

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cp1, cp1-1, cp1-2

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: cp1

Bond precision:	C-C = 0.0098 A	Wavelength=0.71073
Cell:	a=14.5978 (6) b=33.6931 (15) c=28.1944 (13)	
	alpha=90 beta=102.552 (1) gamma=90	
Temperature:	120 K	
	Calculated	Reported
Volume	13535.8 (10)	13535.8 (10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10, 2 (H2 O)	2 (C35 H24 Cd Cl4 N2 O5), 2 (H2 O)
Sum formula	C70 H52 Cd2 Cl8 N4 O12	C70 H52 Cd2 Cl8 N4 O12
Mr	1649.58	1649.55
Dx, g cm-3	1.619	1.619
Z	8	8
Mu (mm-1)	1.010	1.010
F000	6624.0	6624.0
F000'	6623.03	
h, k, lmax	17, 40, 33	17, 40, 33
Nref	23935	23907
Tmin, Tmax	0.886, 0.904	0.685, 0.746
Tmin'	0.886	

Correction method= # Reported T Limits: Tmin=0.685 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.999 Theta(max)= 25.027

R(reflections)= 0.0690 (17350)

wR2(reflections)=
0.1969 (23907)

S = 1.064

Npar= 1796

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 Bond Without Acceptor O17 --H17 . Please Check

Author Response: The O17-H17 / O18-H18A / O19-H19A / O20-H20A / O23-H23A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O18 --H18A . Please Check

Author Response: The O17-H17 / O18-H18A / O19-H19A / O20-H20A / O23-H23A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O19 --H19A . Please Check

Author Response: The O17-H17 / O18-H18A / O19-H19A / O20-H20A / O23-H23A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O20 --H20A . Please Check

Author Response: The O17-H17 / O18-H18A / O19-H19A / O20-H20A / O23-H23A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O23 --H23A . Please Check

Author Response: The O17-H17 / O18-H18A / O19-H19A / O20-H20A / O23-H23A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

 Alert level C

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C70 H48 Cd2 Cl8 N4 O10, 2(H2 O)

Rep.: 2(C35 H24 Cd Cl4 N2 O5), 2(H2 O)

PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.9 Ratio

PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 3.2 Ratio

PLAT220_ALERT_2_C NonSolvent Resd 2 Cl Ueq(max)/Ueq(min) Range 4.1 Ratio

PLAT220_ALERT_2_C NonSolvent Resd 2 O Ueq(max)/Ueq(min) Range 3.6 Ratio

PLAT222_ALERT_3_C	NonSolvent Resd 1	H	Uiso(max)/Uiso(min) Range	6.6	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 2	H	Uiso(max)/Uiso(min) Range	5.2	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C10	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C31	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C50	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O22		0.120	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O23		0.110	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O24		0.169	Check
PLAT336_ALERT_2_C	Long Bond Distance for	 C132	-C118	2.020	Ang.
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds		0.00979	Ang.
PLAT354_ALERT_3_C	Short	O-H (X0.82,N0.98A)	O23 - H23B	0.70	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C99 - C100	1.54	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C113 - C114	1.53	Ang.
PLAT414_ALERT_2_C	Short Intra	D-H..H-X	H12 ..H17	1.95	Ang.
			x,y,z =	1_555	Check
PLAT414_ALERT_2_C	Short Intra	D-H..H-X	H20A ..H50B	1.98	Ang.
			x,y,z =	1_555	Check
PLAT414_ALERT_2_C	Short Intra	D-H..H-X	H20A ..H77B	1.97	Ang.
			-x,1/2+y,3/2-z =	2_556	Check
PLAT415_ALERT_2_C	Short Inter	D-H..H-X	H19A ..H76	2.08	Ang.
			-x,-1-y,2-z =	3_547	Check
PLAT751_ALERT_4_C	Bond Calc	0.90000, Rep	0.902(8)		Senseless s.u.
	O21 -H21A	1_555	1_555	#	316 Check
PLAT751_ALERT_4_C	Bond Calc	0.89000, Rep	0.885(10)		Senseless s.u.
	O21 -H21B	1_555	1_555	#	317 Check
PLAT751_ALERT_4_C	Bond Calc	0.86000, Rep	0.863(10)		Senseless s.u.
	O23 -H23A	1_555	1_555	#	320 Check
PLAT751_ALERT_4_C	Bond Calc	0.70000, Rep	0.697(8)		Senseless s.u.
	O23 -H23B	1_555	1_555	#	321 Check
PLAT752_ALERT_4_C	Angle Calc	97.00, Rep	97.3(8)		Senseless s.u.
	H21A -O21 -H21B	1_555	1_555 1_555	#	588 Check
PLAT752_ALERT_4_C	Angle Calc	110.00, Rep	110.0(12)		Senseless s.u.
	H23A -O23 -H23B	1_555	1_555 1_555	#	590 Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance	...		-1.548	Report
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			5	Note
	1 0 0, 0 2 0, 0 1 1, 0 2 1, 0 0 2,				
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595		23	Report
	4 0 0, 0 4 0, -1 2 1, 0 3 1, 1 3 1, -1 4 1,				
	0 4 1, -1 0 2, -1 1 2, -4 2 2, 0 2 2, -1 3 2,				
	0 3 2, 0 4 2, -1 1 3, 0 1 3, -1 2 3, 3 2 3,				
	0 3 3, -1 8 3, -1 0 4, -1 1 4, 1 4 13,				
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF			5	Note
	4 0 0, 0 0 2, -4 2 2, 3 2 3, -1 8 3,				
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.84Ang From C11C		2.12	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.80Ang From Cd1		1.91	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.86Ang From C19A		1.78	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.34Ang From C77		1.76	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.77Ang From Cd4		1.73	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	2.57Ang From C116		1.71	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.89Ang From C11B		1.69	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.84Ang From C116		1.57	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.82Ang From C15A		1.52	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.19Ang From C11B		-2.11	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Cd2		1.32	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Cd4		1.05	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H10A	.	-0.43	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H10B	.	-0.53	eA-3

PLAT977_ALERT_2_C	Check Negative Difference Density on H19A	.	-0.44 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H24A	.	-0.32 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H50A	.	-0.34 eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		25	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms		43	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		12	Report
	H17 H18A H19A H20A H21A H21B H22A H22B H23A H23B H24A			
	H24B			
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		146.02	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		4	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		21	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		5	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		12	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0010	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0010	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0010	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0010	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0010	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)		11%	Note
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 2)		6%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C11B ..C60	.	3.20	Ang.
	-1-x,-1/2+y,3/2-z =		2_446	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C112 ..C104	.	3.23	Ang.
	-1-x,-1/2+y,3/2-z =		2_446	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C116 ..C24	.	3.21	Ang.
	-x,-1/2+y,3/2-z =		2_546	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C11C ..C60	.	3.19	Ang.
	-1-x,-1/2+y,3/2-z =		2_446	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C118 ..C104	.	2.97	Ang.
	-1-x,-1/2+y,3/2-z =		2_446	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C118 ..C105	.	3.01	Ang.
	-1-x,-1/2+y,3/2-z =		2_446	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact C17 ..C114	.	3.22	Ang.
	x,-3/2-y,-1/2+z =		4_545	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact C17 ..C117	.	3.36	Ang.
	x,-3/2-y,-1/2+z =		4_545	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact C115 ..C119	.	3.40	Ang.
	x,-3/2-y,-1/2+z =		4_545	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd1 (II)	.	2.03	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd2 (II)	.	1.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd3 (II)	.	2.09	Info

PLAT794_ALERT_5_G Tentative Bond Valency for Cd4 (II) . 2.06 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 283 Note
 PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 49% Note
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
 0 3 3, 0 4 0, 1 4 13,
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.617 Note
 Predicted wR2: Based on SigI**2 4.27 or SHELX Weight 18.52
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

Datablock: cp1-1

Bond precision:	C-C = 0.0124 A	Wavelength=1.34138
Cell:	a=14.8185(15) alpha=90	b=33.726(3) beta=103.239(3) c=28.389(3) gamma=90
Temperature:	273 K	

	Calculated	Reported
Volume	13811(2)	13811(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	2(C35 H24 Cd Cl4 N2 O5)
Sum formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Mr	1613.55	1613.52
Dx, g cm-3	1.552	1.552
Z	8	8
Mu (mm-1)	5.585	5.585
F000	6464.0	6464.0
F000'	6498.35	
h, k, lmax	17, 39, 33	17, 39, 33
Nref	23541	23147
Tmin, Tmax	0.672, 0.756	0.455, 0.752
Tmin'	0.609	

Correction method= # Reported T Limits: Tmin=0.455 Tmax=0.752
AbsCorr = NONE

Data completeness= 0.983 Theta(max)= 52.096

R(reflections)= 0.1027(13948) wR2(reflections)=
0.3294(23147)

S = 1.066 Npar= 1551

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 Bond Without Acceptor O17 --H17A . Please Check

Author Response: The O17-H17A / O18-H18 / O19-H19A / O20A-H20A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O18 --H18 . Please Check

Author Response: The O17-H17A / O18-H18 / O19-H19A / O20A-H20A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O19 --H19A . Please Check

Author Response: The O17-H17A / O18-H18 / O19-H19A / O20A-H20A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O20A --H20A . Please Check

Author Response: The O17-H17A / O18-H18 / O19-H19A / O20A-H20A hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Cd4 1.57 eA-3

Author Response: Cd4 is a heavy atom and this alert is often found for molecules of this type.

Alert level C

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

THETM01_ALERT_3_C The value of $\sin(\theta_{\max})/\lambda$ is less than 0.590

Calculated $\sin(\theta_{\max})/\lambda = 0.5882$

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.13 Do !

PLAT084_ALERT_3_C High wR_2 Value (i.e. > 0.25) 0.33 Report

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O11 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C126 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cd3 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cd4 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C52 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C76 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C88 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C89 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C90 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C91 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C93 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C98 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C109 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cd1 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 C27 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C116 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C117 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C118 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C136 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C137 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C139 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cd3 0.109 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cd1 0.102 Check

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01239 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.337 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.115 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.588 392 Report

4	0	0,	0	4	0,	0	12	0,	0	34	0,	-1	2	1,	-4	3	1,
0	32	1,	0	0	2,	4	0	2,	3	1	2,	-4	2	2,	-1	3	2,
0	4	2,	-1	7	2,	0	8	2,	-1	2	3,	3	2	3,	0	3	3,
0	5	3,	-1	8	3,	3	1	4,	0	4	4,	2	4	4,	-1	5	4,
-1	7	4,	-1	9	4,	3	15	4,	0	31	4,	2	3	5,	-1	6	5,
-1	33	5,	1	1	6,	-1	5	6,	0	6	6,	-1	9	6,	0	31	6,
0	5	7,	-1	33	7,	-15	1	8,	2	36	8,	1	30	10,	2	32	11,
-4	34	12,	1	4	13,	1	29	13,	1	34	13,	0	0	14,	1	29	15,
0	0	16,	1	0	16,	0	1	16,	1	1	16,	0	2	16,	1	4	16,
0	1	17,	1	1	17,	0	2	17,	1	2	17,	1	3	17,	1	4	17,
-6	20	17,	-12	0	18,	-1	0	18,	0	0	18,	1	0	18,	-1	1	18,
0	1	18,	1	1	18,	0	2	18,	1	2	18,	0	3	18,	1	3	18,
0	4	18,	1	4	18,	1	5	18,	0	6	18,	-6	17	18,	-1	1	19,
0	1	19,	1	1	19,	4	1	19,	-1	2	19,	0	2	19,	1	2	19,
-2	3	19,	0	3	19,	4	3	19,	0	4	19,	-6	16	19,	-7	19	19,
-3	22	19,	-2	0	20,	-1	0	20,	0	0	20,	1	0	20,	-2	1	20,

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 12 Note

4	0	0,	0	0	2,	-4	2	2,	0	4	2,	-1	7	2,	0	8	2,
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3 2 3, 0 3 3, -1 8 3, -1 9 4, -1 5 6, -1 9 6,	
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.30Ang From Cd2	1.66 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Cd4	-1.52 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Cd1	1.05 eA-3

Author Response: Cd4 is a heavy atom and this alert is often found for molecules of this type.

PLAT977_ALERT_2_C Check Negative Difference Density on H17A	.	-0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H61	.	-0.38 eA-3



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.		
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite		27 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms		166 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension		1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms		6 Report
H19A H20A H20 H17A H18 H18A		
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ		Please Check
Calc: C70 H48 Cd2 Cl8 N4 O10		
Rep.: 2(C35 H24 Cd Cl4 N2 O5)		
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large		0.17 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large		60.03 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records		19 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records		1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records		2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records		3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records		11 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used		0.0010 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used		0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used		0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par		0.0001 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar		0.0020 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par		0.0001 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar		0.0002 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K)		273 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K)		273 Check
PLAT301_ALERT_3_G Main Residue Disorder (Resd 1)		2% Note
PLAT301_ALERT_3_G Main Residue Disorder (Resd 2)		6% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H3 ..H7 .		2.08 Ang.
	x,y,z =	1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H6 ..H17 .		2.12 Ang.
	x,y,z =	1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H9 ..H14 .		2.07 Ang.
	x,y,z =	1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H9 ..H14A .		2.13 Ang.
	x,y,z =	1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H17 ..H6A .		2.10 Ang.
	x,y,z =	1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H24 ..H13A .		2.08 Ang.
	x,y,z =	1_555 Check
PLAT414_ALERT_2_G Short Intra D-H...H-X H19A ..H77D .		1.68 Ang.
	2-x,-1/2+y,1/2-z =	2_745 Check
PLAT414_ALERT_2_G Short Intra D-H...H-X H20A ..H72 .		1.97 Ang.

PLAT415_ALERT_2_G Short Inter D-H...H-X	H9	x,y,z = ..H18	.	1_555 Check
		1-x,-y,1-z =	.	1.90 Ang.
PLAT415_ALERT_2_G Short Inter D-H...H-X	H9	..H18A	.	3_656 Check
		1-x,-y,1-z =	.	1.83 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C17	..C68	.	3_656 Check
		x,y,z =	.	3.20 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C113	..C131	.	1_555 Check
		x,-1+y,z =	.	3.20 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact	C13	..C111	.	1_545 Check
		1-x,-y,1-z =	.	3.23 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure				3_656 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C12		--C13A		122 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1		(II)	.	1.73 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2		(II)	.	2.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd3		(II)	.	1.98 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd4		(II)	.	2.04 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints				2.02 Info
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed				2790 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).				! Info
0 2 0, 0 1 1,				2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File				5 Note
0 1 1, 0 5 7, 0 6 6, 1 4 13, 3 15 4,				
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity				4.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value				4.137 Note
Predicted wR2: Based on SigI**2 7.96 or SHELX Weight 30.91				
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.				0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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20 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
7 ALERT type 5 Informative message, check

Datablock: cp1-2

Bond precision:	C-C = 0.0105 A	Wavelength=1.34138
Cell:	a=14.8687(7)	b=33.5918(15) c=28.2887(13)
	alpha=90	beta=103.812(2) gamma=90
Temperature:	273 K	

	Calculated	Reported
Volume	13720.7(11)	13720.7(11)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H48 Cd2 C18 N4 O10 [+ solvent]	2(C35 H24 Cd C14 N2 O5), [+ solventS]
Sum formula	C70 H48 Cd2 C18 N4 O10 [+ solvent]	C70 H48 Cd2 C18 N4 O10
Mr	1613.55	1613.52
Dx, g cm ⁻³	1.562	1.562
Z	8	8
Mu (mm ⁻¹)	5.622	5.622
F000	6464.0	6464.0
F000'	6498.35	
h, k, lmax	19, 43, 36	19, 43, 36
Nref	31594	31050
Tmin, Tmax	0.535, 0.570	0.503, 0.752
Tmin'	0.485	

```
Correction method= # Reported T Limits: Tmin=0.503 Tmax=0.752
AbsCorr = NONE
```

Data completeness= 0.983 Theta (max)= 60.699

[illegible]

S = 1.070 Npar= 1690

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 Bond Without Acceptor 017 --H17A . Please Check

Author Response: The O17-H17A / O18-H18A / O19-H19 / O20-H20 hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor 018 --H18A . Please Check

Author Response: The O17-H17A / O18-H18A / O19-H19 / O20-H20 hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O19 --H19 . Please Check

Author Response: The O17-H17A / O18-H18A / O19-H19 / O20-H20 hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.

PLAT420_ALERT_2_B D-H Bond Without Acceptor O20 --H20 . Please Check

Author Response: The O17-H17A / O18-H18A / O19-H19 / O20-H20 hydroxo groups are a little unstable in their positions. No suitable acceptor has been located for this hydroxo group.



Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.27	Report
PLAT213_ALERT_2_C	Atom Cl4 has ADP max/min Ratio	3.1	prolat
PLAT215_ALERT_3_C	Disordered Cl4A has ADP max/min Ratio	3.3	Note
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	3.4	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	4.1	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	011	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C110	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C111	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C118	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C134	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	01	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	02	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	03	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	04	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	05	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	08	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C39	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C54	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C66	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C102	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C109	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C117	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C119	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C127	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C128	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C132	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C135	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Cd1	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	C47	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C49	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C53	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C56	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C64	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C65	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C68	Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C70 Check
 PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C43 -C45 . 1.37 Ang.
 PLAT336_ALERT_2_C Long Bond Distance for C130 -C112 1.970 Ang.
 PLAT336_ALERT_2_C Long Bond Distance for C70 -C14A 1.967 Ang.
 PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01054 Ang.
 PLAT414_ALERT_2_C Short Intra D-H..H-X H10B ..H20 . 1.90 Ang.
 x,y,z = 1_555 Check
 PLAT415_ALERT_2_C Short Inter D-H..H-X H19 ..H84 . 2.10 Ang.
 2-x,-y,1-z = 3_756 Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.030 Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 246 Report
 2 0 0, 4 0 0, 6 0 0, 7 1 0, 3 3 0, 7 3 0,
 0 4 0, 4 4 0, 6 4 0, 2 8 0, 4 8 0, 0 12 0,
 4 1 1, -3 2 1, -1 2 1, 1 2 1, 3 2 1, 7 2 1,
 -4 3 1, -4 4 1, -1 6 1, -4 7 1, 0 7 1, 0 9 1,
 3 10 1, -11 28 1, 0 0 2, 4 0 2, 6 0 2, -7 1 2,
 -3 1 2, -1 1 2, 3 1 2, -4 2 2, 2 2 2, -3 3 2,
 -1 3 2, 0 4 2, 6 4 2, -3 5 2, -1 5 2, 0 6 2,
 -1 7 2, 0 8 2, 6 8 2, -1 9 2, 1 17 2, -14 19 2,
 7 22 2, -1 26 2, -4 1 3, 0 1 3, -4 2 3, -1 2 3,
 3 2 3, 7 2 3, -8 3 3, -6 3 3, -4 3 3, -2 3 3,
 0 3 3, 2 3 3, -5 4 3, 1 4 3, -2 5 3, 0 5 3,
 -1 6 3, 3 6 3, 7 6 3, -8 7 3, -1 8 3, 3 22 3,
 0 23 3, -12 0 4, -6 0 4, 10 0 4, 14 0 4, -1 1 4,
 1 1 4, 3 1 4, -4 2 4, -2 2 4, 0 2 4, -8 4 4,
 -4 4 4, 0 4 4, 2 4 4, -5 5 4, -3 5 4, -1 5 4,
 3 5 4, -1 7 4, -8 8 4, -1 8 4, 0 8 4, 4 8 4,
 PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 42 Note
 4 0 0, 7 1 0, 0 4 0, 3 2 1, 7 2 1, -4 3 1,
 0 0 2, 4 0 2, -7 1 2, -4 2 2, 0 4 2, -1 7 2,
 0 8 2, 0 1 3, -1 2 3, 3 2 3, 7 2 3, -4 3 3,
 0 3 3, 0 5 3, -1 8 3, 0 4 4, -5 5 4, -1 5 4,
 PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 5 Check
 PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
 4 2 0,
 PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Cdl 1.85 eA-3
 PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.04Ang From O18 -2.15 eA-3
 PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.75Ang From Cdl -1.54 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H17A . -0.36 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H18A . -0.32 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H19 . -0.38 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H20 . -0.33 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H40 . -0.37 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
 not performed for this radiation type.
 PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
 PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 14 Report
 PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
 H19 H20 H17A H18A
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: C70 H48 Cd2 Cl8 N4 O10
 Rep.: 2(C35 H24 Cd Cl4 N2 O5),
 PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.16 Report

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	17.33	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		4	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		3	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0010	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	 (K)	273	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	 (K)	273	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl17	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	1%	Note
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 2)	1%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact Cl9	..C51	3.25	Ang.
		x,y,z =	1_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl1	..Cl14	3.32	Ang.
		1-x,1-y,1-z =	3_666	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl3	..Cl11	3.27	Ang.
		1-x,1-y,-z =	3_665	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		151	A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd1	(II)	2.01	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd2	(II)	1.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd3	(II)	2.06	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd4	(II)	2.07	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		88	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks	Suppressed	!	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).		2	Note
	0 2 0, 0 1 1,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	296	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		17	Note
	-13 2 15, -13 3 15, -2 1 9, -2 6 8, -1 3 5,	0 1 1,		
	0 2 0, 0 2 7, 0 6 6, 0 23 3, 1 4 3,	1 17 2,		
	2 0 0, 2 2 2, 2 23 7, 3 22 3, 4 0 0,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.6	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		4.360	Note
	Predicted wR2: Based on SigI**2	6.30 or SHELX Weight	25.67	
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
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 35 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 61 ALERT type 2 Indicator that the structure model may be wrong or deficient
 16 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 7 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.

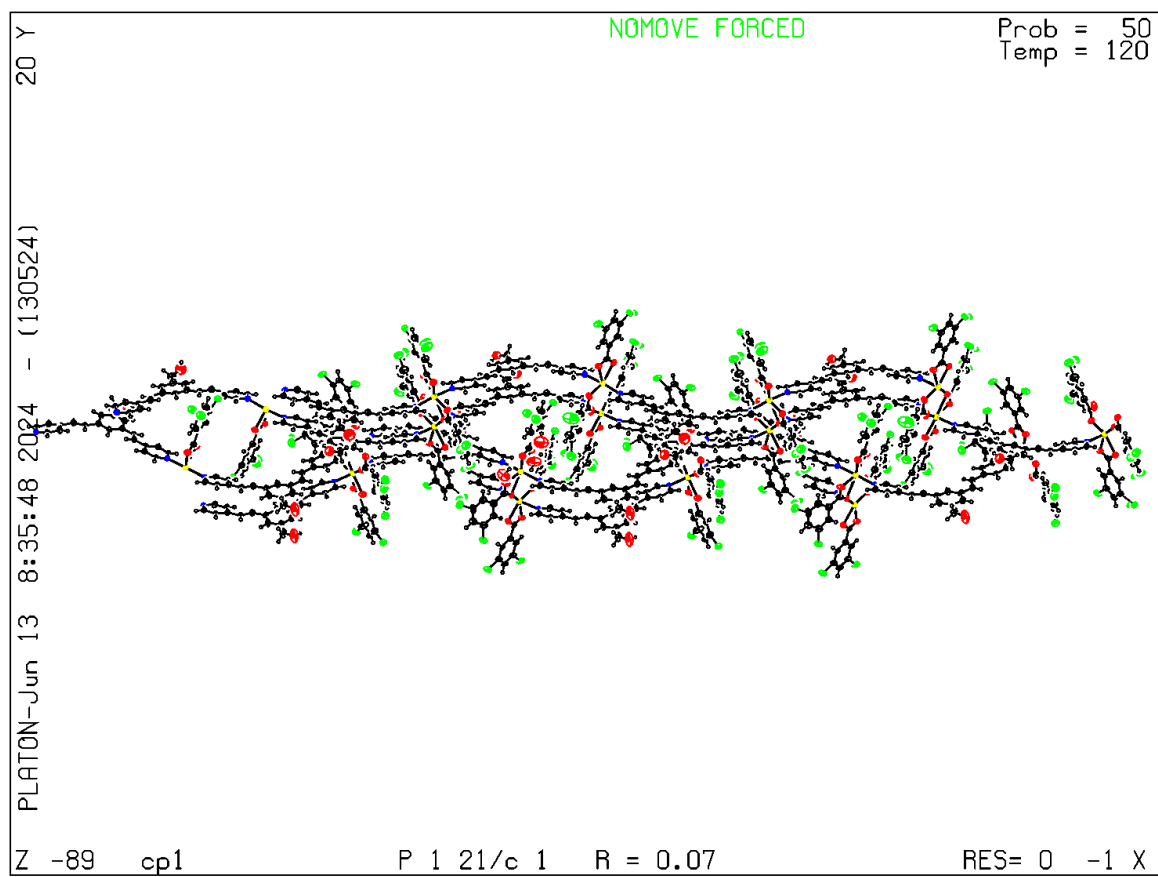
Publication of your CIF in IUCr journals

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.

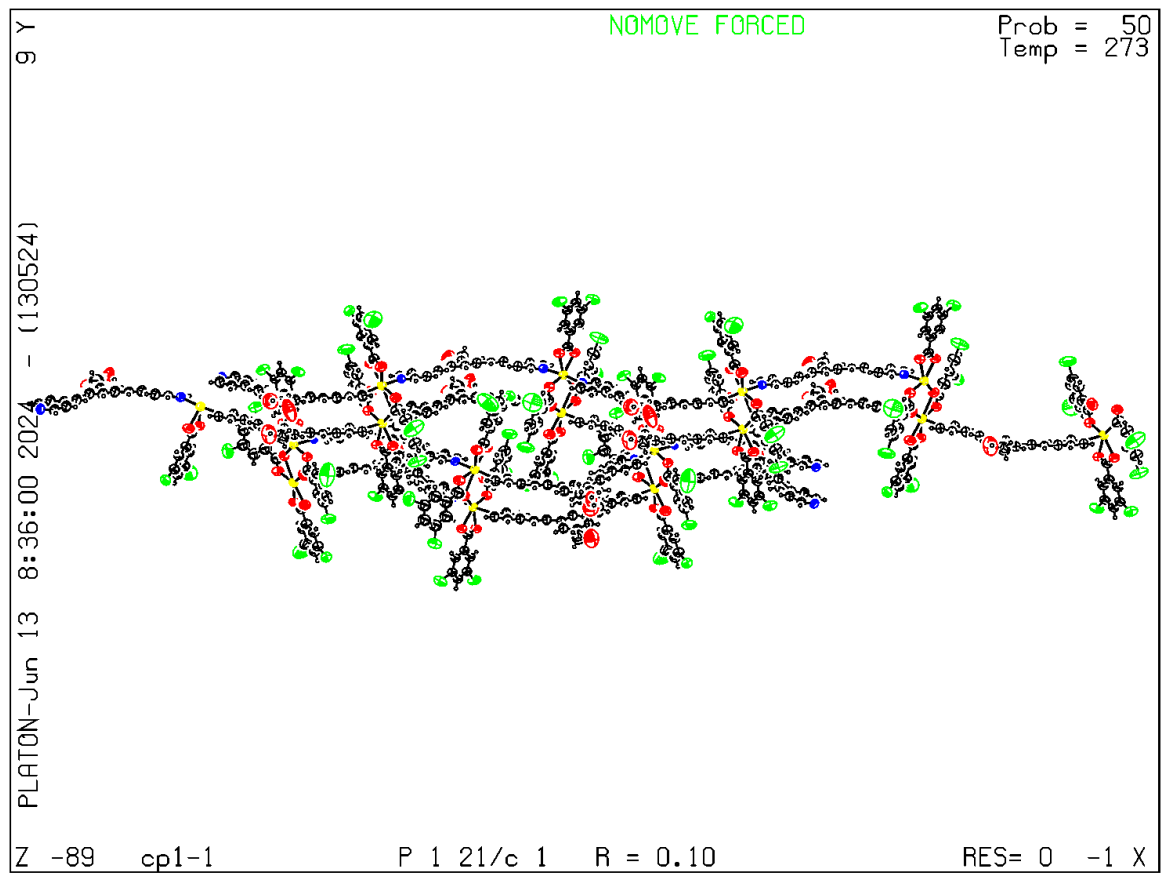
Publication of your CIF in other journals

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

Datablock cp1 - ellipsoid plot



Datablock cp1-1 - ellipsoid plot



Datablock cp1-2 - ellipsoid plot

