checkCIF/PLATON report (publication check)

No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: complex1

Bond precision: C-C = 0.0065 A Wavelength=0.71073

Cell: a=11.6822(8) b=11.7376(8) c=6.2220(4)
alpha=90 beta=90.0466 (18) gamma=90

Temperature: 295 K

	Calculated	Reported
Volume	853.17(10)	853.17(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C6 H3 Ag2 Cl O4 S	C6 H3 Ag2 Cl O4 S
Sum formula	C6 H3 Ag2 Cl O4 S	C6 H3 Ag2 Cl O4 S
Mr	422.34	422.33
Dx,g cm-3	3.288	3.288
Z	4	4
Mu (mm-1)	5.125	5.125
F000	792.0	792.0
F000'	786.19	
h,k,lmax	15,15,8	15,15,8
Nref	1941	1937
Tmin,Tmax	0.427,0.541	0.476,0.578
Tmin'	0.414	

Correction method= MULTI-SCAN
Data completeness= 0.998 Theta(max)= 27.470
R(reflections)= 0.0250(1830) wR2(reflections)= 0.0614(1937)
S = 1.060 Npar= 128

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

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag1 -- O3_d .. 5.32 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag2 -- O2 .. 6.38 su

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Alert level G

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.38 Ratio
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Ag1 ..... 1.02
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Ag2 ..... 0.85

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0 **ALERT level A** = In general: serious problem
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3 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: complex2

Bond precision: C-C = 0.0043 A Wavelength=0.71073
Cell: a=9.6946(19) b=11.245(2) c=9.2827(19)
alpha=90 beta=100.76(3) gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	994.2(3)	994.2(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C6 H5 Ag2 Cl O5 S	C6 H5 Ag2 Cl O5 S
Sum formula	C6 H5 Ag2 Cl O5 S	C6 H5 Ag2 Cl O5 S
Mr	440.36	440.35
Dx,g cm-3	2.942	2.942

Z	4	4
Mu (mm-1)	4.411	4.412
F000	832.0	832.0
F000'	826.23	
h,k,lmax	12,14,12	12,14,12
Nref	2267	2264
Tmin,Tmax	0.535,0.616	0.539,0.642
Tmin'	0.489	

Correction method= MULTI-SCAN
Data completeness= 0.999 Theta(max)= 27.420
R(reflections)= 0.0282(2125) wR2(reflections)= 0.0710(2264)
S = 1.071 Npar= 142

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 O	Ueq(max)/Ueq(min) ...	3.44 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H	Uiso(max)/Uso(min) ...	5.22 Ratio
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Ag1 -- Cl1_b ..		8.17 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Ag1 -- C3_f ..		5.66 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Ag2 -- O1W ..		6.43 su
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for		Ag2
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond C3 - C4 ...		1.39 Ang.
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond C4 - C5 ...		1.39 Ang.

Alert level G

PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.29 Ratio
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Ag1	0.80
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Ag2	1.01

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0 **ALERT level A** = In general: serious problem
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8 **ALERT level C** = Check and explain
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   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   2 ALERT type 5 Informative message, check
```

Datablock: complex3

```
Bond precision:     C-C = 0.0053 A              Wavelength=0.71073
Cell:       a=9.7366(19)   b=11.322(2)    c=9.4589(19)
            alpha=90       beta=101.22(3) gamma=90
Temperature: 295 K
                   Calculated                    Reported
Volume             1022.8(4)                     1022.8(4)
Space group        P 21/c                        P 21/c
Hall group         -P 2ybc                       -P 2ybc
Moiety formula     C6 H5 Ag2 Br O5 S             C6 H5 Ag2 Br O5 S
Sum formula        C6 H5 Ag2 Br O5 S             C6 H5 Ag2 Br O5 S
Mr                 484.81                        484.81
Dx,g cm-3          3.148                         3.148
Z                  4                             4
Mu (mm-1)          7.934                         7.934
F000               904.0                         904.0
F000'              896.59
h,k,lmax           12,14,12                      12,14,12
Nref               2339                          2335
Tmin,Tmax          0.332,0.490                   0.382,0.535
Tmin'              0.292
Correction method= MULTI-SCAN
Data completeness= 0.998       Theta(max)= 27.440
R(reflections)= 0.0296( 2061)     wR2(reflections)= 0.0748( 2335)
S = 1.073            Npar= 142
```

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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag1 -- Br1_d .. 15.86 su

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Alert level C

PLAT220_ALERT_2_C Large Non-Solvent O Ueq(max)/Ueq(min) ... 3.20 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uso(min) ... 4.78 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag2 -- O1W .. 5.76 su
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Ag2
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C3 - C4 ... 1.38 Ang.

Alert level G

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.40 Ratio
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Ag1 ..... 0.68
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Ag2 ..... 0.95

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Datablock: complex4

Bond precision: C-C = 0.0068 A Wavelength=0.71073
Cell: a=11.761(2) b=23.561(5) c=5.7475(11)
alpha=90 beta=91.35(3) gamma=90
Temperature: 295 K

	Calculated	Reported

Volume	1592.2(5)	1592.2(5)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	C6 H2 Ag4 N O11 S2, Ag H6 N2	C6 H2 Ag4 N O11 S2, Ag H6 N2
Sum formula	C6 H8 Ag5 N3 O11 S2	C6 H8 Ag5 N3 O11 S2
Mr	901.64	901.62
Dx,g cm-3	3.761	3.761
Z	4	4
Mu (mm-1)	6.370	6.370
F000	1680.0	1680.0
F000'	1663.71	
h,k,lmax	15,30,7	15,30,7
Nref	1879	1868
Tmin,Tmax	0.273,0.410	0.348,0.469
Tmin'	0.252	

Correction method= MULTI-SCAN

Data completeness= 0.994 Theta(max)= 27.470

R(reflections)= 0.0494(1736) wR2(reflections)= 0.1259(1868)

S = 1.083 Npar= 139

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

PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for			N1	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for			O5	
PLAT420_ALERT_2_C	D-H Without Acceptor	N2	-	H2N2 ...	?	
PLAT420_ALERT_2_C	D-H Without Acceptor	N3	-	H3N1 ...	?	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of				Ag3	

Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	16.35	
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	13	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	4	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.64	Ratio
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Ag1	0.75	

PLAT794_ALERT_5_G Note: Tentative Bond Valency for Ag2 ..... 1.09

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checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
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

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
missing. This is required for a full paper submission (but is
optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

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7 **ALERT level A** = Data missing that is essential or data in wrong format
2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should always 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 the submission requirements of the journal and these should be commented upon in the discussion or experimental section of a paper - after all, they might represent an interesting feature.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

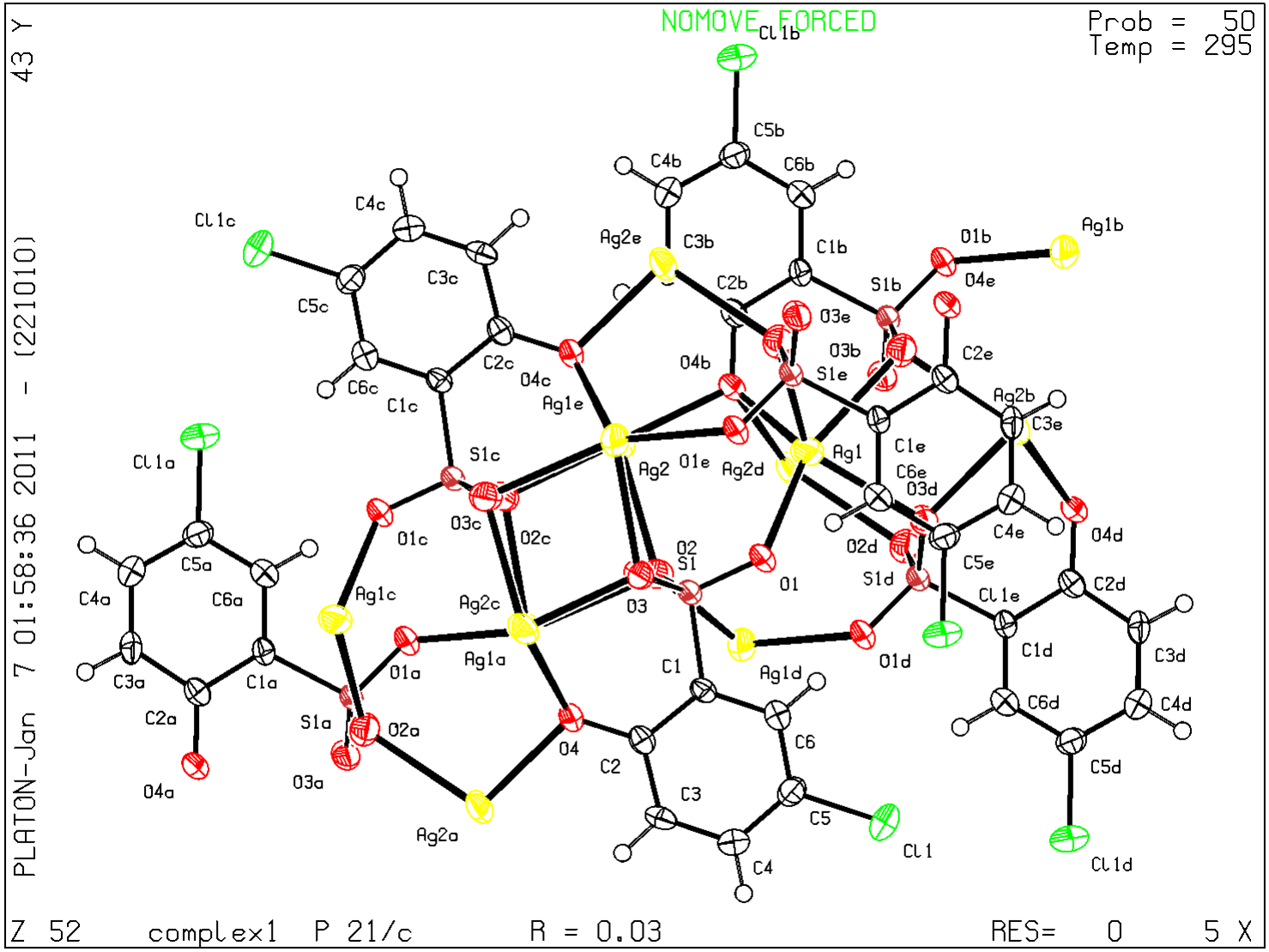
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
```

```
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_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 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 22/10/2010; check.def file version of 11/10/2010

Datablock complex1 - ellipsoid plot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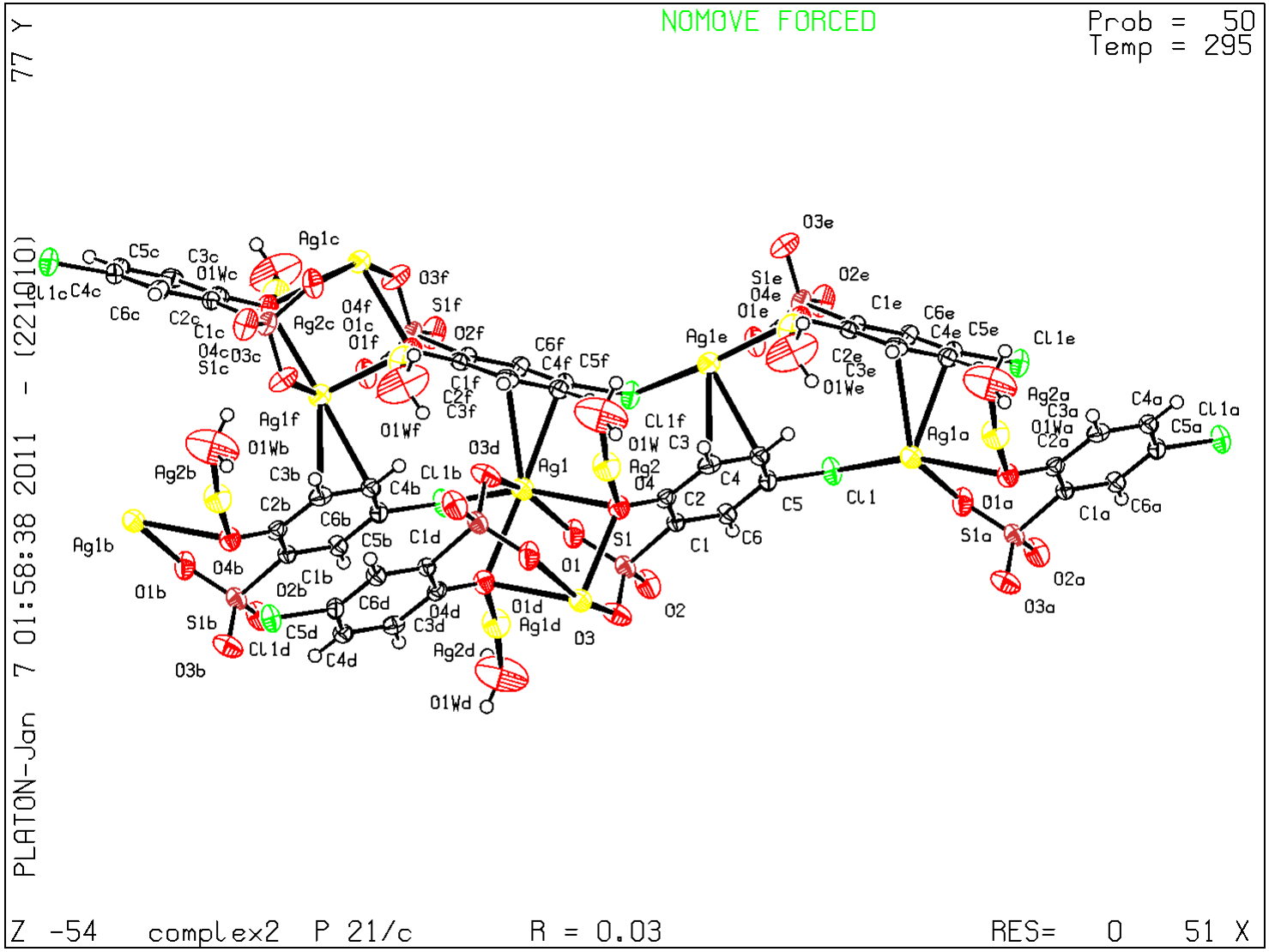
Prob = 50
Temp = 295
PLATON-Jan 7 01:58:36 2011 - (221010)
43 Y
Z 52 complex1 P 21/c R = 0.03 RES= 0 5 X
Cl1b
C5b
C4b
C6b
C1b
C4c
Cl1c
C3b
Ag2e
O1b
Ag1b
O4e
C3c
C5c
C2b
S1b
O3e
O3b
C2e
C2c
O4c
O4b
S1e
C6c
C1c
Ag1e
Ag2b
C3e
Cl1a
S1c
Ag2
O1e
Ag2d
Ag1
C1e
C6e
O3d
O1c
O3c
O2c
O2
S1
O2d
C4e
O4d
C5a
C5e
C4a
C6a
Ag1c
Ag2c
O3
O1
S1d
Cl1e
C2d
C1d
C3d
O1a
Ag1a
C1
Ag1d
O1d
C3a
C1a
C6d
C4d
C2a
S1a
O2a
O4
C2
C6
C5d
O4a
O3a
C3
C5
Cl1
Ag2a
C4
Cl1d

Datablock complex2 - ellipsoid plot


NOMOVE FORCED
Prob = 50
Temp = 295
PLATON-Jan 7 01:58:38 2011 - (221010) 77 Y
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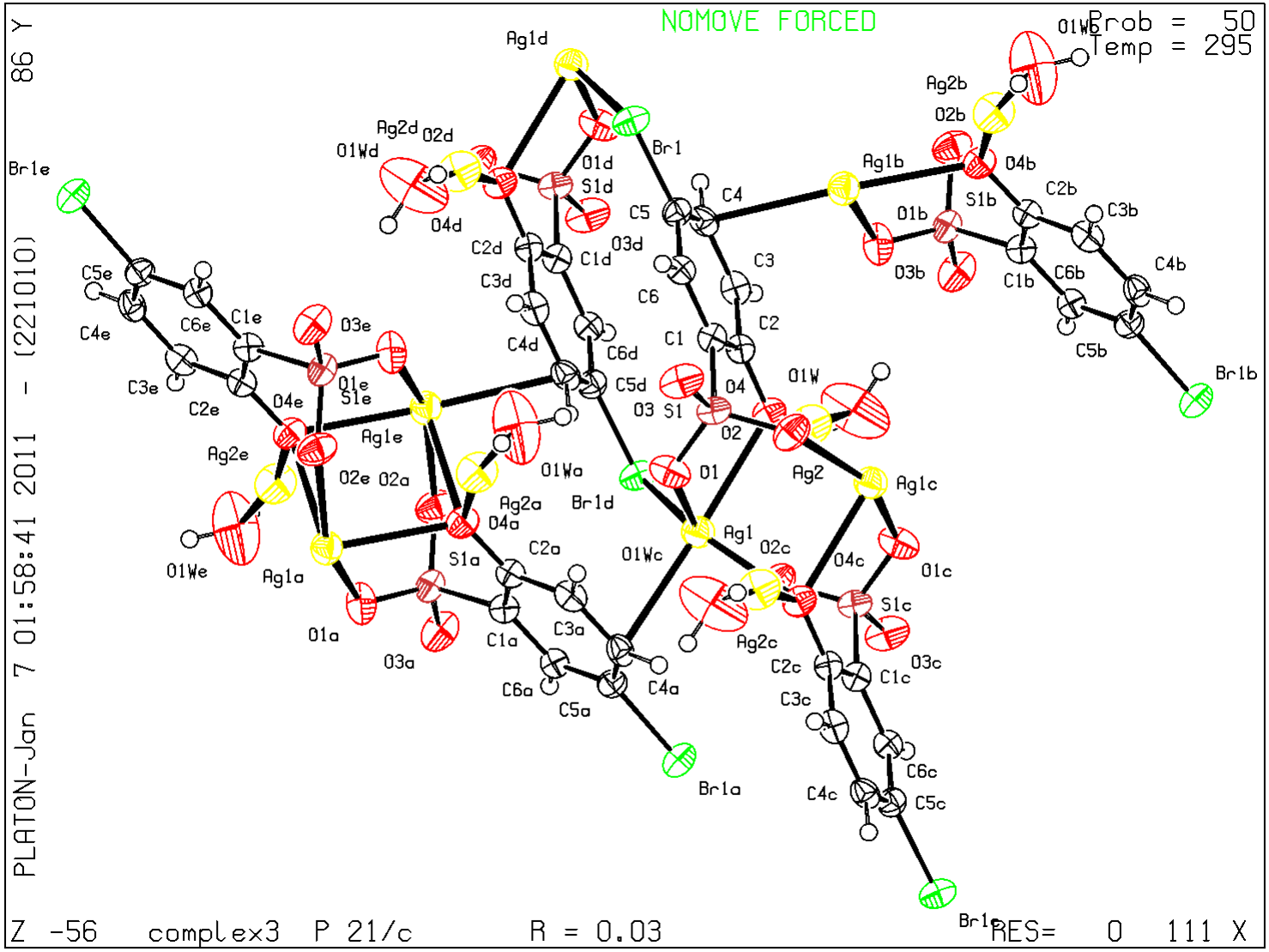
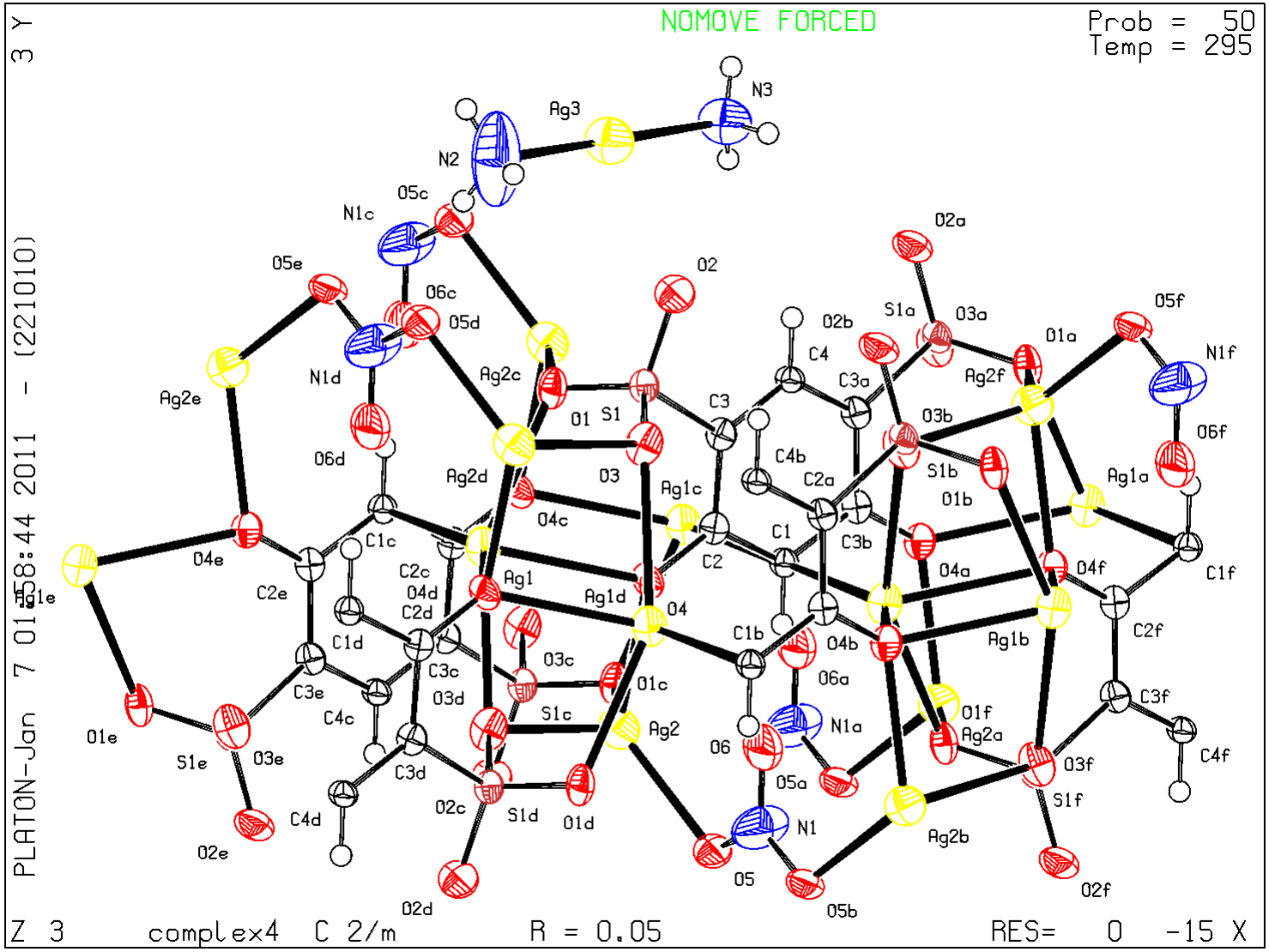
Ag1c
O3f
S1f
O2f
O4f
O1c
O1f
C6f
C4f
C5f
C1f
C2f
C3f
O1WF
Cl1f
O1W
C3
Ag2
O4
C4
C2
C5
Cl1
C1
C6
S1
O1
O2
O3
Ag1
O3d
Cl1b
C4b
C3b
C2b
C6b
C5b
C1d
C1b
O2b
O4b
Ag1b
O1b
S1b
Cl1d
O3b
C5d
C4d
C6d
O4d
C3d
O1d
Ag1d
Ag2d
O1Wd
Ag2b
O1Wb
Ag1f
C5c
C3c
O1Wc
Cl1c
C4c
C6c
C2c
C1c
O4c
O3c
S1c
Ag2c
O3e
S1e
O4e
O1e
O2e
C1e
C6e
C4e
C5e
Cl1e
C2e
C3e
O1We
Ag1e
Ag2a
C3a
O1Wa
C2a
C4a
Cl1a
C5a
Ag1a
O1a
S1a
O2a
O3a
C1a
C6a

Datablock complex3 - ellipsoid plot


NOMOVE FORCED
Prob = 50
Temp = 295
PLATON-Jan 7 01:58:41 2011 - (221010) 86 Y
Z -56 complex3 P 21/c R = 0.03
RES= 0 111 X
Ag1d
Br1
Ag2d
O2d
O1Wd
O4d
O1d
S1d
O3d
C1d
C2d
C3d
C4d
C5d
C6d
C5
C4
C3
C6
C1
C2
O4
O3
S1
O2
O1
O1W
Ag2
Ag1c
O1c
S1c
O4c
O2c
Ag2c
C2c
C1c
O3c
C3c
C6c
C4c
C5c
Br1c
Ag1
O1Wc
Br1d
Ag2a
O1Wa
O4a
S1a
C2a
C1a
C3a
C4a
C5a
C6a
O1a
O3a
Ag1a
O1We
Ag2e
O2e
O2a
Ag1e
S1e
O4e
O1e
O3e
C1e
C6e
C5e
C4e
C3e
C2e
Br1e
Ag1b
O2b
Ag2b
O1Wb
O4b
S1b
O1b
O3b
C2b
C3b
C4b
C5b
C6b
C1b
Br1b

Datablock complex4 - ellipsoid plot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Prob = 50
Temp = 295
3 Y
PLATON-Jan 7 01:58:44 2011 - (221010)
Z 3 complex4 C 2/m R = 0.05 RES= 0 -15 X
Ag3
N3
N2
O5c
N1c
O5e
O6c
O5d
N1d
Ag2e
O6d
Ag2c
O2
O1
S1
C3
O2a
O2b
S1a
O3a
C4
C3a
O1a
Ag2f
O5f
N1f
O6f
O3b
S1b
Ag1a
O1b
Ag2d
O3
Ag1c
C4b
C2a
C1
C3b
O4a
O4f
C1f
C2f
C3f
C4f
Ag1b
O4b
C1b
O6a
N1a
O1f
Ag2a
O3f
S1f
O2f
Ag2b
O5b
O5
N1
O6
O5a
O4
Ag1d
Ag1
O4c
O4d
C2c
C1c
O4e
C2e
Ag1e
O1e
S1e
O3e
C4c
C3e
C1d
C2d
C3c
O3d
O3c
O1c
S1c
Ag2
C3d
O2c
S1d
O1d
C4d
O2e
O2d

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