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Metadata for raw data from X-ray diffraction and other structural techniques
Rovinj, Croatia, 2015

X-ray Origins;

Protection or Paranoia?

Natalie Johnson
Newcastle University

Newcastle University

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X-ray Origins

- Storing raw diffraction images could provide a 'greater hurdle' against false structure solutions.[1]
- This is only the case if the manufacture of raw data is sufficiently difficult.
- This talk covers:
  - The need for a method to validate our diffraction frames.
  - Suggestion of a method to ensure that the diffraction frames archived are from genuine experimental data.

1: L. M. J. Kroon-Batenburg & J. R. Helliwell, *Acta Crystallogr. Sect. D: Biol. Crystallogr.*, 2013, **70**, 2502-2509

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Anesthesiologist Fabricates 172 Papers

A researchers in Japan faked patient data on nearly 200 studies over the past 2 decades, according to an investigating committee.

By Jef Akst | July 3, 2012

NATURE NEWS BLOG

Former chemistry grad student found guilty of fraud

BBC NEWS

S Korea cloning research was fake

Research by South Korea's top human cloning scientist - hailed as a breakthrough earlier this year - was fabricate

Nature retracts epigenetics paper by author who lost two Science papers last year

Posted by Ivan Oransky

Grad student blamed for research misconduct at Utah

13 November 2014 Rebecca Trager

Suspicious Data in a JACS Paper from 2009

November 7th, 2013

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J|A|C|S

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Addition/Correction

Retraction of "Bimetallic Effects for Enhanced Polar Co Enchainment Selectivity in Catalytic Ethylene Polymeri

Brandon A. Rodriguez, Massimiliano Delferro, and Tobin J. Marks*

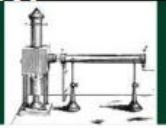
J. Am. Chem. Soc. **2009**, *131*, 5902–5919. DOI: 10.1021/ja900257k

The authors have been unable to reproduce the synthesis and spectroscopic characterization of the ethylene/acrylate copolymer described in this article. Accordingly, the authors are retracting this publication due to concerns over the validity of the aforementioned data. The authors regret any confusion that may have been created by publication of this work.

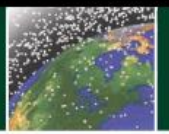
In contrast, the results reported in related publications regarding the synthesis of a binuclear catalyst and its ethylene

COMMENTARY

Helical spin order 338



Space junk 340



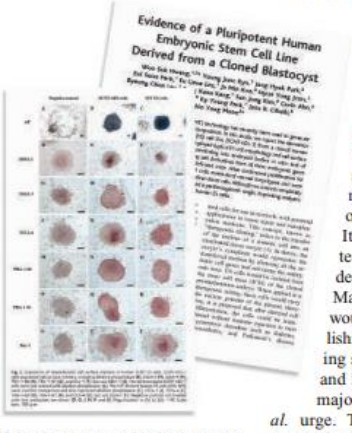
Bottling blue sky 344

LETTERS | POLICY FORUM | ESSAYS | BOOKS | PERSPE

LETTERS

edited by Etta Kavanagh

Editorial Retraction



NVESTIGATION COMMITTEE
NU) (*1*) has concluded that
shed in *Science* (*2*, *3*) have
and that the papers contain
Hwang *et al.*, 2004 (*2*), the
rted that the data showing
nic stem cell line NT-1 is
invalid because they are the
idence that NT-1 is a bona
committee found that the
3) that 11 patient-specific
derived from cloned blasto-
. According to the report of
e laboratory "does not pos-
ines or any scientific basis
." Because the final report
ted that a significant amount of the data presented in both papers
nce feel that an immediate and unconditional retraction of both
retract these two papers and advise the scientific community that
deemed to be invalid.
en of the 15 authors of Hwang *et al.*, 2004 (*2*) have agreed to retract
Hwang *et al.*, 2005 (*3*) have agreed to retract their paper.
he peer reviewers and others spent evaluating these papers as well as
ientific community may have spent trying to replicate these results.

advocating not pure bottom-up dive
new Constitution replacing the
Confederation with an overarching
institutional framework to g
mobilize both the
the private sector i
mon interest.

Victor *et al.* also
terize the plurilate
approach advocated
and Wiener (*1*). This
involves building a
among plural coalitions
nations to create parall
of international emissio
It would not be a "top-d
tem, nor would it app
degree of centralization
Madison's version of fed
would avoid the difficultie
lishing a single universal ca
ing system under the Kyot
and focus on cooperation
major emitting countries, a
al. urge. The plurilateral cap
approach would foster a variety of t
tems to encourage precisely the div
experimentation in policy and pra
Victor *et al.* favor. But it would al
binding mutual commitments by pa

In contrast to both Madisonian
and plurilateral trading, Victor *et al*
bottom-up local policies that they

Retraction: Histone methylation by the *Drosophila* epigenetic transcriptional regulator Ash1

Christian Beisel, Axel Imhof, Jaime Greene, Elisabeth Kremmer & Frank Sauer

Nature (2015) | doi:10.1038/nature14421
Published online 15 April 2015

Nature **419**, 857–862 (2002); doi:10.1038/nature01126

The authors and the University of California Riverside wish to retract this Letter owing to inappropriate image manipulation in the published figures. The figure panels affected are Figure 1b, d, Figure 2b, e, Figure 3a and Figure 4d. *Nature* has not received a response from Frank Sauer to approve this retraction.

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addenda and errata

Acta Crystallographica Section D
Biological Crystallography
ISSN 0907-4449

addenda and errata

Retraction of articles by H. M. Krishna Murthy *et al.*

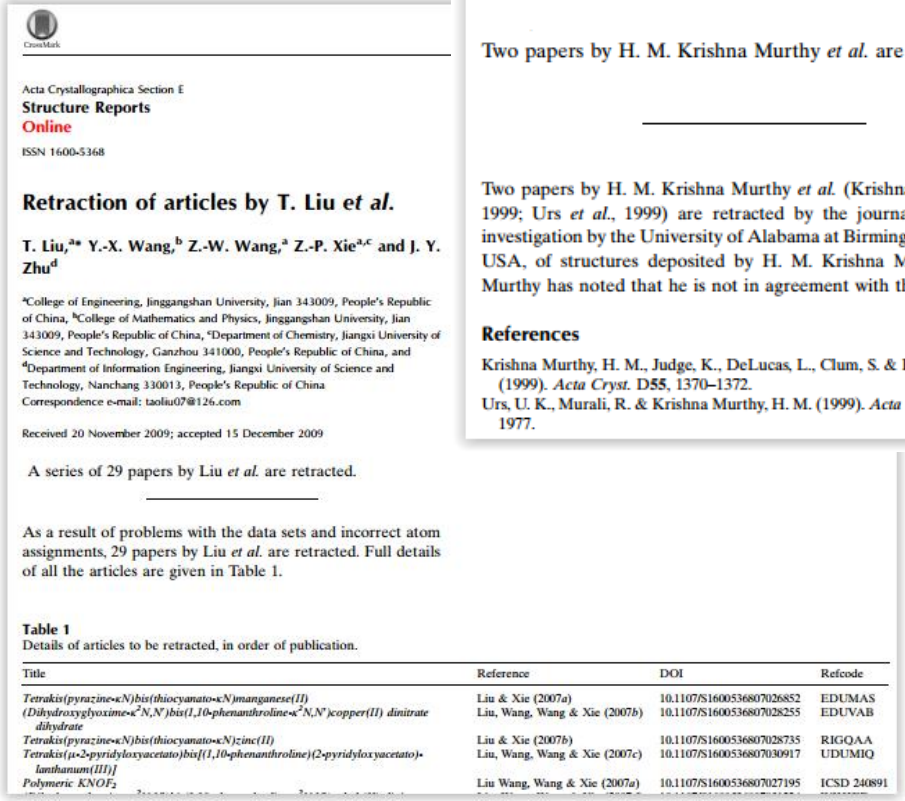
Two papers by H. M. Krishna Murthy *et al.* are retracted.

Two papers by H. M. Krishna Murthy *et al.* (Krishna Murthy *et* 1999; Urs *et al.*, 1999) are retracted by the journal. This follo investigation by the University of Alabama at Birmingham, Alaban USA, of structures deposited by H. M. Krishna Murthy. Krish Murthy has noted that he is not in agreement with the retraction

References

Krishna Murthy, H. M., Judge, K., DeLucas, L., Clum, S. & Padmanabhan, (1999). *Acta Cryst.* D**55**, 1370–1372.

Urs, U. K., Murali, R. & Krishna Murthy, H. M. (1999). *Acta Cryst.* D**55**, 197 1977.



Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles by T. Liu *et al.*

T. Liu,[a]* Y.-X. Wang,[b] Z.-W. Wang,[a] Z.-P. Xie[a,c] and J. Y. Zhu[d]

[a]College of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, [b]College of Mathematics and Physics, Jinggangshan University, Jian 343009, People's Republic of China, [c]Department of Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, People's Republic of China, and [d]Department of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China
Correspondence e-mail: taoliu07@126.com

Received 20 November 2009; accepted 15 December 2009

A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891

addenda and errata

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles by H. Zhong *et al.*

H. Zhong,[a]* S.-H. Duan,[a] Y.-P. Hong,[a] M.-L. Li,[a] Y.-Q. Liu,[a] C.-J. Luo,[a] Q.-Y. Luo,[a] S.-Z. Xiao,[a] H.-L. Xie,[a] Y.-P. Xu,[a] X.-M. Yang,[b,a] X.-R. Zeng[a] and Q. Y. Zhong[c]

[a]College of Chemistry and Chemical Engineering, Provincial Key Laboratory of Coordination Chemistry, Jinggangshan University, Jian 343009, People's Republic of China, [b]Institute of Applied Materials, Jiangxi University of Finance and Economics, Nanchang 330032, People's Republic of China, and [c]Jian Training School, Jian 343000, People's Republic of China
Correspondence e-mail: huazhong06@126.com

Received 20 November 2009; accepted 15 December 2009

A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ

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- Discovered during the testing of *checkCIF.*
- Structure factor files were discovered to be almost identical.
- One set of intensities were taken and refined, unit cell size and elements within were manually changed to produce data for other ‘structures’.

editorial

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Editorial

William T. A. Harrison,[a] Jim Simpson[b] and Matthias Weil[c]

[a]Department of Chemistry, University of Aberdeen, Aberdeen AB24 3UE, Scotland, [b]Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand, and [c]Institute of Chemical Technologies and Analytics, Division of Structural Chemistry, Vienna University of Technology, Getreidemarkt 9/164-SC, Austria

Regrettably, this editorial is to alert readers and authors of *Acta Crystallographica Section E* and the wider scientific community to the fact that we have recently uncovered evidence for an extensive series of scientific frauds involving papers published in the journal, principally during 2007. Although several thousands of structures published in *Acta Crystallographica Section E* every year will continue to reflect results of serious scientific work, the extent of these problems is significant with at least 70 structures demonstrated to be falsified and meanwhile acknowledged by the authors as such. Our work is ongoing and it is likely that this figure will rise further.

These problems were first discovered by Ton Spek during testing of the checking programs for the journal. Testing is routinely carried out using cifs and structure-factor files from back issues of *Acta Crystallographica Sections E* or *C*. Initially, unexplained Hirshfeld rigid-bond alerts and unusual metal–ligand donor-atom distances led to the discovery that metal atoms had been transposed and that more than one structure had been ‘determined’ using identical sets of data. Investigation of these cases sparked a search of papers written by the correspondence authors involved.

A program written by Toine Schreurs of Utrecht University that can examine and compare two structure-factor files was then used to examine the data deposited for the structures under investigation. For all of the problem structures, the program revealed that the data sets used to refine two or more supposedly unique structures were in fact identical, but with the cell parameters apparently manually altered by the authors concerned.

The falsified structures have many features in common: in each case, a *bona fide* set of intensity data, usually on a compound whose structure had been correctly determined and reported in the literature, was used to produce a number of papers, with the authors changing one or more atoms in the structure to produce what appeared to be a genuine structure determination of a new compound. The worst example generated no fewer than 18 supposedly original structures from a single common set of data. There is nothing to suggest that the authors of the original papers describing the real structures are in any way aware of, or complicit in, this fraud.

W. T. A. Harrison, Jim Simpson, and Matthias Weil, *Acta Crystallogr., Sect. E*, 2010, **66**, e1-e2

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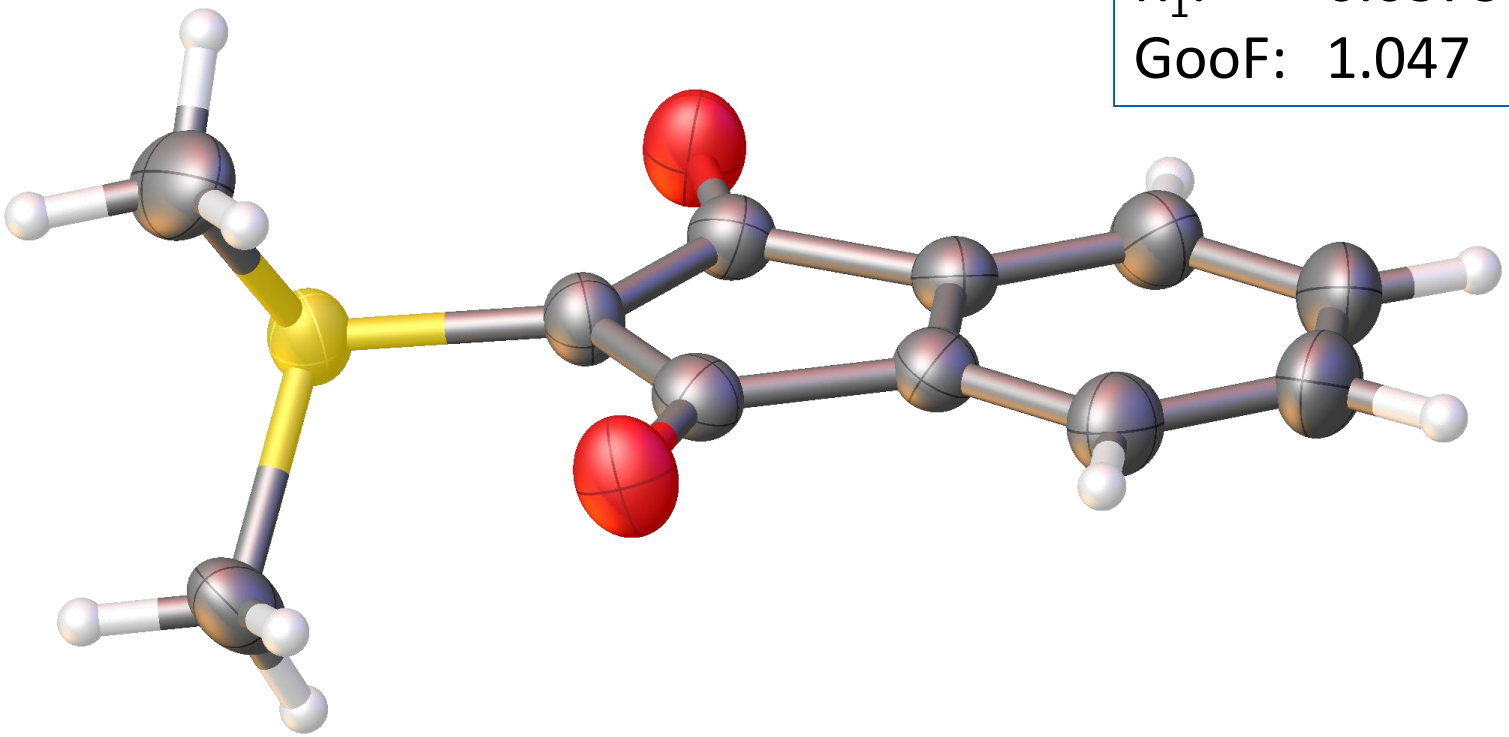

R_1:	0.0373
GooF:	1.047

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R(reflections)= 0.0279(1749) wR2(reflections)= 0.0787(1799)

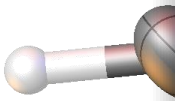
S = 1.100 Npar= 129

Alert level G

PLAT912 ALERT 4 G Missing # of FCF Reflections Above STh/L= 0.600 111 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
0 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.

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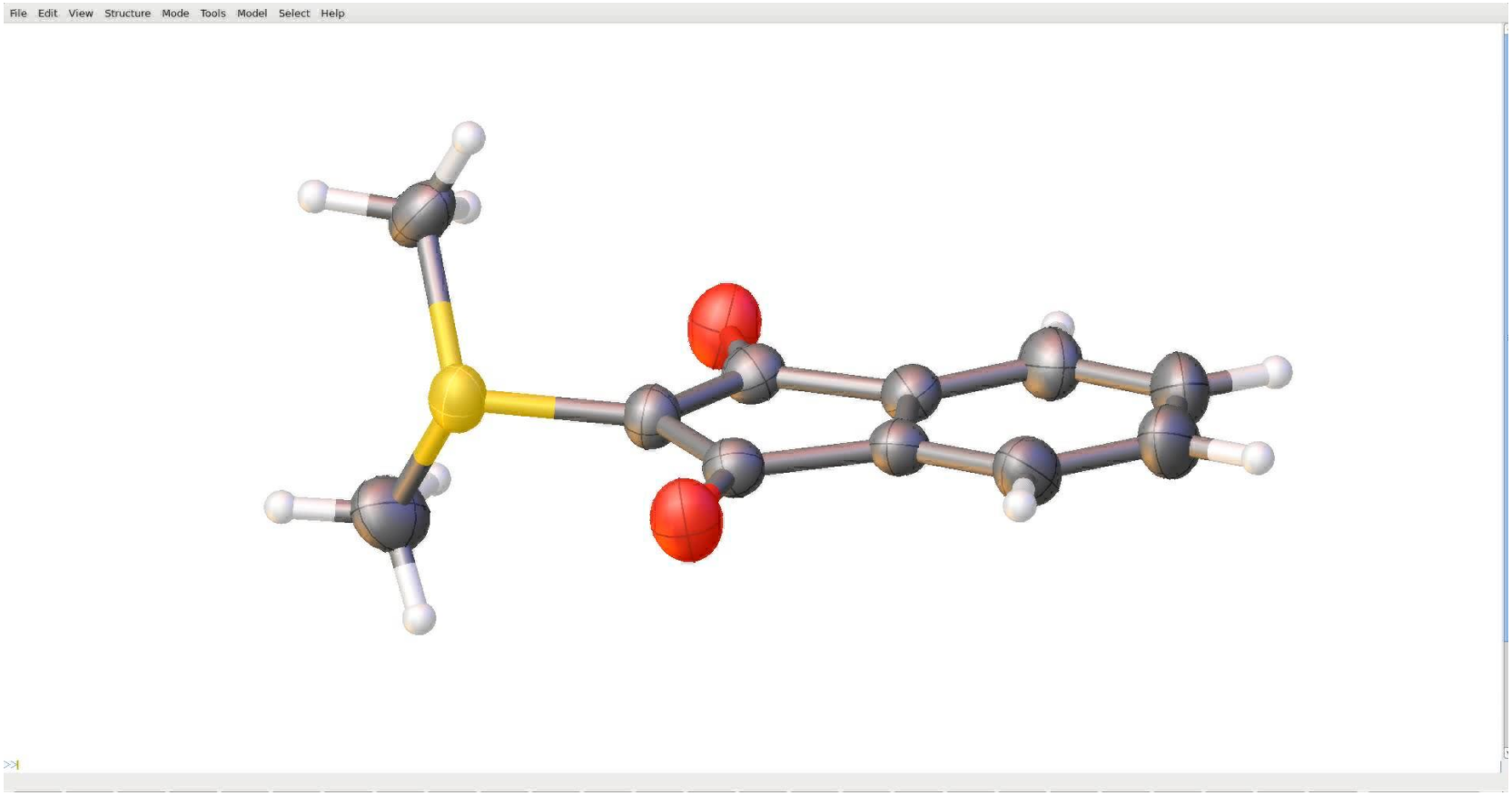

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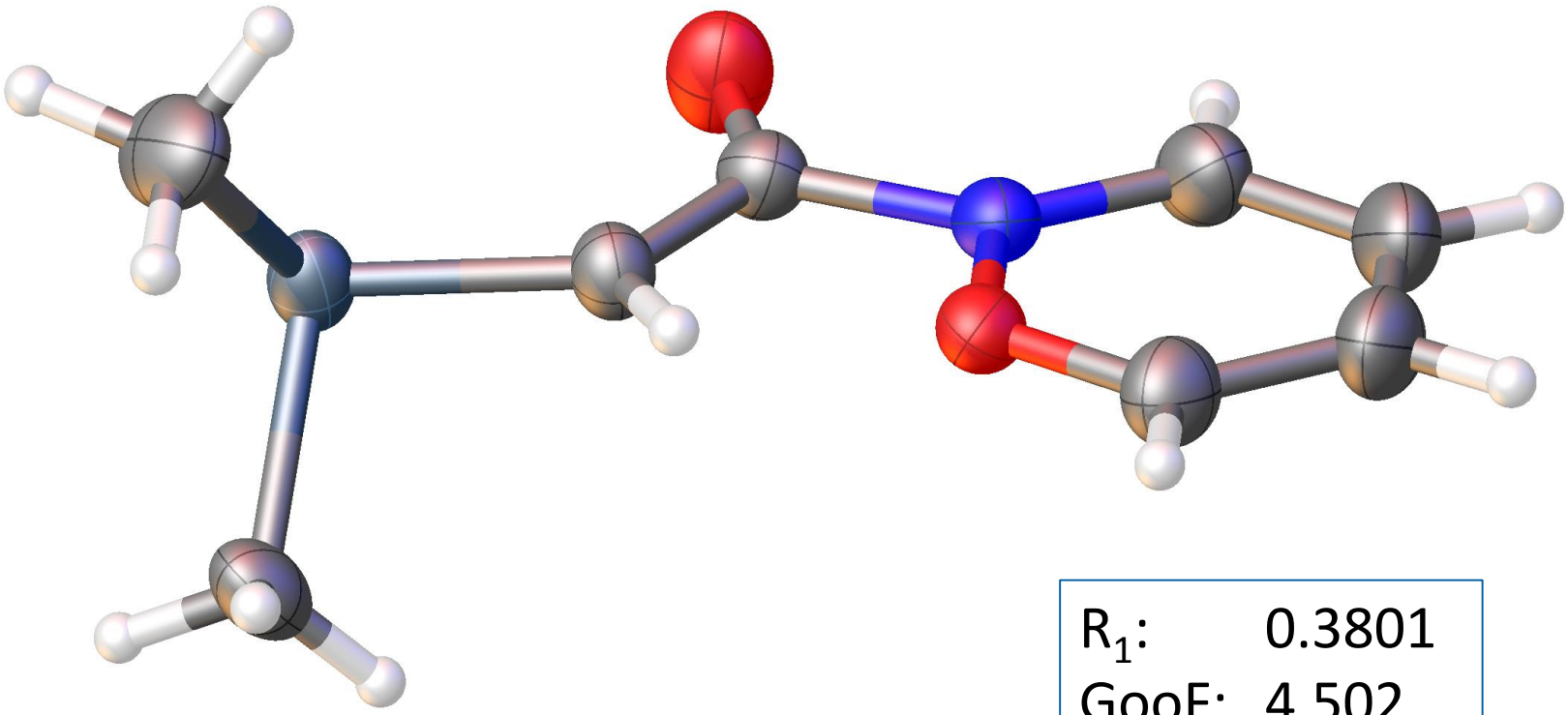

R_1:	0.3801
GooF:	4.502

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

 18 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 60 ALERT type 2 Indicator that the structure model may be wrong or deficient
 12 ALERT type 3 Indicator that the structure quality may be low
 41 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
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R_1: 0.3801

GooF: 4.502

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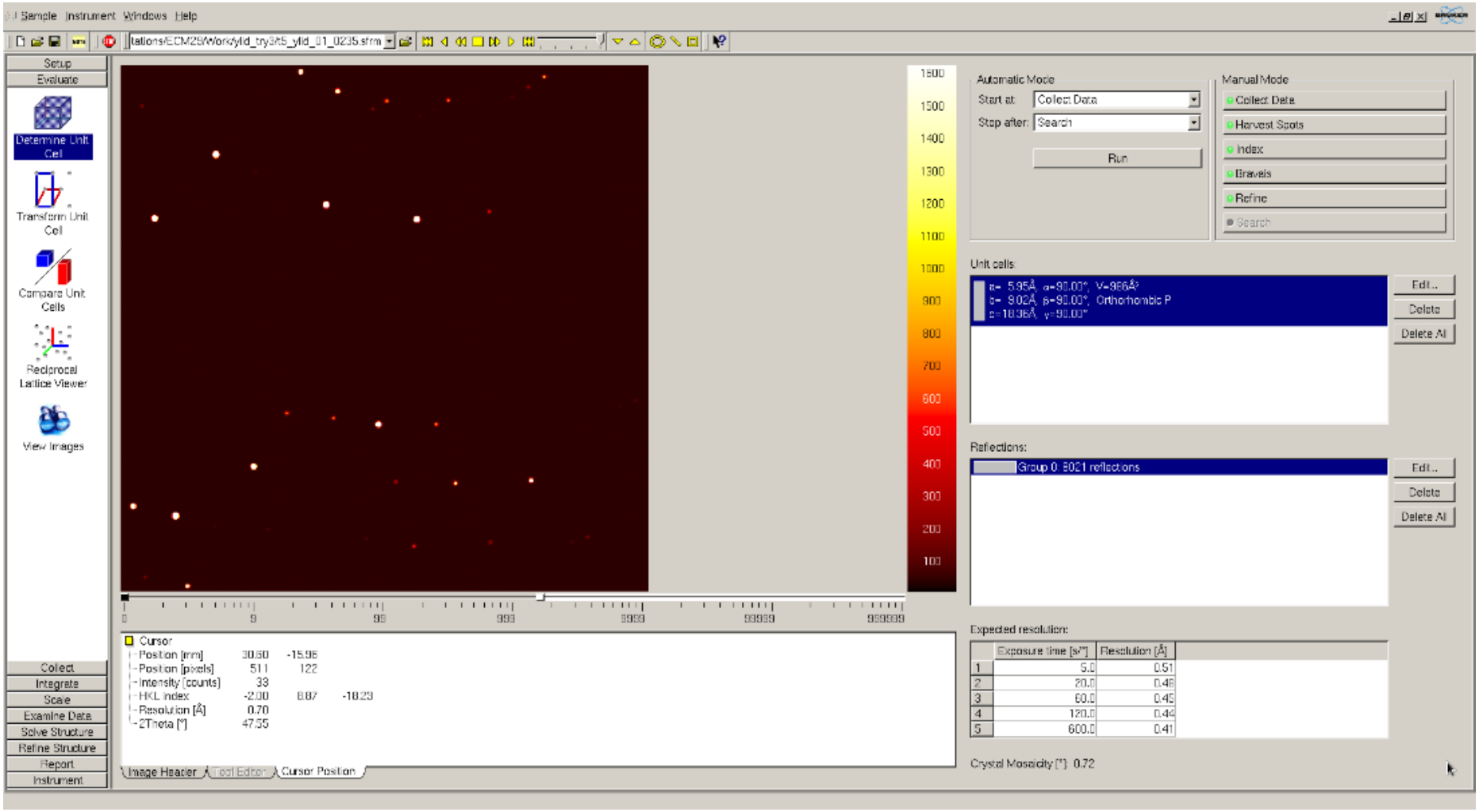

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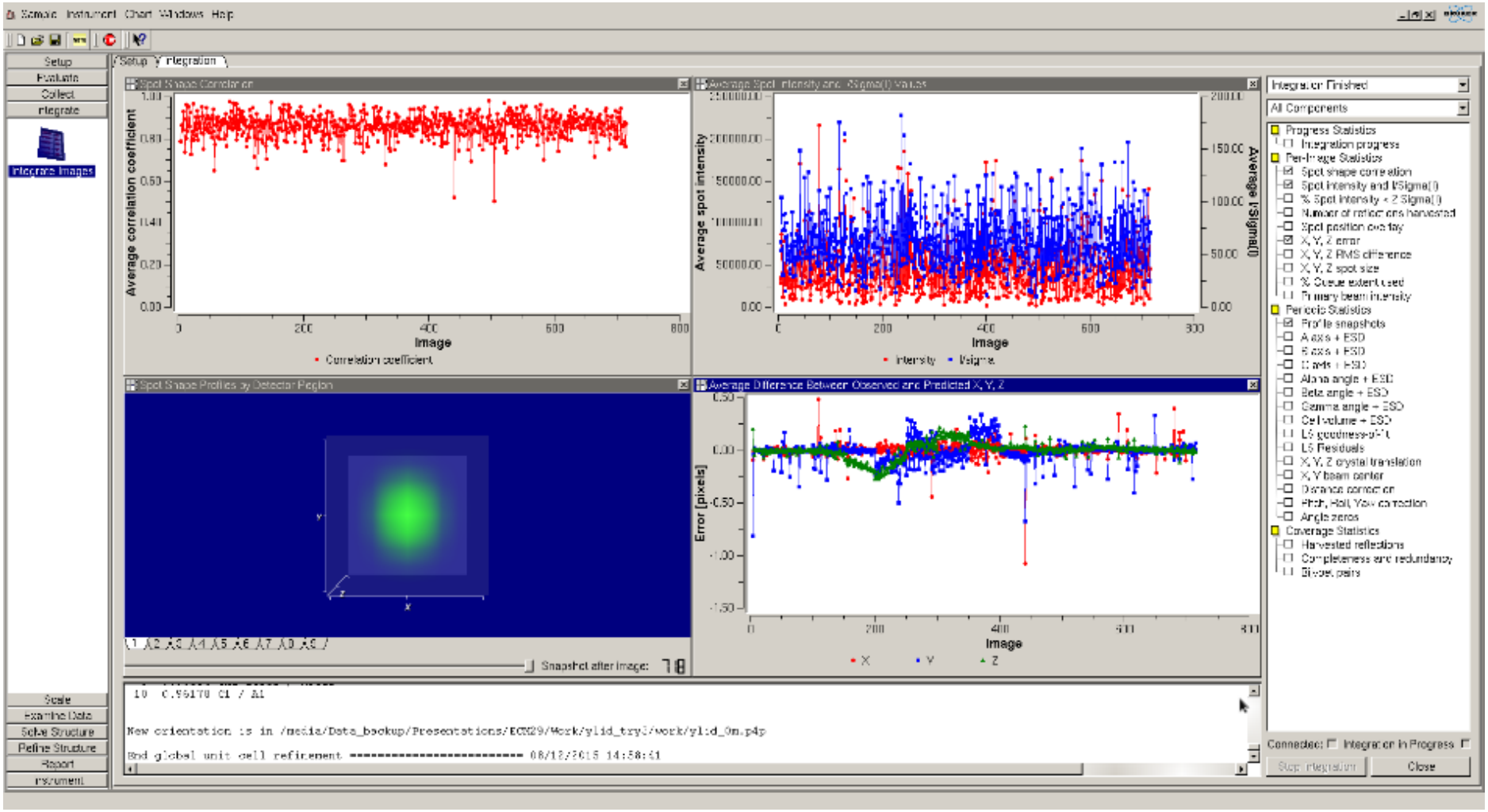

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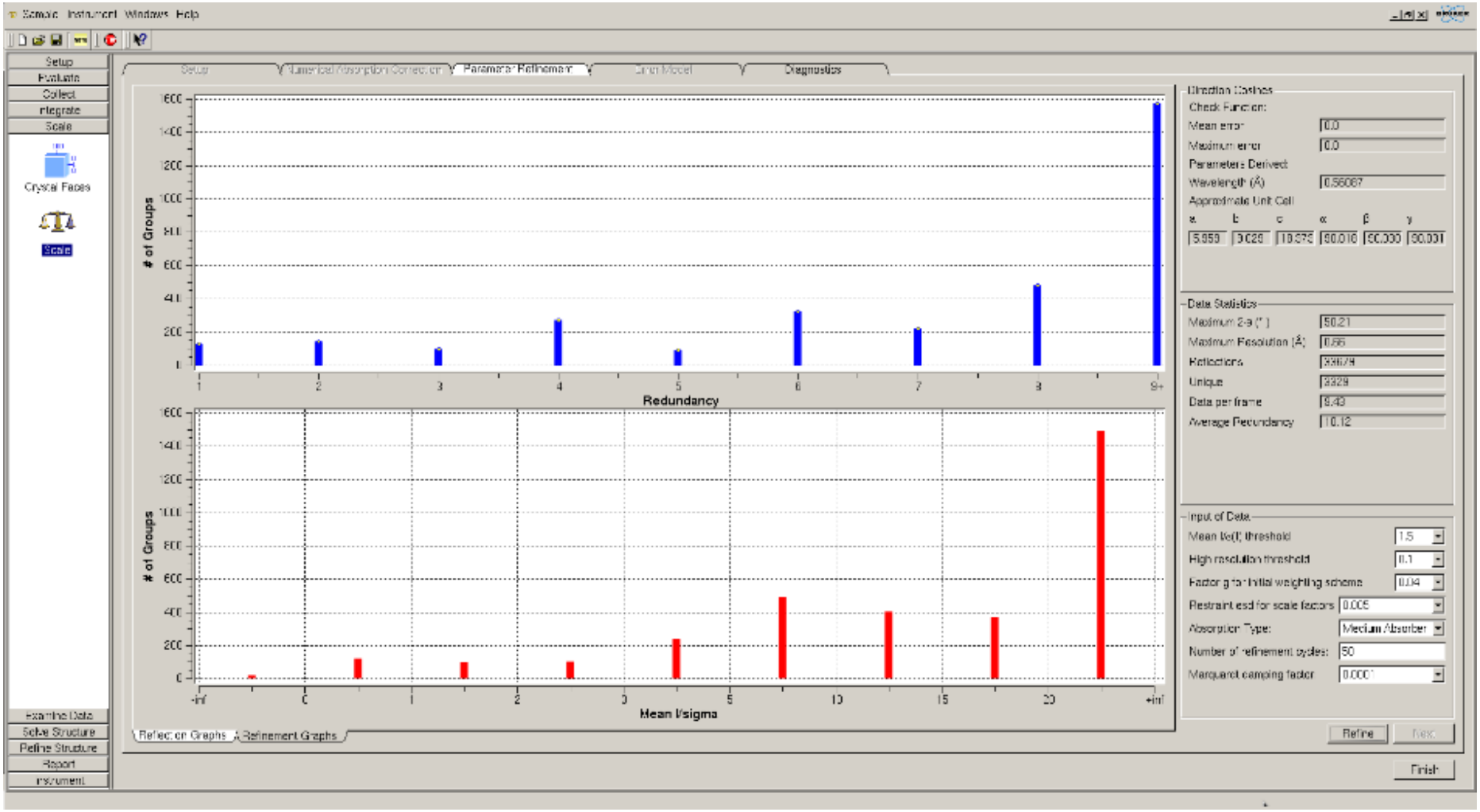

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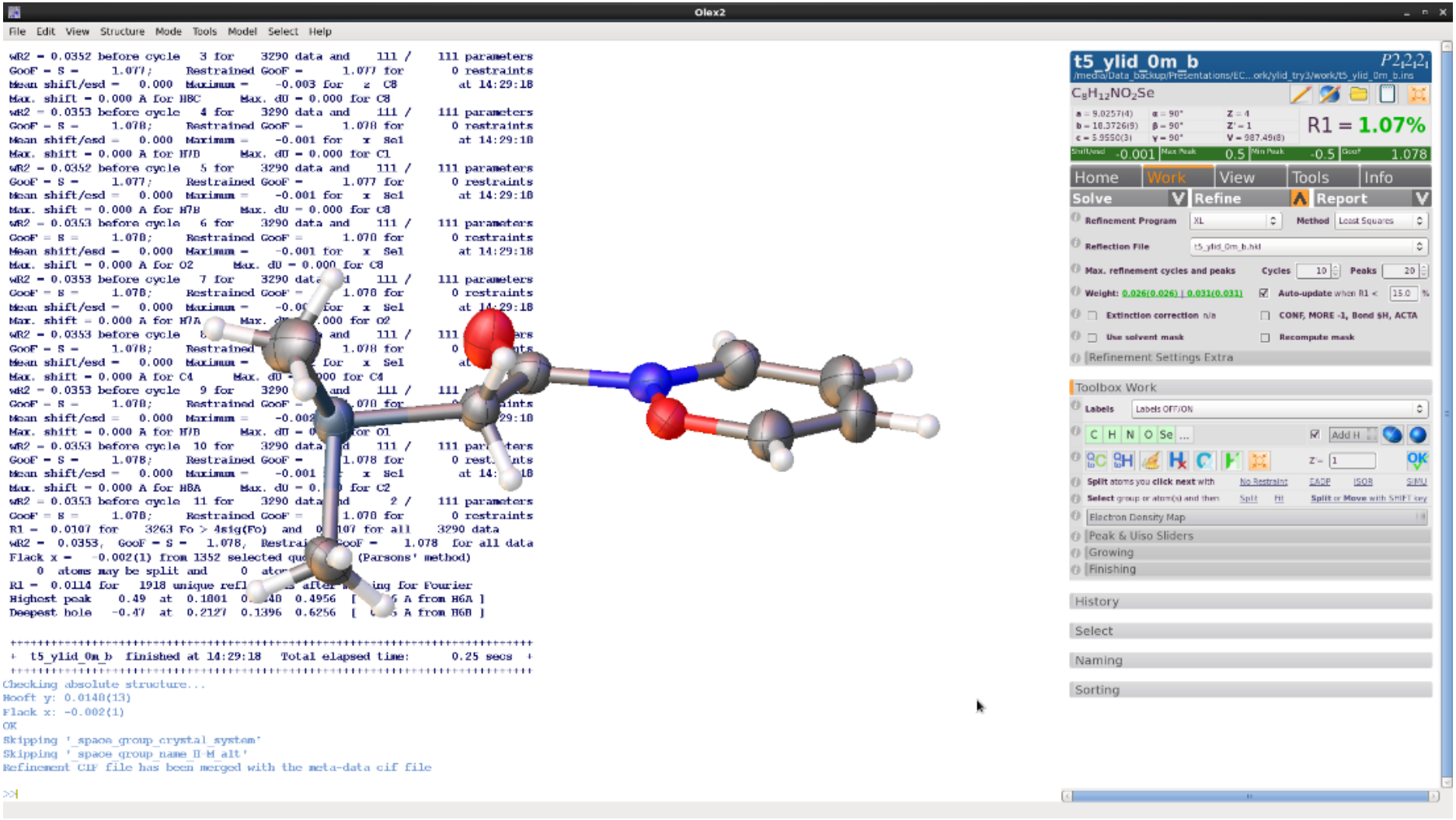

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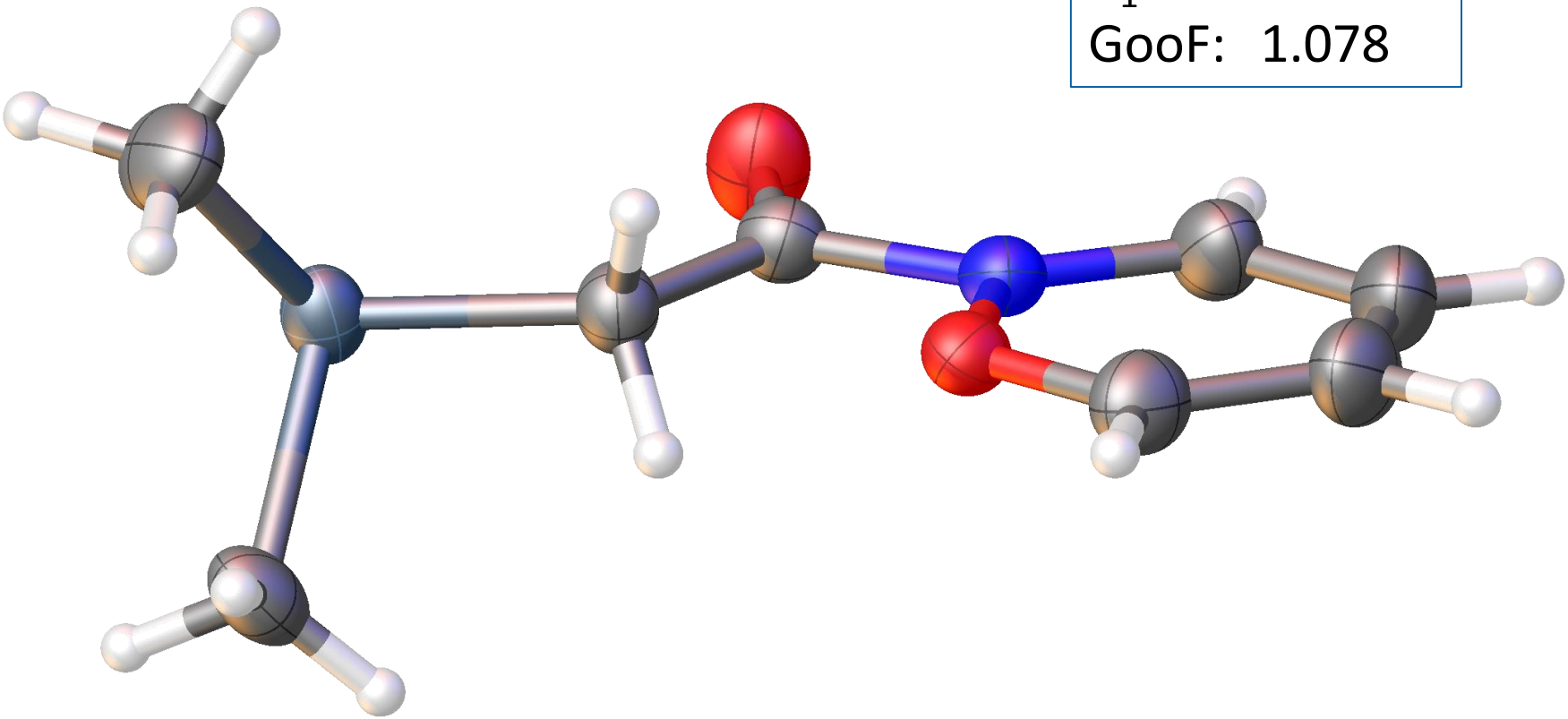

R_1:	0.0107
GooF:	1.078

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R_1: 0.0107

GooF: 1.078

Alert level C

PLAT911 ALERT 3 C Missing # FCF Refl Between THmin & STh/L= 0.600 9 Report

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0 ALERT type 5 Informative message, check

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How is it done?

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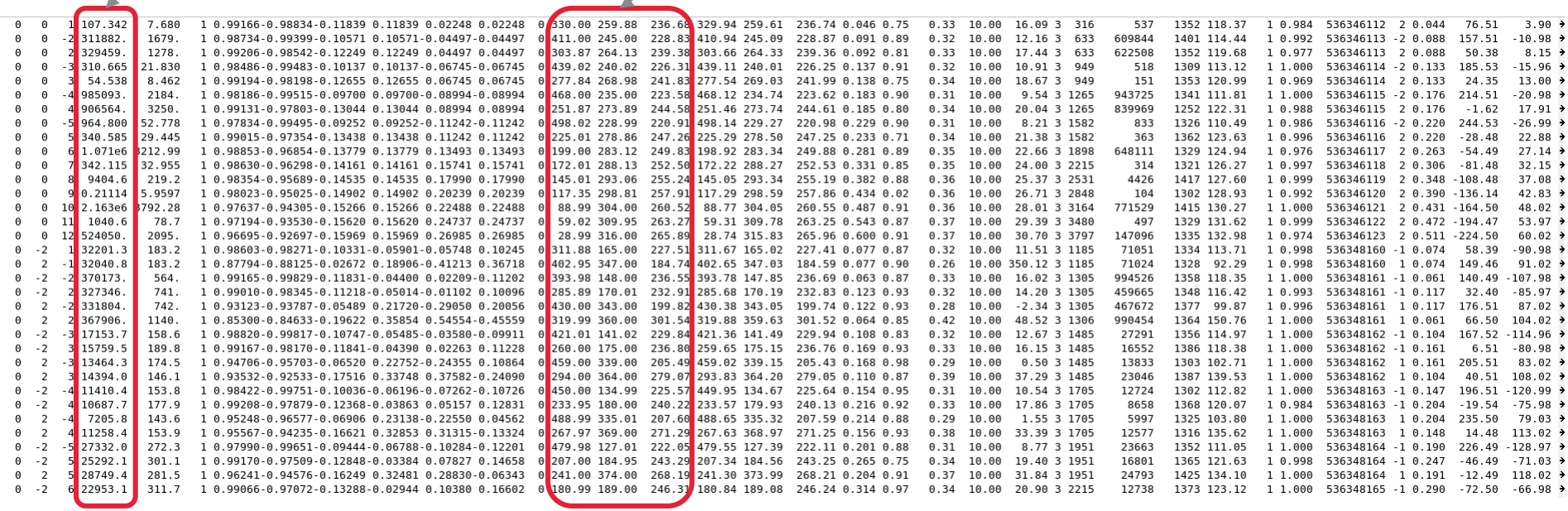
.raw file

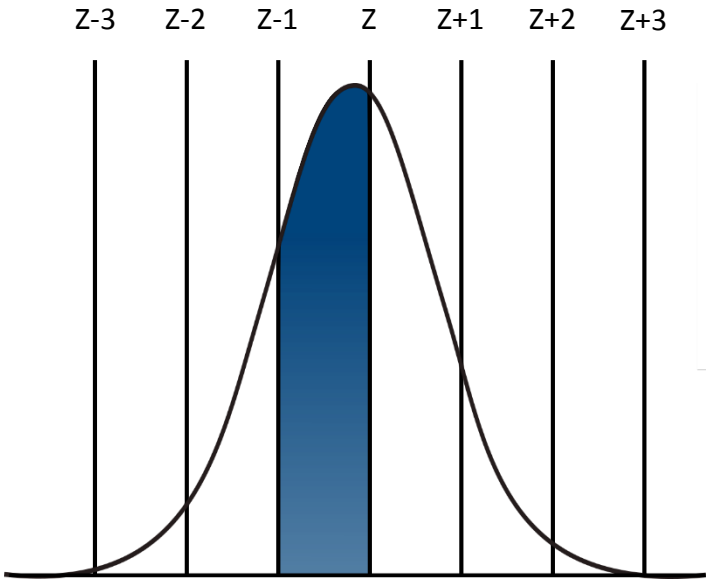
Integrated Intensity

X, Y, Z coordinates of spots



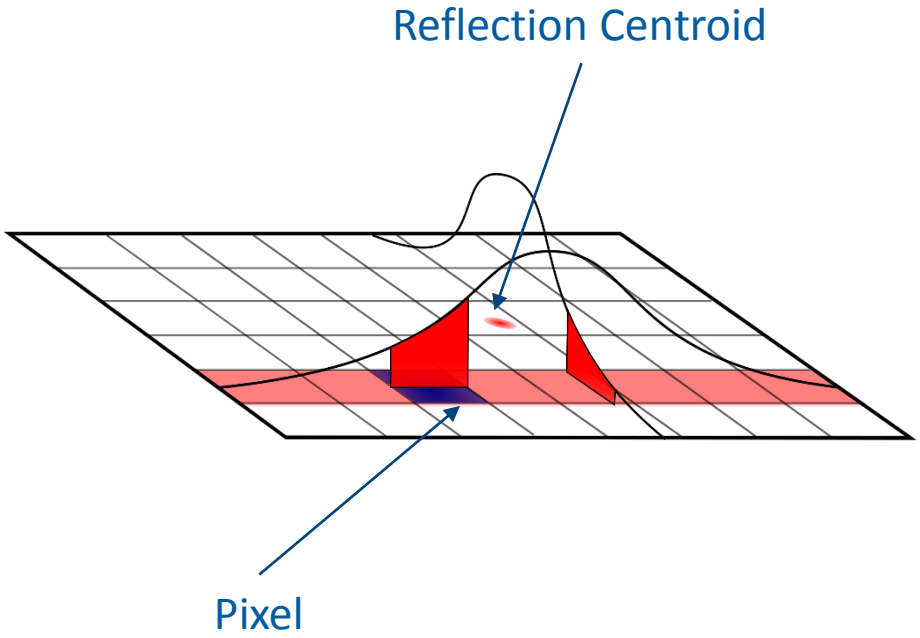
0	0	1	107.342	7.680	1	0.99166	-0.98834	-0.11839	0.11839	0.02248	0.02248	0	330.00	259.88	236.68	329.94	259.61	236.74	0.046	0.75	0.33	10.00	16.09	3	316	537	1352	118.37	1	0.984	536346112	2	0.044	76.51	3.90
0	0	-2	311882.	1679.	1	0.98734	-0.99399	-0.10571	0.10571	-0.04497	-0.04497	0	411.00	245.00	228.83	410.94	245.09	228.87	0.091	0.89	0.32	10.00	12.16	3	633	609844	1401	114.44	1	0.992	536346113	-2	0.088	157.51	-10.98
0	0	2	329459.	1278.	1	0.99206	-0.98542	-0.12249	0.12249	0.04497	0.04497	0	303.87	264.13	239.38	303.66	264.33	239.36	0.092	0.81	0.33	10.00	17.44	3	633	622508	1352	119.68	1	0.977	536346113	2	0.088	50.38	8.15
0	0	-3	310.665	21.830	1	0.98486	-0.99483	-0.10137	0.10137	-0.06745	-0.06745	0	439.02	240.02	226.31	439.11	240.01	226.25	0.137	0.91	0.32	10.00	10.91	3	949	518	1309	113.12	1	1.000	536346114	-2	0.133	185.53	-15.96
0	0	3	54.538	8.462	1	0.99194	-0.98198	-0.12655	0.12655	0.06745	0.06745	0	277.84	268.98	241.83	277.54	269.03	241.99	0.138	0.75	0.34	10.00	18.67	3	949	151	1353	120.99	1	0.969	536346114	2	0.133	24.35	13.00
0	0	-4	985093.	2184.	1	0.98186	-0.99515	-0.09700	0.09700	-0.08994	-0.08994	0	468.00	235.00	223.58	468.12	234.74	223.62	0.183	0.90	0.31	10.00	9.54	3	1265	943725	1341	111.81	1	1.000	536346115	-2	0.176	214.51	-20.98
0	0	4	906564.	3250.	1	0.99131	-0.97803	-0.13044	0.13044	0.08994	0.08994	0	251.87	273.89	244.58	251.46	273.74	244.61	0.185	0.80	0.34	10.00	20.04	3	1265	839969	1252	122.31	1	0.988	536346115	2	0.176	-1.62	17.91
0	0	-5	964.800	52.778	1	0.97834	-0.99495	-0.09252	0.09252	-0.11242	-0.11242	0	498.02	228.99	220.91	498.14	229.27	220.98	0.229	0.90	0.31	10.00	8.21	3	1582	833	1326	110.49	1	0.986	536346116	-2	0.220	244.53	-26.99
0	0	5	340.585	29.445	1	0.99015	-0.97354	-0.13438	0.13438	0.11242	0.11242	0	225.01	278.86	247.26	225.29	278.50	247.25	0.233	0.71	0.34	10.00	21.38	3	1582	363	1362	123.63	1	0.996	536346116	2	0.220	-28.48	22.88
0	0	6	1.071e6	4212.99	1	0.98853	-0.96854	-0.13779	0.13779	0.13493	0.13493	0	199.00	283.12	249.83	198.92	283.34	249.88	0.281	0.89	0.35	10.00	22.66	3	1898	648111	1329	124.94	1	0.976	536346117	2	0.263	-54.49	27.14
0	0	7	342.115	32.955	1	0.98630	-0.96298	-0.14161	0.14161	0.15741	0.15741	0	172.01	288.13	252.50	172.22	288.27	252.53	0.331	0.85	0.35	10.00	24.00	3	2215	314	1321	126.27	1	0.997	536346118	2	0.306	-81.48	32.15
0	0	8	9404.6	219.2	1	0.98354	-0.95689	-0.14535	0.14535	0.17990	0.17990	0	145.01	293.06	255.24	145.05	293.34	255.19	0.382	0.88	0.36	10.00	25.37	3	2531	4426	1417	127.60	1	0.999	536346119	2	0.348	-108.48	37.08
0	0	9	0.21114	5.9597	1	0.98023	-0.95025	-0.14902	0.14902	0.20239	0.20239	0	117.35	298.81	257.91	117.29	298.59	257.86	0.434	0.02	0.36	10.00	26.71	3	2848	104	1302	128.93	1	0.992	536346120	2	0.390	-136.14	42.83
0	0	10	2.163e6	9792.28	1	0.97637	-0.94305	-0.15266	0.15266	0.22488	0.22488	0	88.99	304.00	260.52	88.77	304.05	260.55	0.487	0.91	0.36	10.00	28.01	3	3164	771529	1415	130.27	1	1.000	536346121	2	0.431	-164.50	48.02
0	0	11	1040.6	78.7	1	0.97194	-0.93530	-0.15620	0.15620	0.24737	0.24737	0	59.02	309.95	263.27	59.31	309.78	263.25	0.543	0.87	0.37	10.00	29.39	3	3480	497	1329	131.62	1	0.999	536346122	2	0.472	-194.47	53.97
0	0	12	524050.	2095.	1	0.96695	-0.92697	-0.15969	0.15969	0.26985	0.26985	0	28.99	316.00	265.89	28.74	315.83	265.96	0.600	0.91	0.37	10.00	30.70	3	3797	147096	1335	132.98	1	0.974	536346123	2	0.511	-224.50	60.02
0	-2	1	32201.3	183.2	1	0.98603	-0.98271	-0.10331	-0.05901	-0.05748	0.10245	0	311.88	165.00	227.51	311.67	165.02	227.41	0.077	0.87	0.32	10.00	11.51	3	1185	71051	1334	113.71	1	0.998	536348160	-1	0.074	58.39	-90.98
0	2	-1	32040.8	183.2	1	0.87794	-0.88125	-0.02672	0.18906	-0.41213	0.36718	0	402.95	347.00	184.74	402.65	347.03	184.59	0.077	0.90	0.26	10.00	350.12	3	1185	71024	1328	92.29	1	0.998	536348160	1	0.074	149.46	91.02
0	-2	-2	370173.	564.	1	0.99165	-0.99829	-0.11831	-0.04400	0.02209	-0.11202	0	393.98	148.00	236.55	393.78	147.85	236.69	0.063	0.87	0.33	10.00	16.02	3	1305	994526	1358	118.35	1	1.000	536348161	-1	0.061	140.49	-107.98
0	-2	2	327346.	741.	1	0.99010	-0.98345	-0.11218	-0.05014	-0.01102	0.10096	0	285.89	170.01	232.91	285.68	170.19	232.83	0.123	0.93	0.32	10.00	14.20	3	1305	459665	1348	116.42	1	0.993	536348161	-1	0.117	32.40	-85.97
0	2	-2	331804.	742.	1	0.93123	-0.93787	-0.05489	0.21720	-0.29050	0.20056	0	430.00	343.00	199.82	430.38	343.05	199.74	0.122	0.93	0.28	10.00	-2.34	3	1305	467672	1377	99.87	1	0.996	536348161	1	0.117	176.51	87.02
0	2	2	367906.	1140.	1	0.85300	-0.84633	-0.19622	0.35854	0.54554	-0.45559	0	319.99	360.00	301.54	319.88	359.63	301.52	0.064	0.85	0.42	10.00	48.52	3	1306	990454	1364	150.76	1	1.000	536348161	1	0.061	66.50	104.02
0	-2	-3	17153.7	158.6	1	0.98820	-0.99817	-0.10747	-0.05485	-0.03580	-0.09911	0	421.01	141.02	229.84	421.36	141.49	229.94	0.108	0.83	0.32	10.00	12.67	3	1485	27291	1356	114.97	1	1.000	536348162	-1	0.104	167.52	-114.96
0	-2	3	15759.5	189.8	1	0.99167	-0.98170	-0.11841	-0.04390	0.02263	0.11228	0	260.00	175.00	236.80	259.65	175.15	236.76	0.169	0.93	0.33	10.00	16.15	3	1485	16552	1386	118.38	1	1.000	536348162	-1	0.161	6.51	-80.98
0	2	-3	13464.3	174.5	1	0.94706	-0.95703	-0.06520	0.22752	-0.24355	0.10864	0	459.00	339.00	205.49	459.02	339.15	205.43	0.168	0.98	0.29	10.00	0.50	3	1485	13833	1303	102.71	1	1.000	536348162	1	0.161	205.51	83.02
0	2	3	14394.0	146.1	1	0.93532	-0.92533	-0.17516	0.33748	0.37582	-0.24090	0	294.00	364.00	279.07	293.83	364.20	279.05	0.110	0.87	0.39	10.00	37.29	3	1485	23046	1387	139.53	1	1.000	536348162	1	0.104	40.51	108.02
0	-2	-4	11410.4	153.8	1	0.98422	-0.99751	-0.10036	-0.06196	-0.07262	-0.10726	0	450.00	134.99	225.57	449.95	134.67	225.64	0.154	0.95	0.31	10.00	10.54	3	1705	12724	1302	112.82	1	1.000	536348163	-1	0.147	196.51	-120.99
0	-2	4	10687.7	177.9	1	0.99208	-0.97879	-0.12368	-0.03863	0.05157	0.12831	0	233.95	180.00	240.22	233.57	179.93	240.13	0.216	0.92	0.33	10.00	17.86	3	1705	8658	1368	120.07	1	0.984	536348163	-1	0.204	-19.54	-75.98
0	2	-4	7205.8	143.6	1	0.95248	-0.96577	-0.06906	0.23138	-0.22550	0.04562	0	488.99	335.01	207.60	488.65	335.32	207.59	0.214	0.88	0.29	10.00	1.55	3	1705	5997	1325	103.80	1	1.000	536348163	1	0.204	235.50	79.03
0	2	4	11258.4	153.9	1	0.95567	-0.94235	-0.16621	0.32853	0.31315	-0.13324	0	267.97	369.00	271.29	267.63	368.97	271.25	0.156	0.93	0.38	10.00	33.39	3	1705	12577	1316	135.62	1	1.000	536348163	1	0.148	14.48	113.02
0	-2	-5	27332.0	272.3	1	0.97990	-0.99651	-0.09444	-0.06788	-0.10284	-0.12201	0	479.98	127.01	222.05	479.55	127.39	222.11	0.201	0.88	0.31	10.00	8.77	3	1951	23663	1352	111.05	1	1.000	536348164	-1	0.190	226.49	-128.97
0	-2	5	25292.1	301.1	1	0.99170	-0.97509	-0.12848	-0.03384	0.07827	0.14658	0	207.00	184.95	243.29	207.34	184.56	243.25	0.265	0.75	0.34	10.00	19.40	3	1951	16801	1365	121.63	1	0.998	536348164	-1	0.247	-46.49	-71.03
0	2	5	28749.4	281.5	1	0.96241	-0.94576	-0.16249	0.32481	0.28830	-0.06343	0	241.00	374.00	268.19	241.30	373.99	268.21	0.204	0.91	0.37	10.00	31.84	3	1951	24793	1425	134.10	1	1.000	536348164	1	0.191	-12.49	118.02
0	-2	6	22953.1	311.7	1	0.99066	-0.97072	-0.13288	-0.02944	0.10380	0.16602	0	180.99	189.00	246.31	180.84	189.08	246.24	0.314	0.97	0.34	10.00	20.90	3	2215	12738	1373	123.12	1	1.000	536348165	-1	0.290	-72.50	-66.98

- *.raw* files contain information on position and intensity of diffraction spots.
- Positional information can be used in conjunction with F^2 values, which are used as the total intensity values.
- Diffraction frames are all well documented, this knowledge allows us to produce frames that can be read within existing processing software.



- The sum of the intensity of each spot is calculated for each frame.
- Cumulative distribution is calculated between each pair of consecutive frames.
- Total intensity of a reflection on frame Z is the cumulative distribution of the Gaussian between Z and Z-1.

- Cumulative distribution is calculated for each row of pixels around the centroid.
- Then the cumulative distribution calculated for each pixel within the row.
- This process takes place for each reflection on a frame.
- After this is complete, a background is added to the image.



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- Frames are then manufactured.
- Header information is recycled from real frames – with minor edits.
- Image is encoded in the required format.

```
FORMAT :100
VERSION:15
HDRBLKS:15
TYPE   :Phi Scan Image
SITE   :XIPHOSIIA
MODEL  :D85 [08/10-2338] with 4-CIRCLE (HUBER)
USER   :BrukerAdministrator
SAMPLE :
SETNAME:
RUN    :1
SAMPNUM:0
TITLE  :
TITLE  :
TITLE  :
TITLE  :
TITLE  :
TITLE  :
TITLE  :
TITLE  :
NCOUNTS:9286403                              0
NOVERFL:-1                       149                     0
MINIMUM:26
MAXIMUM:12316
NONTIME:-2
NLATE  :-1
FILENAM:\\XIPHOSIIa\frames\guest\ylid_28_02_12\ylid_28_02_12_01_0025.sfrm
CREATED:02/28/12                             12:21:28
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ELAPSDR:3.000000
ELAPSDA:2.999000
OSCILLA:0
NSTEPS :1
RANGE  :0.500000
START  :193.000000
INCREME:0.500000
NUMBER :25
CSIZE  :
DNSMET :
DARK   :0482_00512_00003._dk
AUTORNG:0.000000E+000 0.000000E+000 0.000000E+000 0.000000E+000 1.251000E+006
ZEROADJ:0.000000          0.000000          0.000000          0.000000
XTRANS :0.000000                0.000000                0.000000
HKL&XY :0.000000      0.000000      0.000000      0.000000      0.000000
AXES2  :0.000000          0.000000          0.000000          1.000000
ENDING2:0.000000          0.000000          0.000000          1.000000
FILTER2:0.000000          0.000000          0.000000          4.170000
LEPTOS :
CFR: HDR:  IMG:
.....................................................................!# " !"! !!!#
!#""&#!#"!"!$$! !"$###    ""  !!""#"# "!!  !'*'!"!!"$"!" "$"##"""!"  !%# !!"$
!"!"&."$""&*!" #" !! !!#%##"#####&$# $#! "#"# $#""!"" ! !"  "# "$!  ""!  !" "#" "
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#!!""##! # ! *$# "$  # ($!!! " "!! #"!"!#!" $!$"$!"$ &$#""$ !!""! !!"!!&$#!!"!#
+&!"!!!!$!)!! %"#← ""&$$!! !#!" !!!!&'#'/""!$"!!! ##$! #!# !"#!""!""!"! !$(%"$!
*&)#!$$  $('!" " #"!!####"" #$#"" #"!"!"#" #!"#"$"#$"  "$ &%# """"# # %$ "  " !!
!"()# !"# #$# #$#!" !%"!" ! #$&' "!$!"!# %&(! """!""!"$ "!&"#")%#"'$!"3$#!$$#1$ !
#! #  %!#'"$ ! %!!!"!!!"!"$!#!*'$  !!'#! $!"#&#(#!!"'("" "#&!!!"! "%!!"$"(%"!"'!
```

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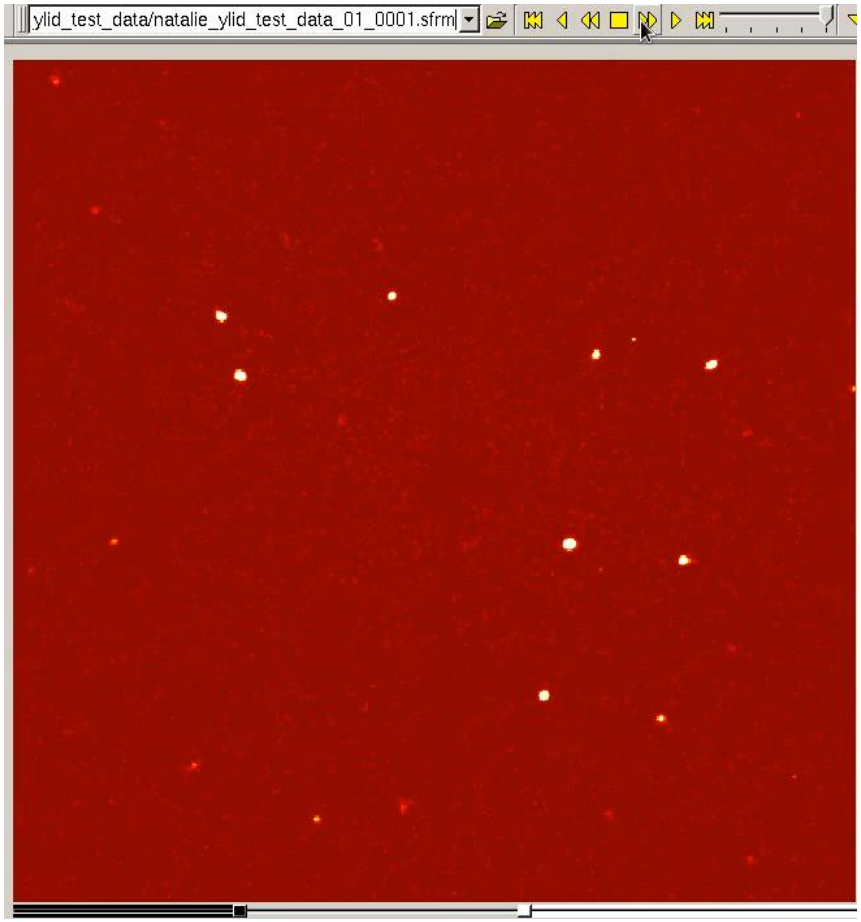
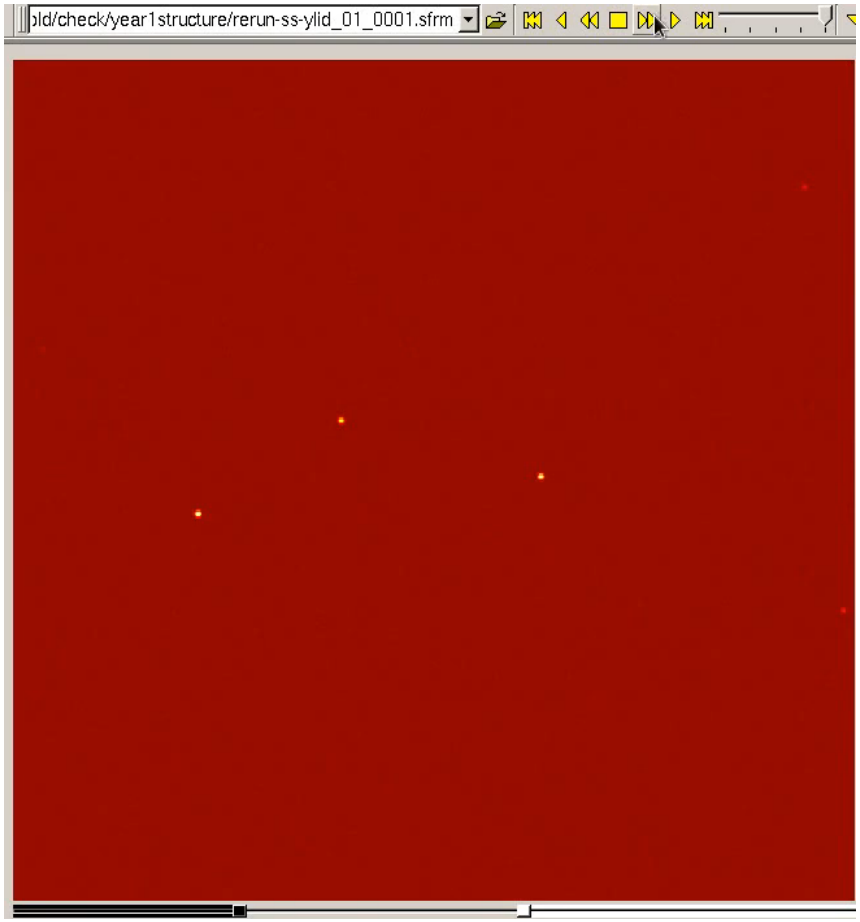
Frame Comparison



Real



Replica

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How Could We Detect Fraud Within Raw Diffraction Frames?

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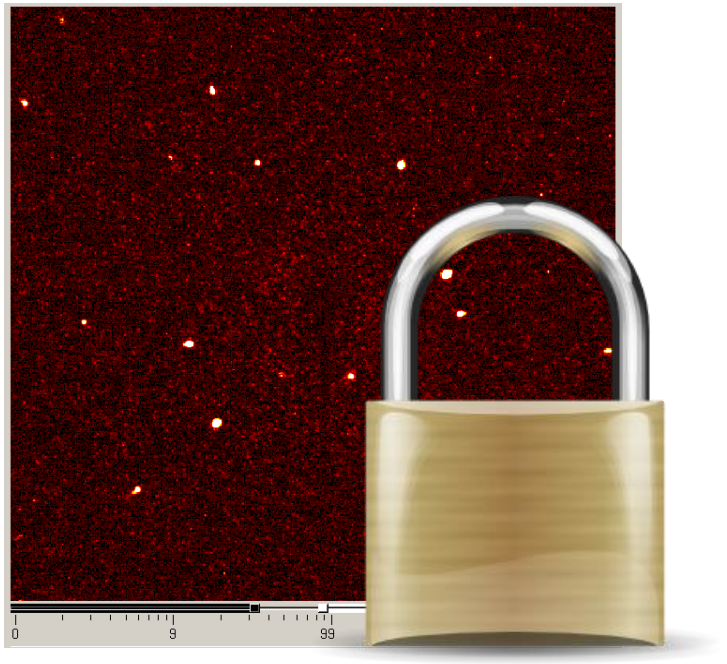
Encrypt Entire Frame

- Fraudsters would have to crack the encryption and be able to re-encrypt files.
- Could slow down diffraction software as the decryptions need to be performed.
- Could hamper the development of current and new diffraction frame formats.



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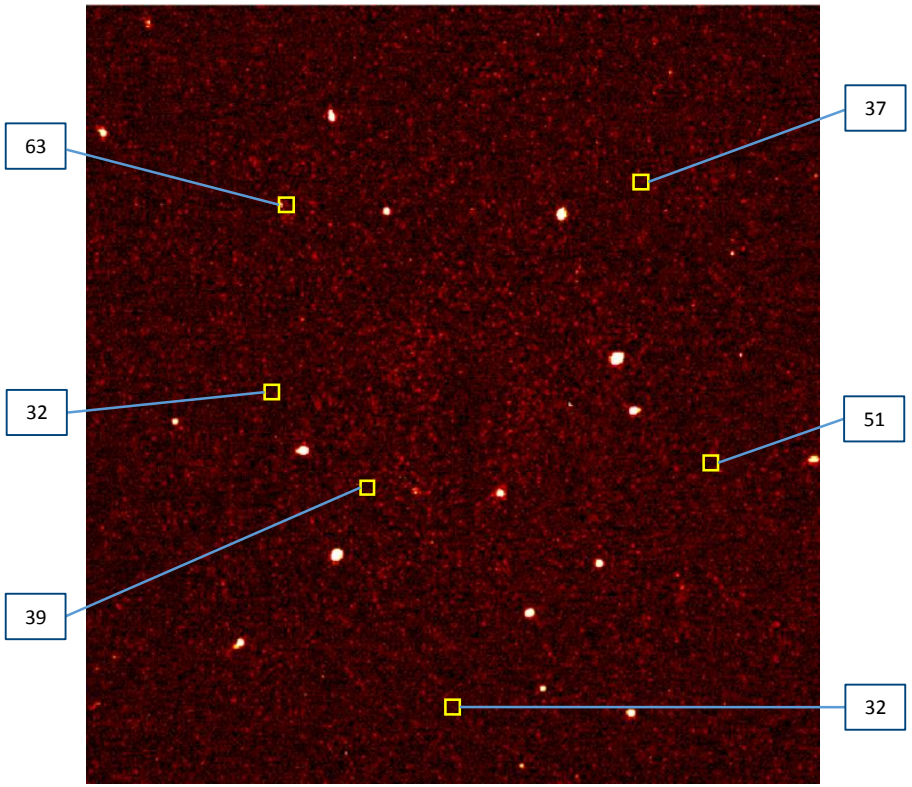
Encryptions within frame header

- Using information from the diffraction image to create an encrypted section within the header.
- Encryption check required when file is submitted.



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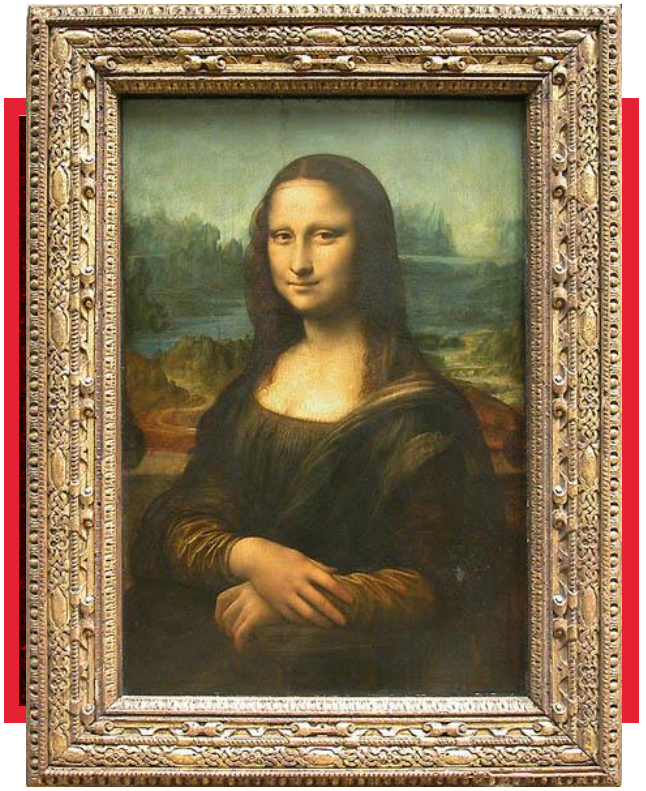
Addition of information

- Fraud is prevented by photographing and cataloguing famous artwork without its frame.
- In a similar way, extra values or information could be added around the image, within the image binary itself.
- Fraudsters would have to know of its existence.



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Certification

- An additional file produced during the diffraction process, which contains encrypted information about the frames.
- Encryption check needed when raw images are submitted.

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Acknowledgements

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Thank you for listening

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Should we rely on the honesty of our peers?

Has anything like this already been done?