -C2B 1.555 1.555 1.555	44.00	Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	2	Note
C5 H4 N4 O3		
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	3	Note
H2 O		
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	4	Note
H2 O		
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PLAT860_ALERT_3_G Number of Least-Squares Restraints	6	Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..		! 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	19	Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.57	Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	4	Note

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Datablock UAD_30_uracdiH_303k - ellipsoid plot

