Electronic Supplementary Material (ESI) for CrystEngComm.
This journal is © The Royal Society of Chemistry 2025

Electronic Supplementary Information

Strong supramolecular synthons assembled by hydrogen bonds and chalcogen bonds

Yu Zhang, Xiaotian Sun and Weizhou Wang*

College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471934, P. R. China

E-mail: wzw@lynu.edu.cn

Contents

S1. Methods

S1.1. Cocrystal synthesis

The 5-nitroisophthalic acid (purity: ⩾98%), 5-bromoisophthalic acid (purity: ⩾98%), 5-methylisophthalic acid (purity: ⩾98%), 5-aminoisophthalic acid (purity: ⩾98%), 4-bromoisophthalic acid (purity: ⩾98%), 2,5-thiophenedicarboxylic acid (purity: ⩾ 98%) and 2,1,3-benzoselenadiazole (purity: ⩾ 98%) were purchased from Alfa Chemical Co., Ltd., Zhengzhou, China. The solvents ethanol (analytical reagent grade) were purchased from local suppliers. All reagents and solvents were used without further purification. The synthetic procedure of each cocrystal is almost the same. Using 20 mL ethanol as solvent, we prepared the solutions of binary mixtures of 2,1,3-benzoselenadiazole (0.2 mmol, 0.0366 g) with 5-nitroisophthalic acid (0.2 mmol, 0.0422 g), 5-bromoisophthalic acid (0.2 mmol, 0.0490 g), 5-methylisophthalic acid (0.2 mmol, 0.0360 g), 5-aminoisophthalic acid (0.2 mmol, 0.0362 g), 4-bromoisophthalic acid (0.2 mmol, 0.0490 g) and 2,5-thiophenedicarboxylic acid (0.2 mmol, 0.0344 g), respectively, by gently stirring in the air at room temperature. After 7-8 days, single crystals of six cocrystals suitable for single-crystal X-ray diffraction analyses were successfully synthesized by slowly evaporating these solutions also in the air and at room temperature.

S1.2. Single-crystal X-ray diffraction

Single-crystal X-ray diffraction data were collected on the Bruker D8 or Oxford Diffraction SuperNova area-detector diffractometer equipped with the Mo-Kα X-ray source (λ = 0.71073 Å). The data reduction was performed using CrysAlisPro software.[1,2] The crystal structure was solved and refined with the SHELXS-97/SHELXS-2014 program.[3-5] Anisotropic thermal parameters were assigned to all non-hydrogen atoms. The hydrogen atoms were set in calculated positions and refined as riding atoms with a common fixed isotropic thermal parameter. Crystallographic data of the six cocrystals were listed in the next section. The CIF files of the thirteen cocrystals (CCDC deposition numbers: 2429784-2429789) can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html. At the same time, the CIF files of the six cocrystals were also provided as the electronic supplementary materials. The

checkcif files for the six cocrystal structures can be found in the Supplementary Materials.

S1.3. Computational details

The geometries of the complexes were not optimized, and taken from the corresponding crystal structures. All the density functional theory (DFT) calculations were carried out at the PBE0-D3(BJ)/def2-TZVPP level of theory with the Gaussian 09 program.[6-10] Previous studies on the noncovalent interactions have shown that the PBE0-D3(BJ)/def2-TZVPP calculations can give comparable results with the "golden standard" coupled cluster calculations.[11,12] It is well known that the accuracy of the DFT calculations also depends on the number of points used in the numerical integration. An "ultrafine" integration grid (99 radial, 590 angular points) was used for all the DFT calculations to avoid the possible integration grid errors. All the interaction energies have been corrected for basis set superposition error by using the counterpoise scheme of Boys and Bernardi.[13] In this study, the interaction energy refers to the sum of the interaction energy of an O−H···N hydrogen bond and the corresponding N−Se···O chalcogen bond. This combined value represents the strength of the supramolecular synthon, making it unnecessary to separately calculate the interaction energies of the O−H···N hydrogen bond and the N−Se···O chalcogen bond.

To further confirm the existence of the synthons, the "atoms in molecules" (AIM) analysis has been performed with the PBE0-D3(BJ)/def2-TZVPP electron density.[14] The AIM2000 software was employed to carry out the AIM analysis.[15]

S2. Supplementary Results

Table S1 The crystallographic data and structure refinement parameters for [IPA-5-NO_2][BSeD], [IPA-5-Br][BSeD], [IPA-5-CH_3][BSeD] and [IPA-5-NH_2][BSeD].

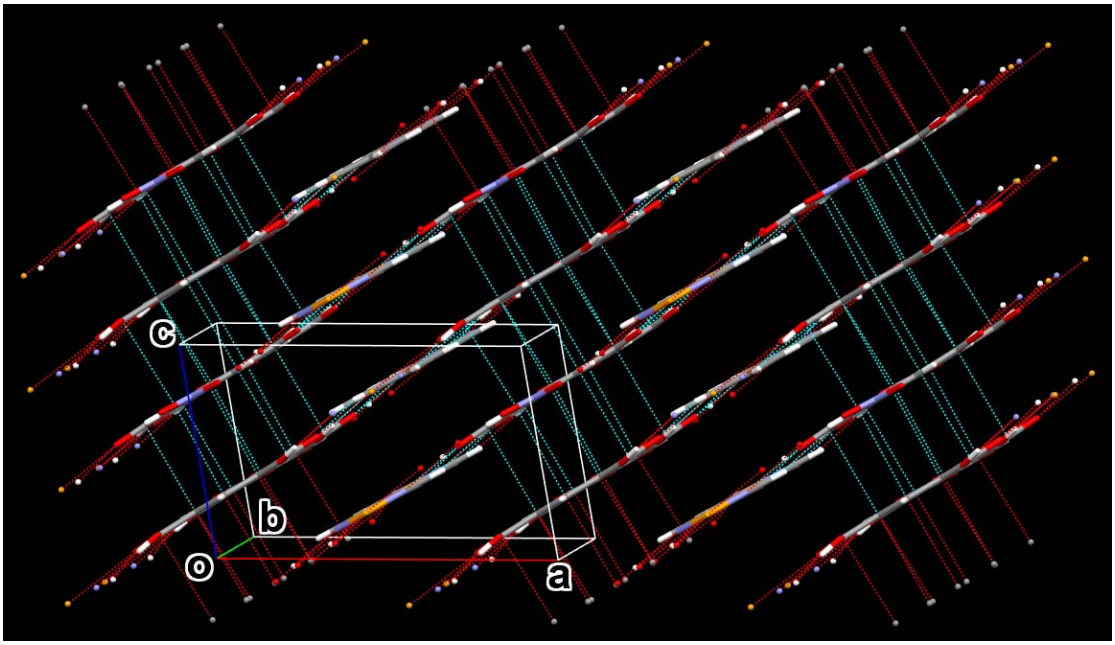
Cocrystal	**[IPA-5-NO_2][BSeD]**	**[IPA-5-Br][BSeD]**
CCDC No.	2429784	2429785
Empirical formula	$C_{14}H_9N_3O_6Se$	$C_{14}H_9BrN_2O_4Se$
Formula weight	394.203	428.10
Crystal size/mm^3	0.3 × 0.25 × 0.18	0.16 × 0.15 × 0.13
Crystal system	monoclinic	monoclinic
Space group	*P*2/c	*P*2/c
a/Å	11.3555(4)	11.154(3)
b/Å	9.1502(3)	9.184(2)
c/Å	7.1692(4)	7.3865(19)
α/°	90	90
β/°	99.648(5)	99.177(9)
γ/°	90	90
V/$Å^3$	734.38(6)	746.9(3)
Z	2	2
ρ_{calc}/$g\cdot cm^{-3}$	1.783	1.903
T/K	293(2)	300(2)
2ϑ range for data collection/°	7.28–58.4	5.776–55.656
Reflections collected	7626	15360
Independent reflections [R_{int}]	1733 [0.0377]	1758 [0.1080]
R_1, wR_2 (I > 2σ(I))	0.0384, 0.0772	0.0515, 0.1006
R_1, wR_2 (all data)	0.0504, 0.0829	0.0860, 0.1144
Goodness-of-fit on F^2	1.076	1.027

Cocrystal	**[IPA-5-CH_3][BSeD]**	**[IPA-5-NH_2][BSeD]**
CCDC No.	2429786	2429787
Empirical formula	$C_{15}H_{12}N_2O_4Se$	$C_{14}H_{11}N_3O_4Se$
Formula weight	363.233	364.22
Crystal size/mm^3	0.26 × 0.25 × 0.20	0.09 × 0.08 × 0.07
Crystal system	monoclinic	monoclinic
Space group	$P2_1/m$	$P2_1/m$
a/Å	7.4596(4)	6.8417(7)
b/Å	12.3445(6)	12.3348(11)
c/Å	8.6525(4)	8.5209(7)
α/°	90	90
β/°	112.155(6)	102.207(4)
γ/°	90	90
V/$Å^3$	737.94(7)	702.83(11)
Z	2	2
ρ_{calc}/$g\cdot cm^{-3}$	1.635	1.721
T/K	293(2)	300(2)
2*ϑ* range for data collection/°	6.76–58.54	13.24–145.57
Reflections collected	7916	1459
Independent reflections [R_{int}]	1873 [0.0301]	1459 [0.0655]
R_1, wR_2 (I > 2σ(I))	0.0346, 0.0669	0.0821, 0.2303
R_1, wR_2 (all data)	0.0451, 0.0702	0.0897, 0.2443
Goodness-of-fit on F^2	1.042	1.086

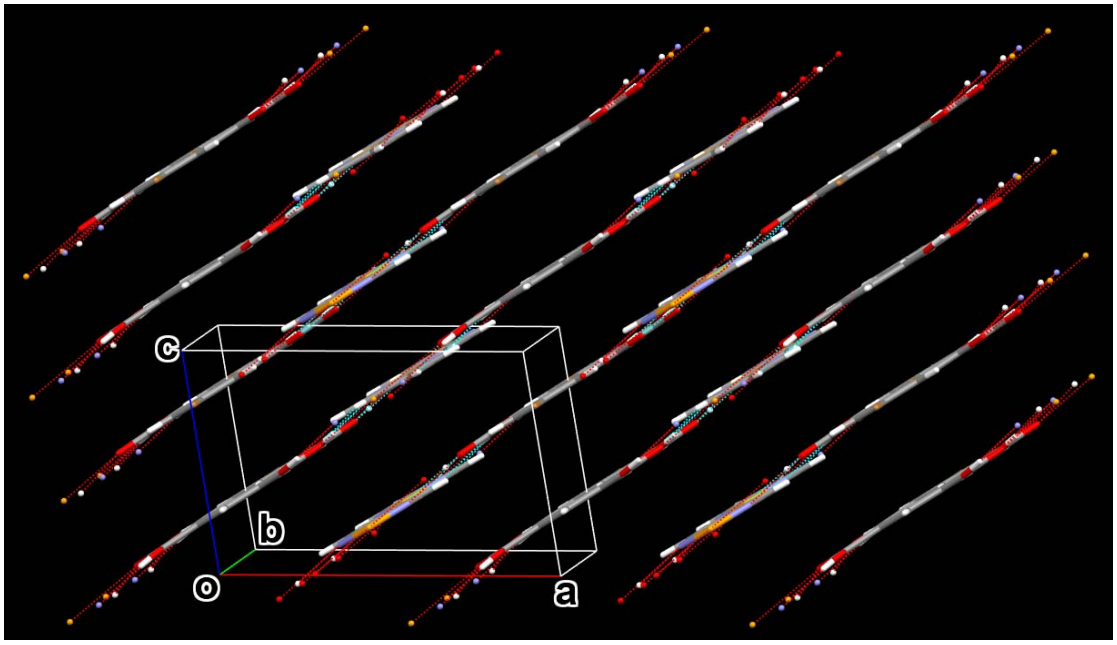
Table S2 The crystallographic data and structure refinement parameters for [IPA-4-Br]$_2$[BSeD] and [TDCA][BSeD].

Cocrystal	**[IPA-4-Br]$_2$[BSeD]**	**[TDCA][BSeD]**
CCDC No.	2429788	2429789
Empirical formula	$C_{11}H_6BrNO_4Se_{0.5}$	$C_{12}H_8N_2O_4SSe$
Formula weight	335.56	355.22
Crystal size/mm^3	0.30 × 0.21 × 0.17	0.18 × 0.15 × 0.13
Crystal system	monoclinic	monoclinic
Space group	$P2_1/m$	$P2_1/c$
a/Å	3.89920(10)	3.8144(11)
b/Å	37.6399(13)	22.357(7)
c/Å	7.7471(2)	15.964(5)
α/°	90	90
β/°	95.702(3)	93.581(9)
γ/°	90	90
V/Å^3	1131.38(6)	1358.7(7)
Z	4	4
ρ_{calc}/g·cm^{-3}	1.970	1.737
T/K	293(2)	300(2)
2ϑ range for data collection/°	6.832–58.26	5.114–54.97
Reflections collected	14800	25654
Independent reflections [R_{int}]	2827 [0.0389]	3070 [0.0641]
R_1, wR_2 (I > 2σ(I))	0.0468, 0.0946	0.0441, 0.0738
R_1, wR_2 (all data)	0.0702, 0.1024	0.0648, 0.0791
Goodness-of-fit on F^2	1.059	1.106

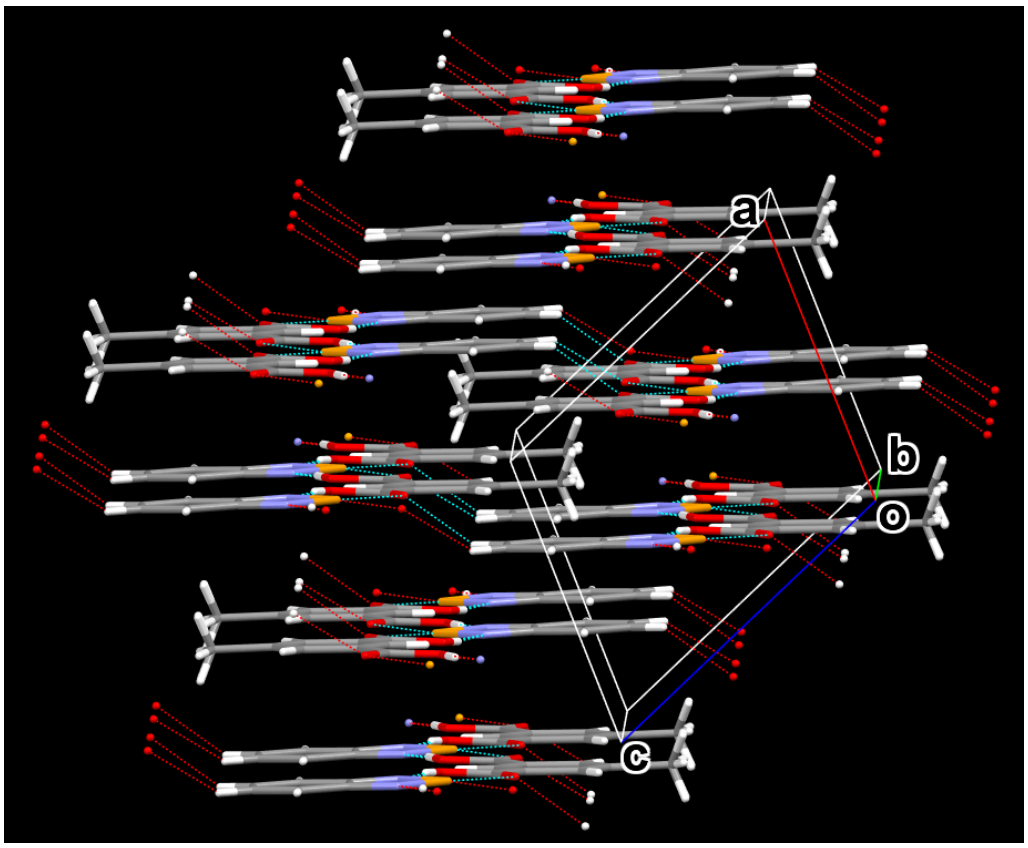
[IPA-5-NO_2][BSeD]



[IPA-5-Br][BSeD]



[IPA-5-CH_3][BSeD]



[IPA-5-NH_2][BSeD]

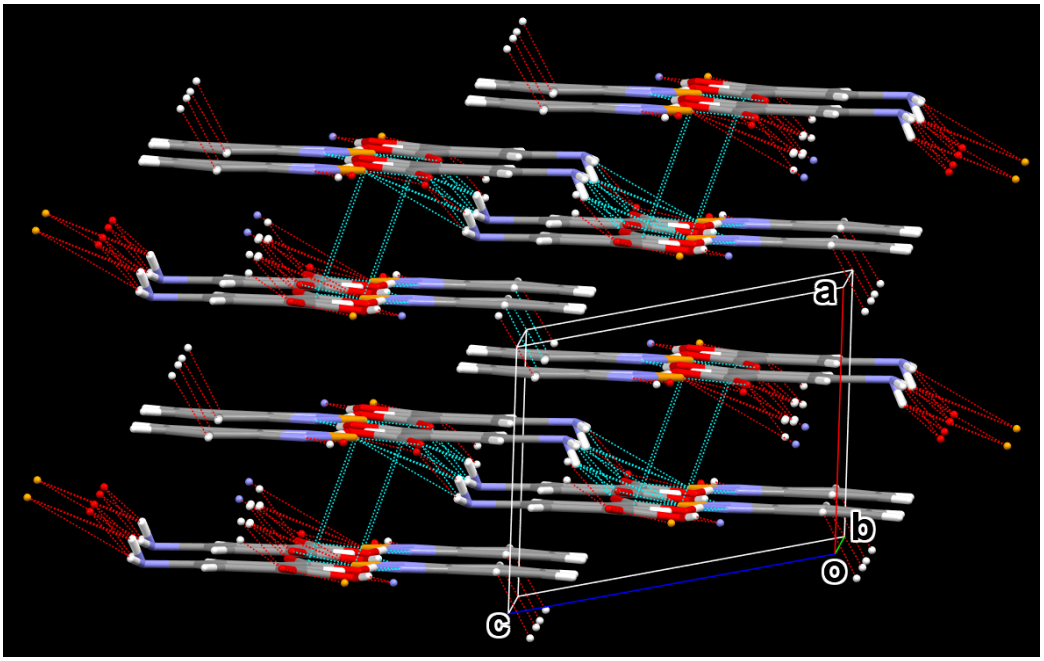
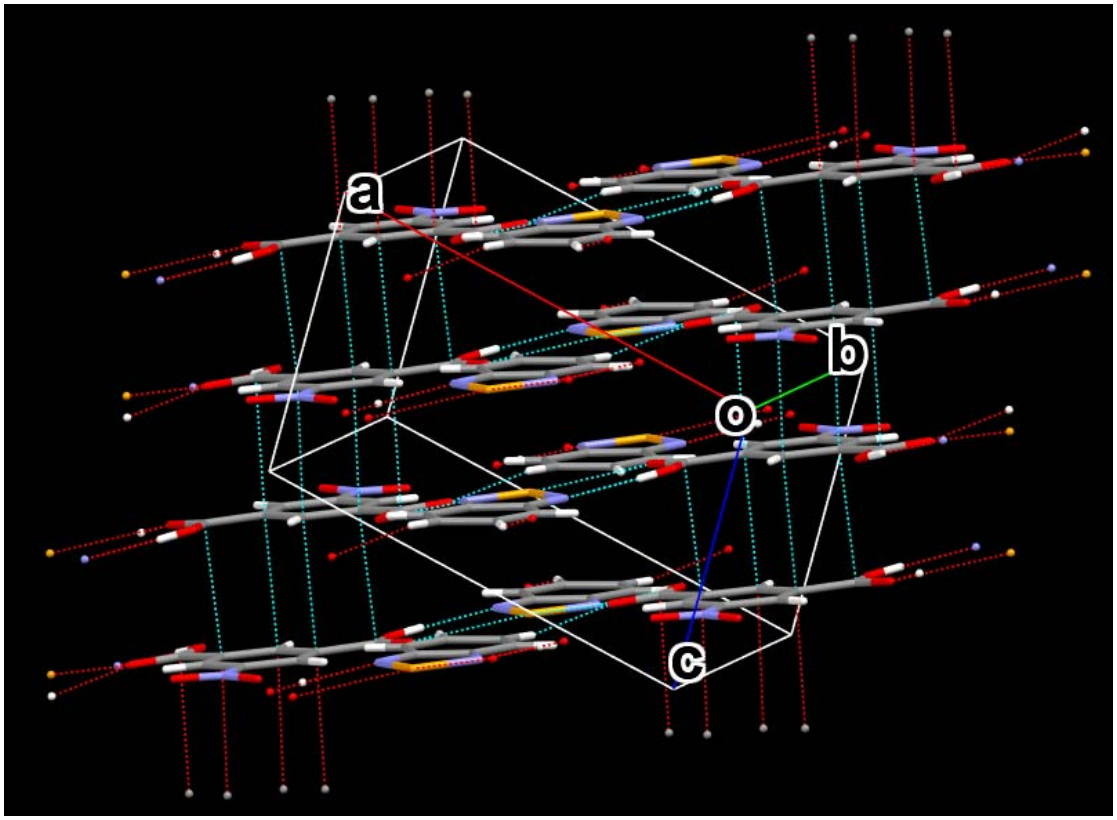
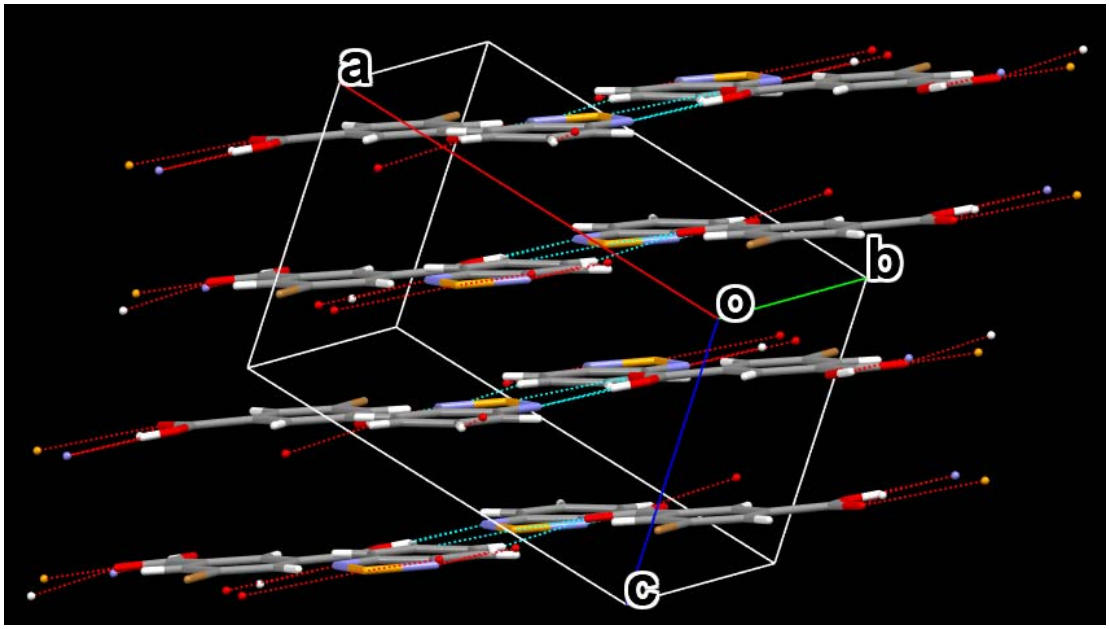


Fig. S1 The 2 × 2 × 2 unit cells of [IPA-5-NO_2][BSeD], [IPA-5-Br][BSeD], [IPA-5-CH_3][BSeD] and [IPA-5-NH_2][BSeD]. Color code: H, white; C, gray; O, red; N, Blue; Se, orange; Br, brown.

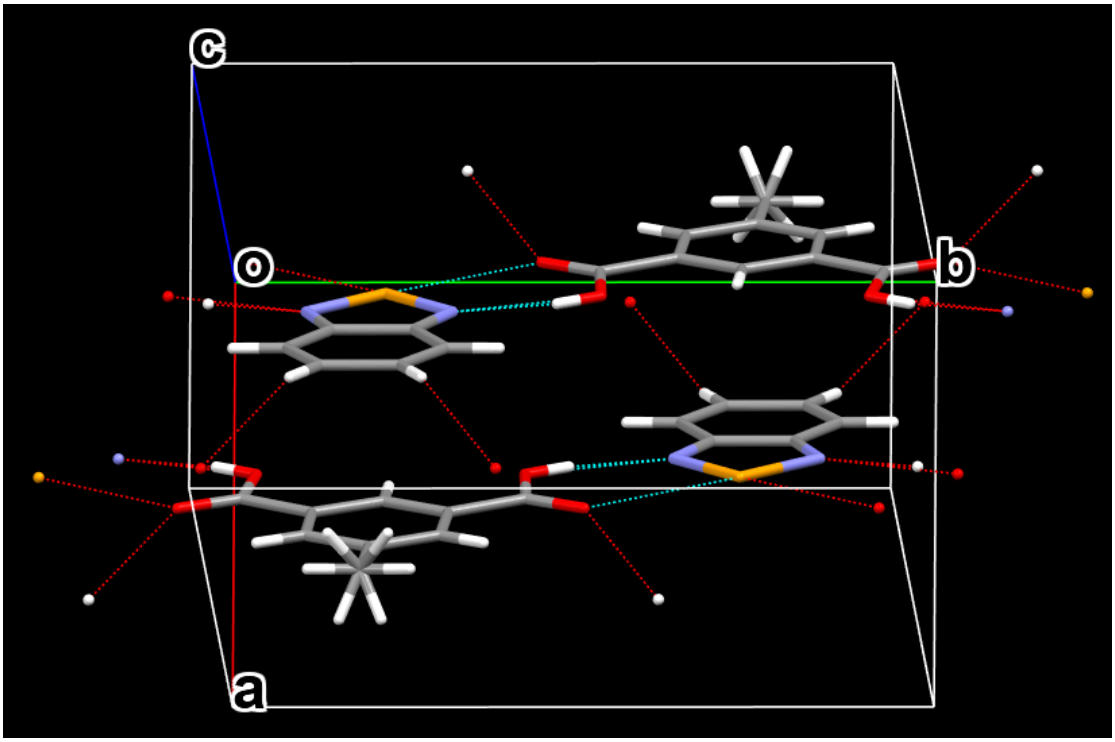
[IPA-5-NO_2][BSeD]



[IPA-5-Br][BSeD]



[IPA-5-CH_3][BSeD]



[IPA-5-NH_2][BSeD]

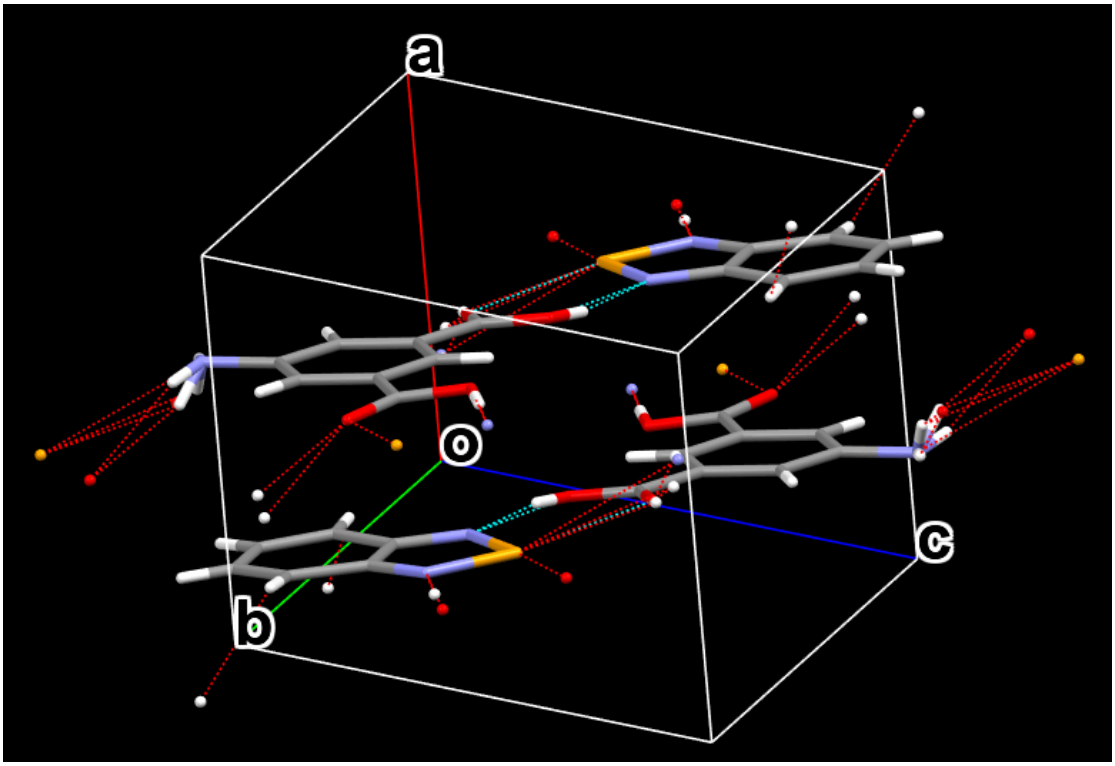
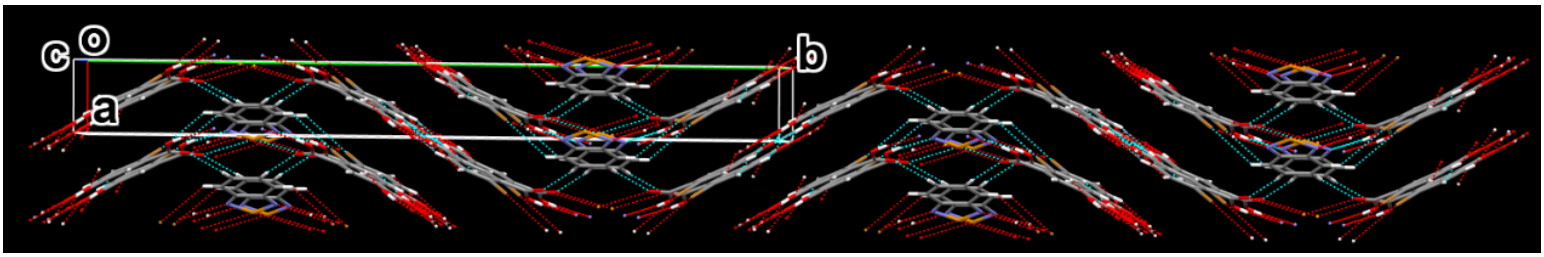


Fig. S2 The π···π stacking interactions in the crystal structures of [IPA-5-NO_2][BSeD], [IPA-5-Br][BSeD], [IPA-5-CH_3][BSeD] and [IPA-5-NH_2][BSeD]. Color code: H, white; C, gray; O, red; N, Blue; Se, orange; Br, brown.

[IPA-4-Br]$_2$[BSeD]



[TDCA][BSeD]

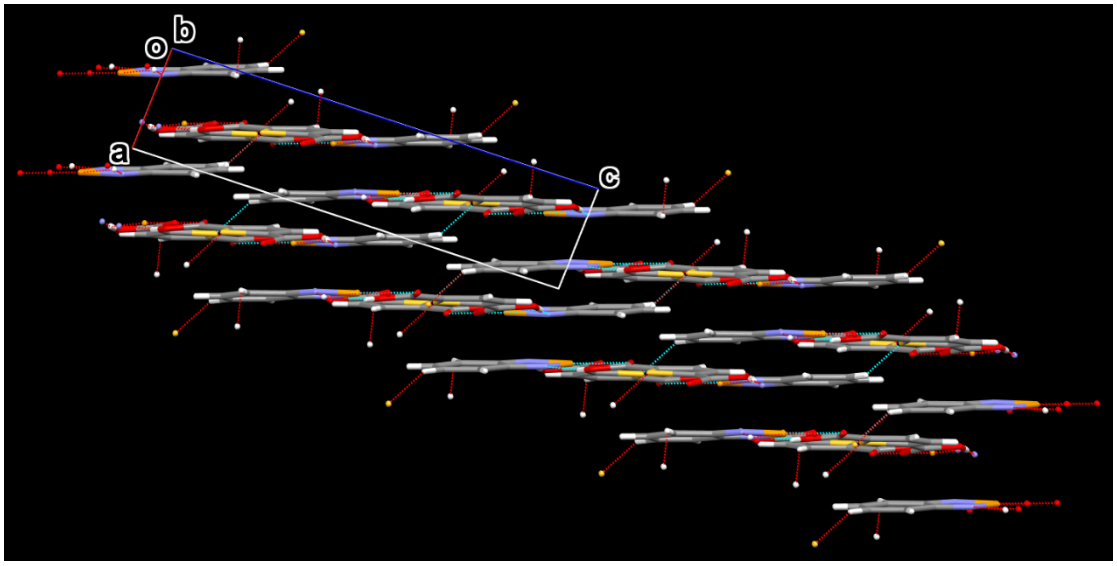
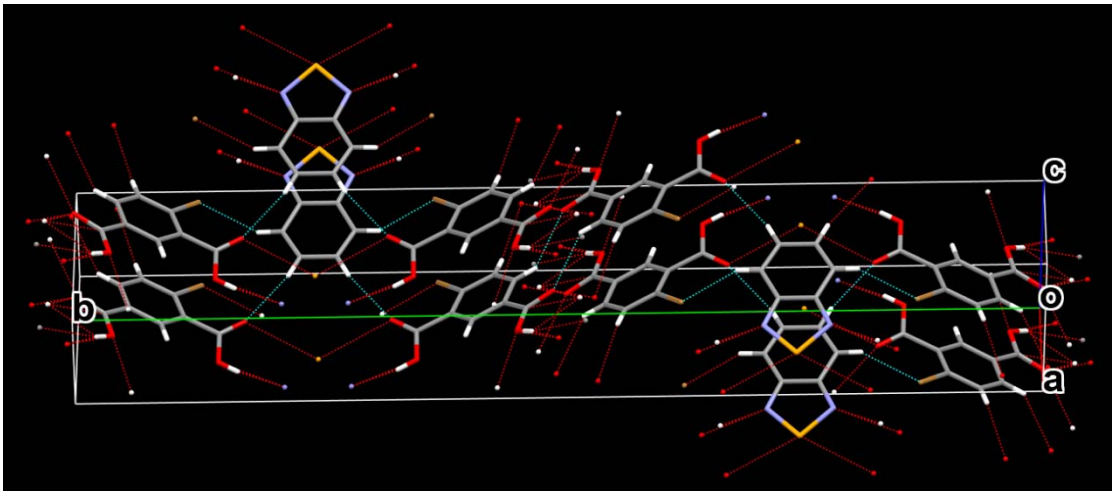


Fig. S3 The 2 × 2 × 2 unit cells of [IPA-4-Br]$_2$[BSeD] and [TDCA][BSeD]. Color code: H, white; C, gray; O, red; N, Blue; S yellow; Se, orange; Br, brown.

[IPA-4-Br]$_2$[BSeD]



[TDCA][BSeD]

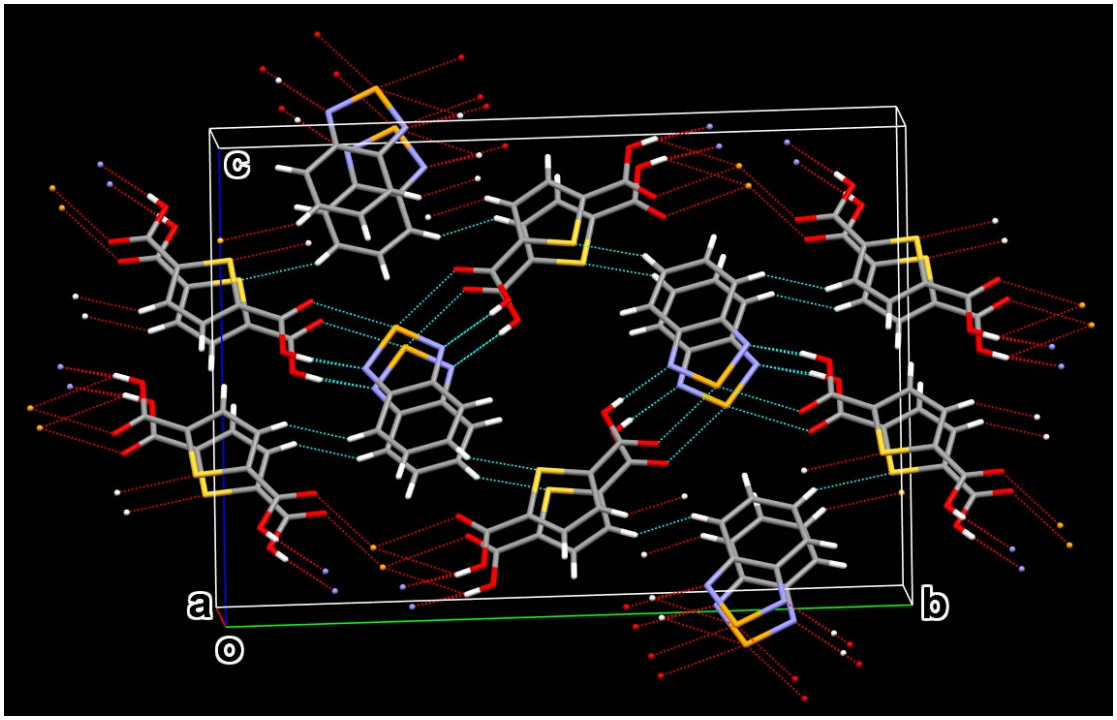


Fig. S4 The π···π stacking interactions in the crystal structures of [IPA-4-Br]$_2$[BSeD] and [TDCA][BSeD]. Color code: H, white; C, gray; O, red; N, Blue; S yellow; Se, orange; Br, brown.

S3. Notes and references

1 CrysAlisPro, Rigaku Oxford Diffraction, Version 1.171.36.32, England, 2013.

2 CrysAlisPro, Rigaku Oxford Diffraction, Version 1.171.38.41r, England, 2015.

3 G. M. Sheldrick, *SHELXS-97: Program for X-ray Crystal Structure Solution*, University of Gottingen: Gottingen, Germany, 1997.

4 G. M. Sheldrick, *SHELXS-97: Program for X-ray Crystal Structure Refinement*, University of Gottingen: Gottingen, Germany, 1997.

5 G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112–122.

6 C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158–6169.

7 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.

8 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.

9 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.

10 Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

11 W. Wang, T. Sun, Y. Zhang and Y. B. Wang, *J. Chem. Phys.*, 2015, **143**, 114312.

12 W. Wang, Y. Zhang and Y. B. Wang, *Int. J. Quantum Chem.*, 2017, **117**, e25345.

13 S. F. Boys and F. Bernardi, *Mol. Phys.* 1970, **19**, 553−566.

14 R. F. W. Bader, *Atoms in Molecules, A Quantum Theory*, Clarendon Press, Oxford, 1990.

15 F. Biegler-König, J. Schönbohm and D. Bayles, *J. Comput. Chem.*, 2001, **22**, 545–559.

S4. The CheckCIF reports for the six cocrystals.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2429784

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: 2429784

```
Bond precision:   C-C = 0.0037 A          Wavelength=0.71073

Cell:             a=11.3555(4)     b=9.1502(3)         c=7.1692(4)
                  alpha=90         beta=99.648(5)      gamma=90
Temperature:      293 K

                 Calculated                  Reported
Volume           734.38(6)                   734.38(6)
Space group      P 2/c                       P 1 2/c 1
Hall group       -P 2yc                      -P 2yc
Moiety formula   C8 H5 N O6, C6 H4 N2 Se     C6 H4 N2 Se, C8 H5 N O6
Sum formula      C14 H9 N3 O6 Se             C14 H9 N3 O6 Se
Mr               394.20                      394.20
Dx,g cm-3        1.783                       1.783
Z                2                           2
Mu (mm-1)        2.595                       2.595
F000             392.0                       392.3
F000'            392.01
h,k,lmax         15,12,9                     15,12,9
Nref             1988                        1733
Tmin,Tmax        0.464,0.627                 0.772,1.000
Tmin'            0.455

Correction method= # Reported T Limits: Tmin=0.772 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.872           Theta(max)= 29.200

R(reflections)= 0.0384( 1484)                    wR2(reflections)=
                                                 0.0829( 1733)
S = 1.076                  Npar= 112
```

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

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.961 Why?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C8 H5 N O6, C6 H4 N2 Se
             Rep.: C6 H4 N2 Se, C8 H5 N O6
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.7 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.227 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         49 Report
               12  0  2,  12  1  2,  12  2  2,   4  1  3,   5  1  3,  10  1  3,
               11  1  3,  11  2  3,  11  3  3,   4  0  4,   4  1  4,   5  0  4,
                5  1  4,   5  2  4,   6  0  4,   6  1  4,   6  2  4,   7  0  4,
                7  1  4,   7  2  4,   8  0  4,   8  1  4,   8  2  4,   9  0  4,
                9  1  4,  10  0  4,  10  1  4,  10  2  4,   4  1  5,   5  1  5,
                6  1  5,   7  1  5,   7  2  5,   8  1  5,   8  2  5,   9  1  5,
                9  2  5,   1  0  6,   2  0  6,   3  0  6,   4  0  6,   4  1  6,
                5  0  6,   5  1  6,   6  0  6,   6  1  6,   7  0  6,   7  1  6,
                8  0  6,
```

Alert level G

```
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT073_ALERT_1_G H-atoms ref., but hydrogen treatment Reported as     constr Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data     Please Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
                  0  1  0,   1  0  0,   1  1  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        203 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.520 Note
             Predicted wR2: Based on SigI**2  3.29 or SHELX Weight  7.70
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
PLAT982_ALERT_1_G The Se-f'=   -0.0811 Deviates from  IT-Value =      -0.0929 Check
PLAT983_ALERT_1_G The Se-f"=    2.3083 Deviates from  IT-Value =       2.2259 Check
```

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

   7 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
   4 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 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

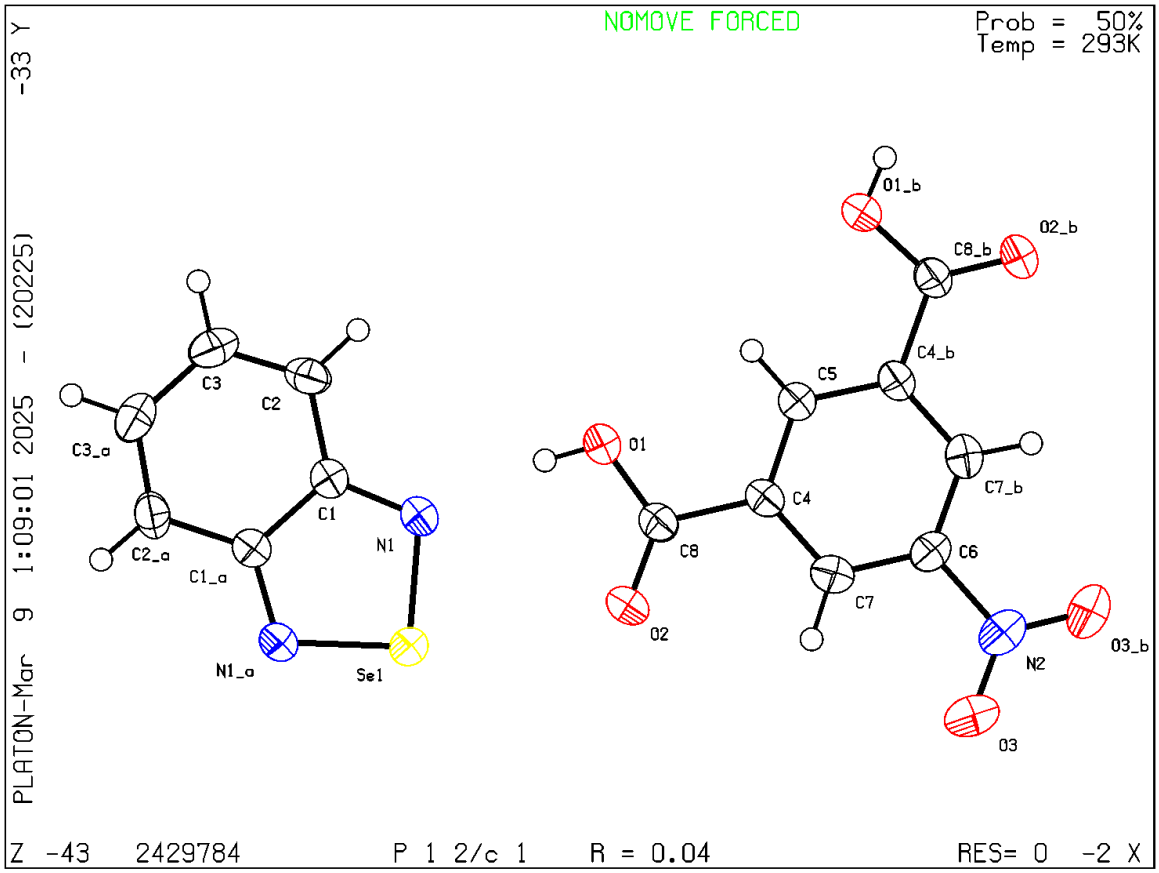
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock 2429784 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2429785

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: 2429785

Bond precision: C-C = 0.0063 A Wavelength=0.71073

Cell: a=11.154(3) b=9.184(2) c=7.3865(19)
alpha=90 beta=99.177(9) gamma=90
Temperature: 300 K

	Calculated	Reported
Volume	747.0(3)	746.9(3)
Space group	P 2/c	P 1 2/c 1
Hall group	-P 2yc	-P 2yc
Moiety formula	C8 H5 Br O4, C6 H4 N2 Se	C6 H4 N2 Se, C8 H5 Br O4
Sum formula	C14 H9 Br N2 O4 Se	C14 H9 Br N2 O4 Se
Mr	428.09	428.10
Dx,g cm-3	1.903	1.903
Z	2	2
Mu (mm-1)	5.206	5.207
F000	416.0	416.0
F000'	415.46	
h,k,lmax	14,12,9	14,11,9
Nref	1780	1758
Tmin,Tmax	0.452,0.508	0.343,0.746
Tmin'	0.418	

Correction method= # Reported T Limits: Tmin=0.343 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.988 Theta(max)= 27.828

R(reflections)= 0.0515(1231) wR2(reflections)= 0.1144(1758)

S = 1.027 Npar= 103

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C8 H5 Br O4, C6 H4 N2 Se
             Rep.: C6 H4 N2 Se, C8 H5 Br O4
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C5       -C8       .       1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00625 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.804 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
               2  0  0,  -2  0  2,   0  0  2,
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
             H2
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               0  1  0,   1  0  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         14 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
               2  0  0,  -2  0  2,   0  0  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               2  0  0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.517 Note
             Predicted wR2: Based on SigI**2  7.54 or SHELX Weight 11.14
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          2 Check
```

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

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

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

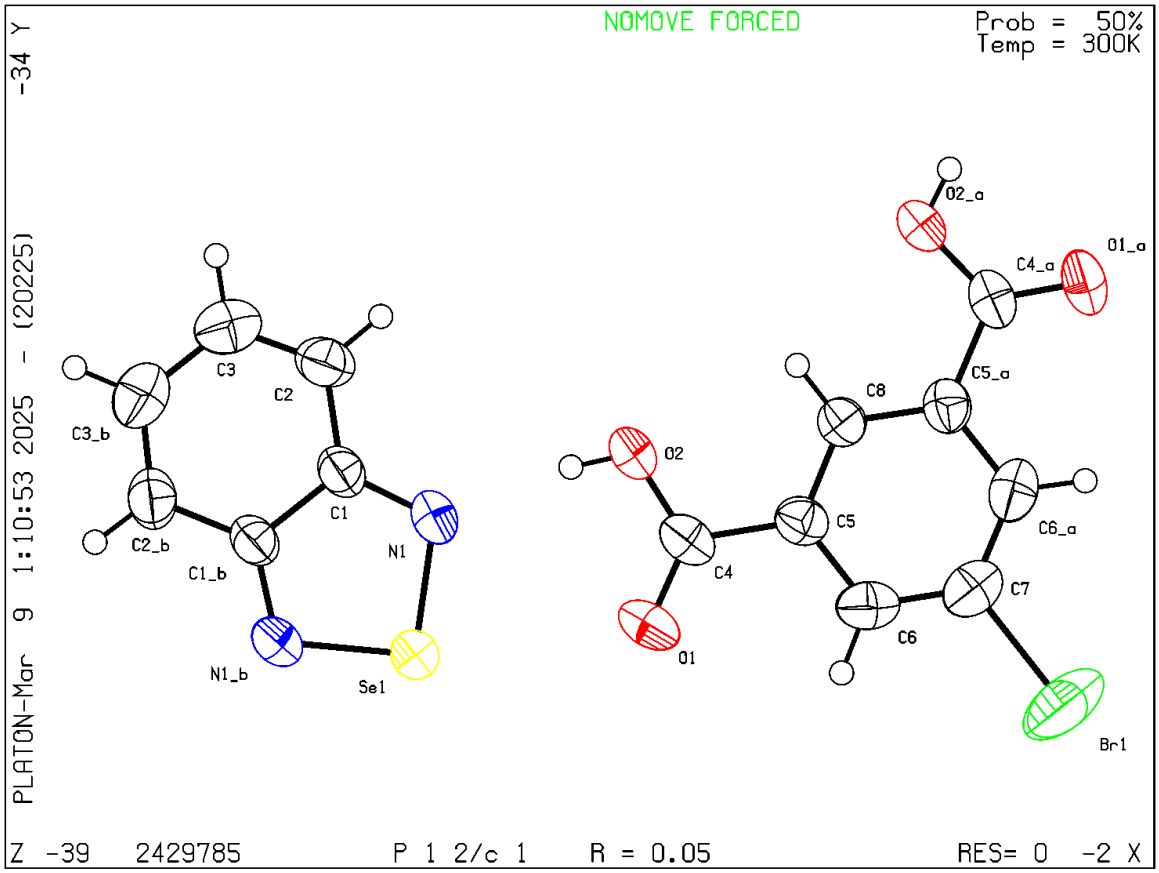
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 02/02/2025; check.def file version of 02/02/2025

Datablock 2429785 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2429786_auto

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: 2429786_auto

```
Bond precision:   C-C = 0.0031 A          Wavelength=0.71073

Cell:             a=7.4596(4)     b=12.3445(6)         c=8.6525(4)
                  alpha=90        beta=112.155(6)      gamma=90
Temperature:      293 K

                 Calculated                  Reported
Volume           737.94(7)                   737.94(7)
Space group      P 21/m                      P 1 21/m 1
Hall group       -P 2yb                      -P 2yb
Moiety formula   C9 H8 O4, C6 H4 N2 Se       C6 H4 N2 Se, C9 H8 O4
Sum formula      C15 H12 N2 O4 Se            C15 H12 N2 O4 Se
Mr               363.23                      363.23
Dx,g cm-3        1.635                       1.635
Z                2                           2
Mu (mm-1)        2.564                       2.564
F000             364.0                       364.2
F000'            363.98
h,k,lmax         10,16,11                    9,16,11
Nref             2098                        1873
Tmin,Tmax        0.519,0.599                 0.847,1.000
Tmin'            0.508

Correction method= # Reported T Limits: Tmin=0.847 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.893          Theta(max)= 29.270

R(reflections)= 0.0346( 1609)                wR2(reflections)=
                                             0.0702( 1873)
S = 1.042                 Npar= 108
```

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C9 H8 O4, C6 H4 N2 Se
             Rep.: C6 H4 N2 Se, C9 H8 O4
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.051 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         5 Note
               1  0  0,   0  2  0,  -1  0  1,   0  0  1,   0  1  1,
```

Alert level G

```
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT073_ALERT_1_G H-atoms ref., but hydrogen treatment Reported as     constr Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             H9A     H9B     H9C
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C6       - C9       .       1.52 Ang.
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data     Please Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          3 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        203 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.967 Note
             Predicted wR2: Based on SigI**2  2.36 or SHELX Weight  6.73
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 Info
PLAT982_ALERT_1_G The Se-f'=   -0.0811 Deviates from  IT-Value =      -0.0929 Check
PLAT983_ALERT_1_G The Se-f"=    2.3083 Deviates from  IT-Value =       2.2259 Check
```

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

   7 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
   2 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 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

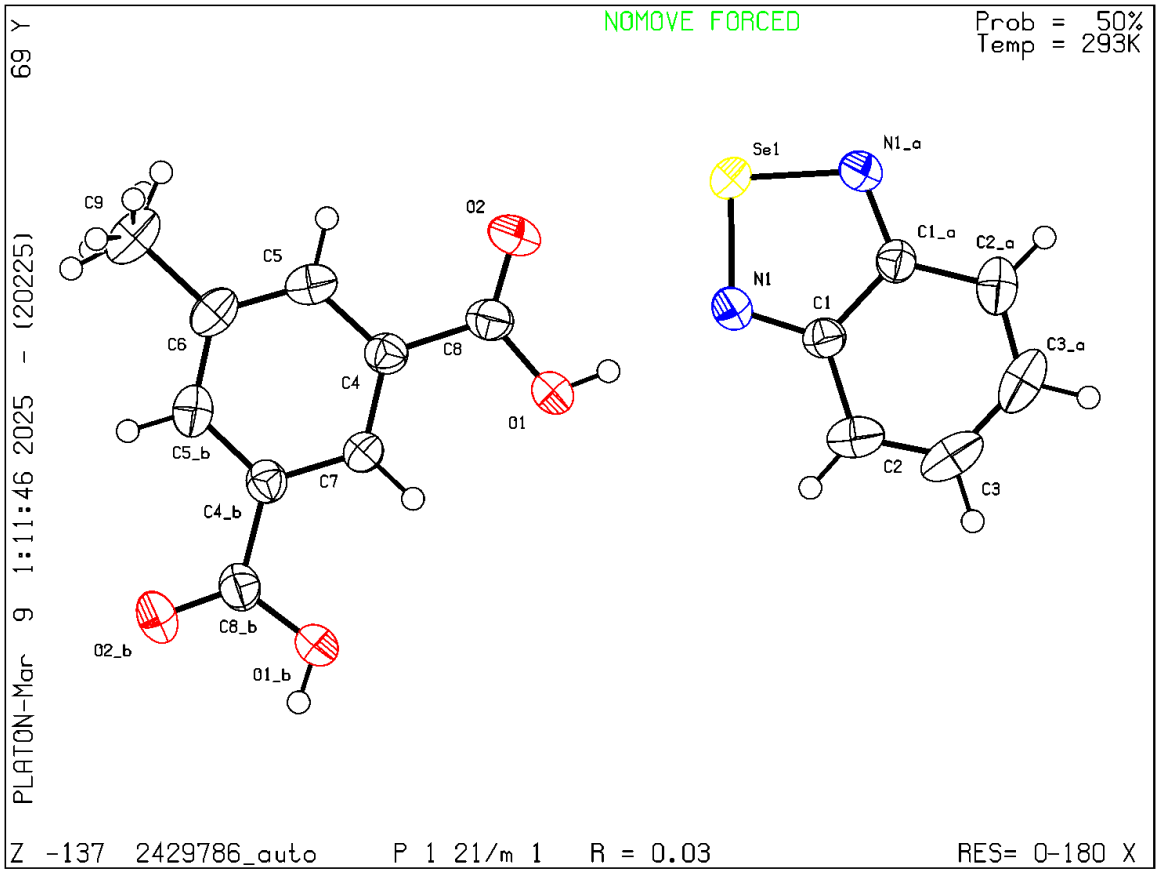
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock 2429786_auto - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2429787

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: 2429787

```
Bond precision:   C-C = 0.0075 A          Wavelength=1.54178

Cell:             a=6.8417(7)     b=12.3348(11)        c=8.5209(7)
                  alpha=90        beta=102.207(4)      gamma=90
Temperature:      300 K

                 Calculated                  Reported
Volume           702.83(11)                  702.83(11)
Space group      P 21/m                      P 1 21/m 1
Hall group       -P 2yb                      -P 2yb
Moiety formula   C8 H7 N O4, C6 H4 N2 Se     C6 H4 N2 Se, C8 H7 N O4
Sum formula      C14 H11 N3 O4 Se            C14 H11 N3 O4 Se
Mr               364.22                      364.22
Dx,g cm-3        1.721                       1.721
Z                2                           2
Mu (mm-1)        3.842                       3.842
F000             364.0                       364.0
F000'            363.43
h,k,lmax         8,15,10                     8,15,10
Nref             1473                        1459
Tmin,Tmax        0.743,0.764                 0.388,0.754
Tmin'            0.674

Correction method= # Reported T Limits: Tmin=0.388 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.990           Theta(max)= 72.785

R(reflections)= 0.0821( 1188)                wR2(reflections)=
                                             0.2443( 1459)
S = 1.086                  Npar= 110
```

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 ....       4.32 Report
```

Author Response: Twinned structure.

```
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       3.52 eA-3
```

Author Response: See above.

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
          The relevant atom site should be identified.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C8 H7 N O4, C6 H4 N2 Se
             Rep.: C6 H4 N2 Se, C8 H7 N O4
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0075 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.500 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          7 Report
               2  0  0,   2  1  0,   0  2  0,  -2  0  1,  -1  3  1,   0  0  2,
               5  0  6,
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
             H1    H2A   H2B
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.18 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             H2A     H2B
PLAT480_ALERT_4_G Long H...A H-Bond Reported H3       ..O2       .       2.75 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      36.30 Deg.
             H2A  -N2   -H2B     1_555   1_555   4_575 ......     #    5 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      36.30 Deg.
             H2B  -N2   -H2A     1_555   1_555   4_575 ......     #    8 Check
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               0  0  1,   0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          5 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
               2  0  0,  -2  0  1,
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law         [ 1 0 4] Est.d BASF       0.28 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.472 Note
             Predicted wR2: Based on SigI**2  7.04 or SHELX Weight 22.50
```

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

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  3 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
  6 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

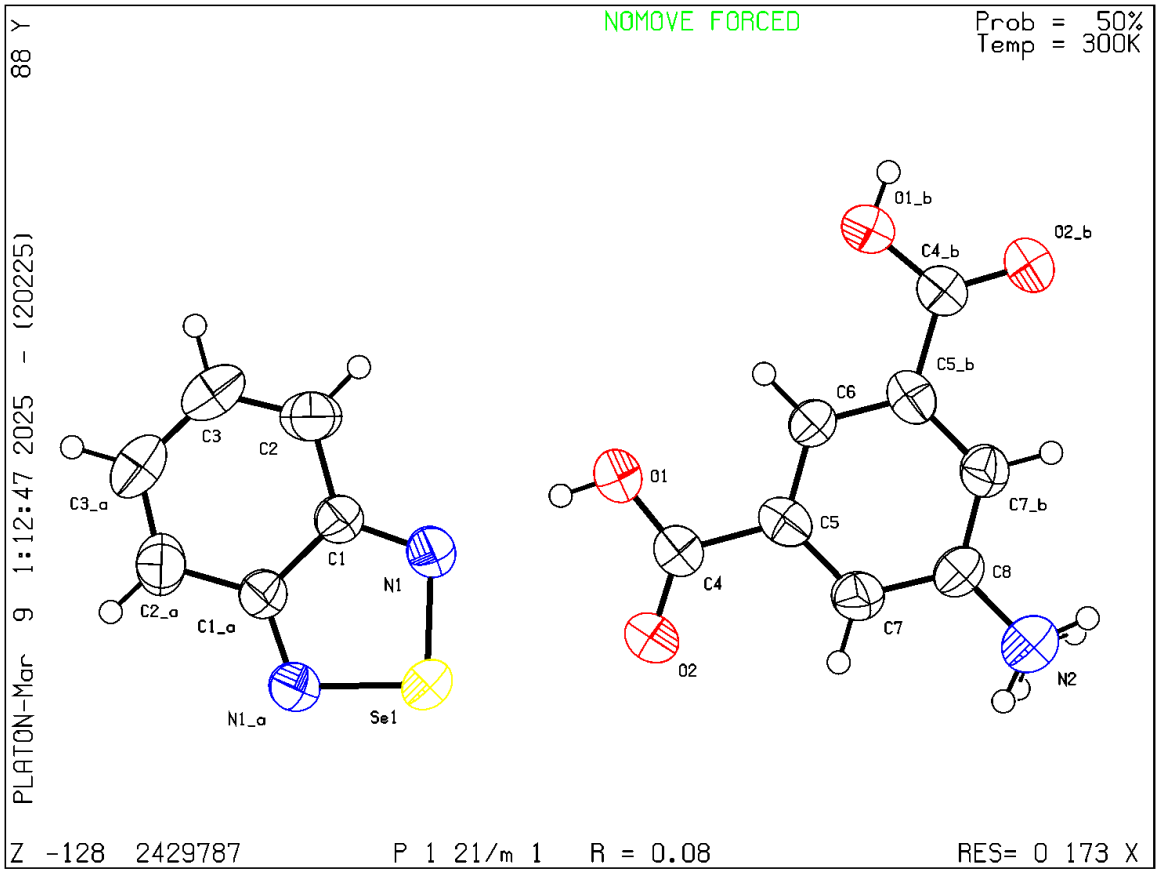
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 02/02/2025; check.def file version of 02/02/2025

Datablock 2429787 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2429788_auto

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: 2429788_auto

```
Bond precision:   C-C = 0.0054 A           Wavelength=0.71073

Cell:              a=3.8992(1)      b=37.6399(13)        c=7.7471(2)
                   alpha=90         beta=95.702(3)       gamma=90
Temperature:       293 K

                 Calculated                  Reported
Volume           1131.38(6)                  1131.38(6)
Space group      P 21/m                      P 1 21/m 1
Hall group       -P 2yb                      -P 2yb
Moiety formula   2(C8 H5 Br O4), C6 H4 N2 Se C8 H5 Br O4, C3 H2 N Se0.5
Sum formula      C22 H14 Br2 N2 O8 Se        C11 H6 Br N O4 Se0.50
Mr               673.11                      335.56
Dx,g cm-3        1.976                       1.970
Z                2                           4
Mu (mm-1)        5.245                       5.245
F000             656.0                       652.0
F000'            655.04
h,k,lmax         5,51,10                     5,50,10
Nref             3108                        2827
Tmin,Tmax        0.277,0.410                 0.650,1.000
Tmin'            0.199

Correction method= # Reported T Limits: Tmin=0.650 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.910            Theta(max)= 29.130

R(reflections)= 0.0468( 2139)                    wR2(reflections)=
                                                 0.1024( 2827)
S = 1.059                  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

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C22 H14 Br2 N2 O8 Se
             Rep.: C11 H6 Br N O4 Se0.50
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C8 H5 Br O4), C6 H4 N2 Se
             Rep.: C8 H5 Br O4, C3 H2 N Se0.5
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       1.99 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.2 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      6.864 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         7 Note
               0  2  0,   0  4  0,   0  6  0,   0  0  1,   0  1  1,   0  2  1,
               0  3  1,
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C11 H6 Br1 N1 O4 Se0.5
           Atom count from _chemical_formula_moiety:C11 H7 Br1 N1 O4 Se0.5
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C11 H6 Br1 N1 O4 Se0.5
           Atom count from the _atom_site data:  C11 H7 Br1 N1 O4 Se0.5
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C11 H6 Br N O4 Se0.50
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         44.00     44.00    0.00
          H         24.00     28.00   -4.00
          Br         4.00      4.00    0.00
          N          4.00      4.00    0.00
          O         16.00     16.00    0.00
          Se         2.00      2.00    0.00
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
             H2
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C6 H4 N2 Se
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        274 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.058 Note
             Predicted wR2: Based on SigI**2  2.52 or SHELX Weight  9.67
```

```
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          6 Info
```

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

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
```

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

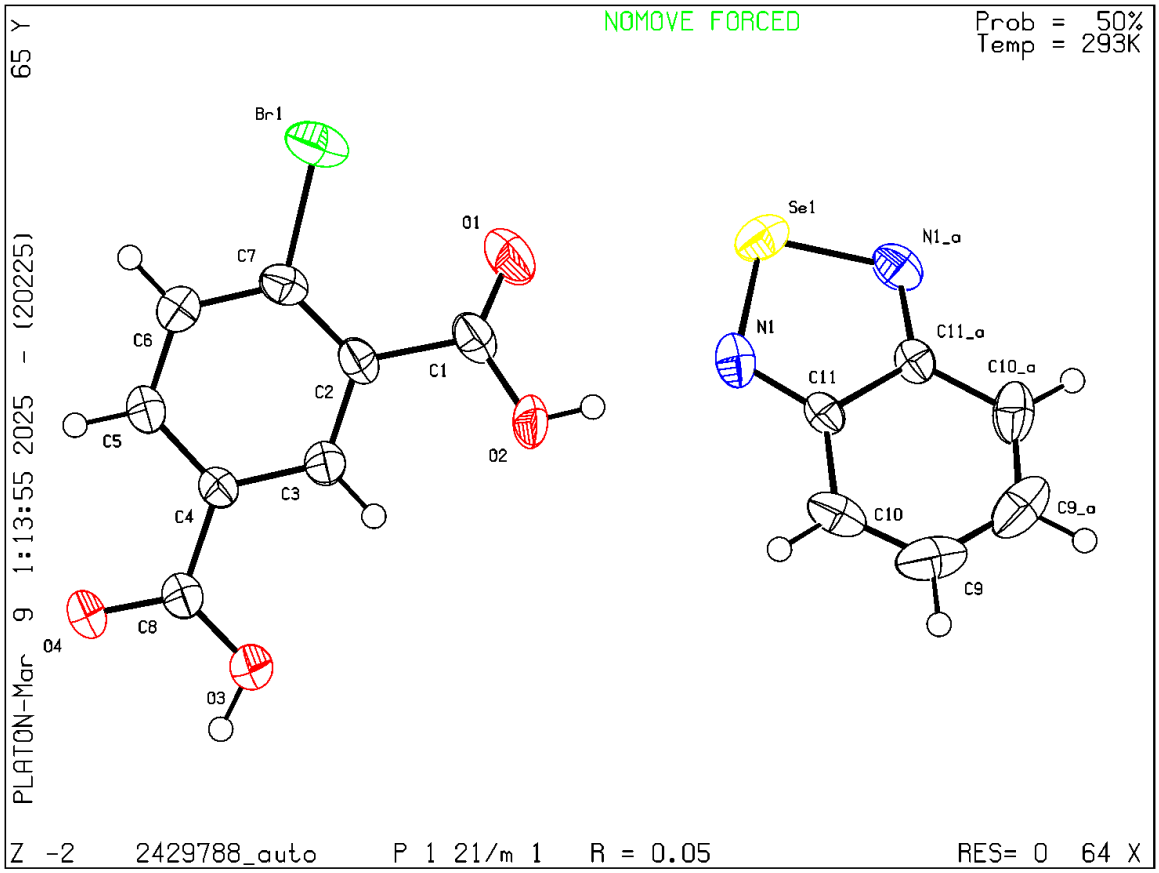
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 02/02/2025; check.def file version of 02/02/2025

Datablock 2429788_auto - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2429789

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: 2429789

```
Bond precision:   C-C = 0.0051 A          Wavelength=0.71073

Cell:             a=3.8144(11)     b=22.357(7)         c=15.964(5)
                  alpha=90         beta=93.581(9)      gamma=90
Temperature:      300 K

                 Calculated                  Reported
Volume           1358.7(7)                   1358.7(7)
Space group      P 21/c                      P 1 21/c 1
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C6 H4 O4 S, C6 H4 N2 Se     C6 H4 N2 Se, C6 H4 O4 S
Sum formula      C12 H8 N2 O4 S Se           C12 H8 N2 O4 S Se
Mr               355.22                      355.22
Dx,g cm-3        1.737                       1.737
Z                4                           4
Mu (mm-1)        2.931                       2.931
F000             704.0                       704.0
F000'            704.43
h,k,lmax         4,29,20                     4,29,20
Nref             3094                        3070
Tmin,Tmax        0.596,0.683                 0.559,0.746
Tmin'            0.584

Correction method= # Reported T Limits: Tmin=0.559 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.992           Theta(max)= 27.485

R(reflections)= 0.0441( 2387)                    wR2(reflections)=
                                                 0.0791( 3070)
S = 1.106                  Npar= 189
```

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

```
PLAT430_ALERT_2_A Short Inter D...A Contact  Se1      ..O2       .       2.89 Ang.
                                                    x,y,z  =      1_555 Check
```

Author Response: It is a chalcogen bond which can not be recognized by the software.

Alert level C

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C6 H4 O4 S, C6 H4 N2 Se
             Rep.: C6 H4 N2 Se, C6 H4 O4 S
PLAT354_ALERT_3_C Short  O-H (X0.82,N0.98A)  O1       - H1       .       0.71 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS   <=         35 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.049 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          7 Report
               1  0  0,   1  1  0,   1  0  2,   0  1  2,   1  1  2,   2  1  2,
               0  2  2,
PLAT977_ALERT_2_C Check Negative Difference Density on H4        .      -0.46 eA-3
```

Alert level G

```
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
               0  2  0,   0  1  1,   0  2  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         13 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
               1  1  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               0  1  2,
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by .          1 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.579 Note
             Predicted wR2: Based on SigI**2  3.06 or SHELX Weight  7.15
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 Info
```

```
   1 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
   8 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
   5 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock 2429789 - ellipsoid plot