

Supplementary data for article :

Pavic, A.; Glišić, B. Đ.; Vojnovic, S.; Waržajtis, B.; Savić, N. D.; Antić, M.; Radenković, S.; Janjić, G. V.; Nikodinovic-Runic, J.; Rychlewska, U.; et al. Mononuclear Gold(III) Complexes with Phenanthroline Ligands as Efficient Inhibitors of Angiogenesis: A Comparative Study with Auranofin and Sunitinib. *Journal of Inorganic Biochemistry* **2017**, *174*, 156–168. <https://doi.org/10.1016/j.jinorgbio.2017.06.009>

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data_1_7phen

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_publ_contact_author_phone      '48 61 8291683'
_publ_contact_author_fax       '48 61 8291555'
_publ_contact_author_email     urszular@amu.edu.pl

_publ_requested_journal        'Journal of Medicinal Chemistry'
_journal_year                  2017
_journal_volume                0000
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  'Rychlewska, Urszula'
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Poland
;
'War\.zajtis, Beata'
;
Department of Chemistry
Adam Mickiewicz University
Umultowska 89B
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Poland
;

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  'Au' 'Au' -2.0133 8.8022
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  _shelx_space_group_comment
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  The symmetry employed for this shelxl refinement is uniquely defined
  by the following loop, which should always be used as a source of
  symmetry information in preference to the above space-group names.
  They are only intended as comments.
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CrysAlisPro (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897,
Agilent Technologies, 2014)
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Reflections were merged by SHELXL according to the crystal

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class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique
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possible theoretically, ignoring centric projections and
systematic absences.
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CrysAlisPro, Agilent Technologies (2014)
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H2 H 0.5770 0.9556 0.6001 0.054 Uiso 1 1 calc R U . . . . .
C3 C 0.6384(4) 0.8315(3) 0.6835(6) 0.0459(11) Uani 1 1 d . . . . .
H3 H 0.7081 0.8539 0.7237 0.055 Uiso 1 1 calc R U . . . . .
C4 C 0.6143(4) 0.7392(3) 0.6974(5) 0.0425(10) Uani 1 1 d . . . . .
H4 H 0.6665 0.6977 0.7499 0.051 Uiso 1 1 calc R U . . . . .
C5 C 0.4785(3) 0.6101(3) 0.6325(5) 0.0381(10) Uani 1 1 d . . . . .
H5 H 0.5290 0.5663 0.6821 0.046 Uiso 1 1 calc R U . . . . .
C6 C 0.3786(3) 0.5799(3) 0.5640(5) 0.0359(9) Uani 1 1 d . . . . .
H6 H 0.3617 0.5160 0.5639 0.043 Uiso 1 1 calc R U . . . . .
C8 C 0.1196(4) 0.6772(3) 0.3581(5) 0.0392(10) Uani 1 1 d . . . . .
H8 H 0.0506 0.6552 0.3132 0.047 Uiso 1 1 calc R U . . . . .
C9 C 0.1407(4) 0.7725(3) 0.3567(6) 0.0420(10) Uani 1 1 d . . . . .
H9 H 0.0862 0.8141 0.3115 0.050 Uiso 1 1 calc R U . . . . .
C10 C 0.2418(3) 0.8056(3) 0.4218(5) 0.0358(9) Uani 1 1 d . . . . .
H10 H 0.2564 0.8699 0.4209 0.043 Uiso 1 1 calc R U . . . . .
C11 C 0.5092(3) 0.7064(3) 0.6317(5) 0.0329(9) Uani 1 1 d . . . . .
C12 C 0.2988(3) 0.6460(3) 0.4917(5) 0.0286(8) Uani 1 1 d . . . . .
C13 C 0.3234(3) 0.7424(2) 0.4898(5) 0.0282(8) Uani 1 1 d . . . . .
C14 C 0.4328(3) 0.7734(3) 0.5594(5) 0.0306(9) Uani 1 1 d . . . . .
N1 N 0.4566(3) 0.8665(2) 0.5488(4) 0.0379(8) Uani 1 1 d . . . . .
N7 N 0.1965(3) 0.6155(2) 0.4231(4) 0.0330(7) Uani 1 1 d . . . . .
C11 Cl 0.11638(9) 0.48806(7) 0.70445(13) 0.0387(2) Uani 1 1 d . . . . .
C12 Cl 0.11800(10) 0.31933(7) 0.42465(14) 0.0462(3) Uani 1 1 d . . . . .
C13 Cl 0.19842(15) 0.46637(8) 0.14247(16) 0.0663(4) Uani 1 1 d . . . . .
Au1 Au 0.15639(2) 0.47532(2) 0.42214(2) 0.03064(7) Uani 1 1 d . . . . .

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C3 0.034(3) 0.050(3) 0.052(3) -0.005(2) -0.002(2) -0.010(2)
C4 0.030(3) 0.049(3) 0.048(3) 0.000(2) 0.0010(19) 0.0031(19)
C5 0.033(3) 0.036(2) 0.044(2) 0.0066(19) 0.0009(19) 0.0080(18)
C6 0.034(2) 0.027(2) 0.046(2) 0.0030(17) 0.0017(19) 0.0013(18)
C8 0.029(2) 0.039(2) 0.048(2) 0.0052(19) -0.0035(19) -0.0001(18)
C9 0.037(3) 0.034(2) 0.054(3) 0.011(2) -0.002(2) 0.0099(19)
C10 0.038(3) 0.028(2) 0.042(2) 0.0047(17) 0.0038(19) -0.0012(18)
C11 0.028(2) 0.037(2) 0.034(2) -0.0013(17) 0.0023(17) -0.0008(17)

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C12 0.023(2) 0.032(2) 0.031(2) 0.0027(16) 0.0025(16) -0.0024(16)
C13 0.029(2) 0.029(2) 0.028(2) 0.0013(16) 0.0054(16) 0.0021(16)
C14 0.031(2) 0.035(2) 0.027(2) -0.0008(16) 0.0076(17) -0.0028(17)
N1 0.040(2) 0.0298(18) 0.044(2) -0.0002(15) 0.0038(16) -0.0028(15)
N7 0.0323(19) 0.0316(18) 0.0349(18) 0.0044(14) 0.0031(14) -0.0008(15)
C11 0.0457(7) 0.0372(6) 0.0331(5) -0.0012(4) 0.0036(5) -0.0030(5)
C12 0.0454(7) 0.0316(6) 0.0609(7) -0.0049(5) 0.0029(5) -0.0047(5)
C13 0.1066(12) 0.0558(8) 0.0399(7) 0.0019(5) 0.0245(7) 0.0080(7)
Au1 0.02950(11) 0.02825(11) 0.03347(10) 0.00100(6) -0.00023(7) -
0.00125(6)

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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C2 C3 1.384(6) . ?

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C3 H3 0.9300 . ?

C4 C11 1.408(6) . ?

C4 H4 0.9300 . ?

C5 C6 1.346(5) . ?

C5 C11 1.418(5) . ?

C5 H5 0.9300 . ?

C6 C12 1.424(5) . ?

C6 H6 0.9300 . ?

C8 N7 1.342(5) . ?

C8 C9 1.377(6) . ?

C8 H8 0.9300 . ?

C9 C10 1.365(6) . ?

C9 H9 0.9300 . ?

C10 C13 1.402(5) . ?

C10 H10 0.9300 . ?

C11 C14 1.407(5) . ?

C12 N7 1.374(5) . ?

C12 C13 1.401(5) . ?

C13 C14 1.453(5) . ?

C14 N1 1.357(5) . ?

N7 Au1 2.049(3) . ?
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C13 Au1 2.2701(12) . ?

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C3 C2 H2 117.8 . . ?
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C3 C4 C11 119.4(4) . . ?
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C11 C4 H4 120.3 . . ?
C6 C5 C11 122.2(4) . . ?
C6 C5 H5 118.9 . . ?
C11 C5 H5 118.9 . . ?
C5 C6 C12 119.9(4) . . ?
C5 C6 H6 120.1 . . ?
C12 C6 H6 120.1 . . ?
N7 C8 C9 121.4(4) . . ?
N7 C8 H8 119.3 . . ?
C9 C8 H8 119.3 . . ?
C10 C9 C8 119.9(4) . . ?
C10 C9 H9 120.1 . . ?
C8 C9 H9 120.1 . . ?
C9 C10 C13 119.7(4) . . ?
C9 C10 H10 120.1 . . ?
C13 C10 H10 120.1 . . ?
C14 C11 C4 117.4(4) . . ?
C14 C11 C5 119.4(4) . . ?
C4 C11 C5 123.3(4) . . ?
N7 C12 C13 119.4(3) . . ?
N7 C12 C6 119.9(3) . . ?
C13 C12 C6 120.6(4) . . ?
C12 C13 C10 119.0(4) . . ?
C12 C13 C14 118.8(3) . . ?
C10 C13 C14 122.2(3) . . ?
N1 C14 C11 123.1(4) . . ?
N1 C14 C13 117.8(3) . . ?
C11 C14 C13 119.1(3) . . ?
C2 N1 C14 116.4(4) . . ?
C8 N7 C12 120.6(3) . . ?
C8 N7 Au1 118.4(3) . . ?
C12 N7 Au1 121.0(2) . . ?
N7 Au1 C12 178.07(10) . . ?

N7 Au1 C13 88.90(9) . . ?
C12 Au1 C13 91.16(4) . . ?
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C13 Au1 C11 178.49(4) . . ?

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C11 C5 C6 C12 -1.7(6) ?
N7 C8 C9 C10 0.2(7) ?
C8 C9 C10 C13 -0.1(6) ?
C3 C4 C11 C14 -2.2(6) ?
C3 C4 C11 C5 176.7(4) ?
C6 C5 C11 C14 0.9(6) ?
C6 C5 C11 C4 -177.9(4) ?
C5 C6 C12 N7 -179.5(4) ?
C5 C6 C12 C13 0.5(6) ?
N7 C12 C13 C10 1.6(5) ?
C6 C12 C13 C10 -178.3(3) ?
N7 C12 C13 C14 -178.6(3) ?
C6 C12 C13 C14 1.4(5) ?
C9 C10 C13 C12 -0.9(6) ?
C9 C10 C13 C14 179.4(4) ?
C4 C11 C14 N1 0.9(6) ?
C5 C11 C14 N1 -178.0(4) ?
C4 C11 C14 C13 179.9(3) ?
C5 C11 C14 C13 1.0(5) ?
C12 C13 C14 N1 177.0(3) ?
C10 C13 C14 N1 -3.3(5) ?
C12 C13 C14 C11 -2.1(5) ?
C10 C13 C14 C11 177.6(3) ?
C3 C2 N1 C14 -1.7(6) ?
C11 C14 N1 C2 1.0(6) ?
C13 C14 N1 C2 -178.1(3) ?
C9 C8 N7 C12 0.6(6) ?
C9 C8 N7 Au1 179.2(3) ?
C13 C12 N7 C8 -1.5(5) ?
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ZERR 4.00 0.0003 0.0003 0.0002 0.000 0.002 0.000
LATT 1
SYMM - X, 1/2 + Y, 1/2 - Z
SFAC C H N CL AU
UNIT 48 32 8 12 4
MERG 2
FMAP 2
PLAN 10
SIZE 0.030 0.050 0.180
ACTA
BOND \$H
CONF
L.S. 20
TEMP 22.00
WGHT 0.019500 0.721600
FVAR 1.81240
C2 1 0.558434 0.892364 0.608876 11.00000 0.04657
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H2 2 0.577049 0.955578 0.600057 11.00000 -1.20000
AFIX 0
C3 1 0.638447 0.831491 0.683534 11.00000 0.03390
0.05034 =
0.05212 -0.00485 -0.00236 -0.01045
AFIX 43
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AFIX 0
C4 1 0.614254 0.739193 0.697413 11.00000 0.02956
0.04945 =
0.04787 0.00039 0.00096 0.00306
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AFIX 0
C5 1 0.478456 0.610074 0.632508 11.00000 0.03339
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C12 1 0.298796 0.646031 0.491728 11.00000 0.02285
0.03194 =
0.03110 0.00269 0.00252 -0.00238
C13 1 0.323400 0.742416 0.489821 11.00000 0.02856
0.02867 =
0.02780 0.00127 0.00540 0.00213
C14 1 0.432768 0.773449 0.559371 11.00000 0.03096
0.03454 =
0.02733 -0.00082 0.00763 -0.00280
N1 3 0.456589 0.866491 0.548827 11.00000 0.03982
0.02981 =
0.04404 -0.00021 0.00378 -0.00283
N7 3 0.196496 0.615468 0.423063 11.00000 0.03232
0.03157 =
0.03493 0.00438 0.00309 -0.00080
CL1 4 0.116384 0.488058 0.704448 11.00000 0.04566
0.03719 =
0.03315 -0.00120 0.00359 -0.00303
CL2 4 0.118000 0.319326 0.424648 11.00000 0.04544
0.03157 =
0.06092 -0.00486 0.00287 -0.00471
CL3 4 0.198421 0.466374 0.142467 11.00000 0.10659
0.05576 =
0.03991 0.00193 0.02449 0.00799
AU1 5 0.156386 0.475316 0.422135 11.00000 0.02950
0.02825 =
0.03347 0.00100 -0.00023 -0.00125
HKLF 4

```

```

REM AuCl3_1_7phen in P2(1)/c
REM R1 = 0.0190 for 2126 Fo > 4sig(Fo) and 0.0230 for all 2336
data

```

REM 163 parameters refined using 0 restraints

END

WGHT 0.0195 0.7216

REM Highest difference peak 0.833, deepest hole -0.564, 1-sigma level 0.113

Q1	1	0.1407	0.4743	0.2505	11.00000	0.05	0.83
Q2	1	0.1762	0.4781	0.5436	11.00000	0.05	0.67
Q3	1	0.2287	0.4772	0.2582	11.00000	0.05	0.63
Q4	1	0.0878	0.4721	0.5351	11.00000	0.05	0.58
Q5	1	0.0551	0.4768	0.2552	11.00000	0.05	0.49
Q6	1	0.0610	0.4788	0.4074	11.00000	0.05	0.47
Q7	1	0.2804	0.5189	0.7363	11.00000	0.05	0.41
Q8	1	0.0270	0.5375	0.5104	11.00000	0.05	0.40
Q9	1	0.3390	0.4751	0.4037	11.00000	0.05	0.39
Q10	1	0.1269	0.4905	0.1207	11.00000	0.05	0.39

;

_shelx_res_checksum 2901

_shelx_hkl_file

;

0	0	-2	110607.	1521.48	1
0	0	2	112898.	1520.47	9
0	0	-2	119195.	1546.10	9
0	0	2	112295.	1730.80	8
0	0	2	111069.	1436.57	2
0	0	-2	118073.	1713.48	8
0	0	-2	111103.	1388.74	2
0	0	2	123637.	1575.50	5
0	0	2	116197.	1563.94	1
0	0	-3	138.779	132.930	2
0	0	3	295.637	129.286	5
0	0	3	-1.93638	94.0133	1
0	0	-3	38.8482	108.822	8
0	0	3	68.2937	107.028	6
0	0	3	137.635	144.042	2
0	0	3	251.743	136.708	9
0	0	3	57.7416	26.5728	4
0	0	-3	167.886	105.301	1
0	0	-3	-60.2397	86.2451	9
0	0	-4	49787.7	1459.50	1
0	0	4	51566.7	1467.34	9
0	0	-4	49742.2	1315.59	2
0	0	-4	52870.2	1201.45	3
0	0	4	47609.8	589.262	4
0	0	-5	45.2828	125.703	1
0	0	5	57.5259	123.044	9
0	0	-5	54.7575	102.477	2
0	0	-5	40.2868	106.010	3
0	0	-6	61597.1	2057.10	1
0	0	-6	60127.6	1799.35	2
0	0	6	60648.1	2006.40	9

0	0	-7	312.465	206.497	2
0	0	-7	328.507	161.236	1
0	0	7	-224.220	225.152	9
0	0	-8	15621.9	1253.76	1
0	0	8	15707.2	1221.12	9
0	0	-8	15395.7	1085.92	2
0	0	-9	-195.561	245.861	2
0	0	9	-102.497	243.188	9
0	0	-9	-267.408	239.609	1
0	1	2	23567.1	700.333	2
0	-1	-2	23968.3	485.547	3
0	1	-2	23532.7	616.849	2
0	1	-2	22965.9	774.103	6
0	1	2	23357.5	660.774	9
0	-1	-2	23106.4	709.433	1
0	-1	2	24967.8	690.651	5
0	-1	2	23227.3	734.329	9
0	-1	-2	23322.1	676.279	2
0	-1	2	23226.7	489.819	4
0	1	2	23198.8	714.395	5
0	-1	-2	23435.9	711.039	5
0	-1	2	23915.1	774.930	6
0	-1	-2	23846.1	666.740	9
0	1	-2	23861.6	708.921	1
0	1	2	25258.4	737.558	1
0	1	-2	23626.6	487.062	4
0	1	2	24671.6	790.463	8
0	-1	-2	24082.9	785.672	8
0	-1	2	22410.7	691.677	1
0	1	-2	24090.6	734.558	9
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0	1	-3	3571.24	311.062	2
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0	1	-3	4482.01	435.640	8
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0	1	3	3332.42	386.158	8
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0	1	-3	3174.25	340.004	9
0	1	-3	3396.93	321.418	1
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0	1	3	3446.03	321.051	2
0	1	3	3251.04	328.412	1
0	-1	3	3346.38	206.986	4
0	-1	-3	3480.29	327.603	9
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0	1	-4	8823.41	534.391	2
0	-1	-4	9119.35	470.095	3

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0	1	-4	9168.03	374.959	4
0	1	-4	9159.42	631.982	1
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0	1	-5	33909.6	1217.09	2
0	-1	-5	35717.4	1062.68	3
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0	1	8	1023.41	309.417	9
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0	3	2	21425.8	689.768	1
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0	3	-2	21182.5	833.926	6
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0	3	2	21368.8	466.077	3
0	3	2	22475.0	961.210	7

0	-3	-2	21370.5	959.983	7
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0	3	8	1536.75	376.928	9
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0	-4	-1	17058.7	757.099	10
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0	-4	3	38641.7	1054.84	5
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0	4	-3	37082.8	1115.56	1
0	4	3	37814.2	926.103	9
0	4	3	39003.3	1141.02	1
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-3	-10	2	142.168	143.705	4
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-3	-10	-1	41464.8	1696.19	9
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-3	15	1	9572.55	994.876	3
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3	15	-1	10497.3	1198.39	6
3	-15	0	847.419	574.864	7
-3	-15	0	473.432	420.244	7
-3	-15	0	-10.2987	190.549	4
3	15	0	212.554	173.412	6
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3	15	1	6053.97	950.800	6
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-3	-15	-2	3962.39	893.886	7
-3	-15	-2	4087.59	623.348	4
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-3	-15	-3	434.928	232.784	2
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3	-15	3	421.192	485.130	7
3	15	3	322.612	350.487	6
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-3	-16	2	6651.55	1351.95	7
3	-16	-2	8279.61	1800.44	7
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-3	16	2	4596.70	692.748	3
-3	16	2	5130.02	727.174	6
-3	-16	1	238.351	240.704	7
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-3	-16	1	836.695	397.848	4
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-3	16	1	18.8189	191.769	6
-3	16	1	192.440	187.044	3
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-3	-16	0	15072.1	1827.85	7

-3	16	0	10260.7	1103.08	3
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-3	16	0	12041.2	1131.66	6
3	-16	0	11123.6	1613.61	7
3	-16	1	644.103	508.550	7
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-3	-16	-1	718.766	453.946	7
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-3	-16	-2	779.032	329.895	4
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-4	-7	-3	4287.20	523.932	2
-4	-7	-3	3608.56	552.849	7
-4	-7	-3	3541.88	360.014	1
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-4	-7	-4	80123.6	1973.54	1
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-4	-10	-4	420.191	197.951	4
4	10	4	549.393	400.742	6
-4	-10	-4	750.923	209.455	1
-4	10	-4	479.712	240.277	1
-4	-10	-4	380.830	196.761	2
-4	10	-4	967.590	330.650	6
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-4	-10	-5	23060.5	1516.01	2
-4	10	-5	21378.5	1326.41	1
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-4	10	-6	194.633	267.399	1
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-4	11	6	7388.15	1191.19	8
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-4	11	5	673.748	494.201	8
-4	-11	5	21.1094	317.781	7
-4	11	5	288.041	191.792	6
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-4	-11	5	370.828	261.458	4
4	-11	-5	433.788	299.476	10

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-4	-11	4	4835.78	655.035	4
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4	-11	-4	5100.98	919.806	7
4	-11	-4	4173.99	525.182	5
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4	-11	-3	1778.58	320.741	5
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-8	-2	5	460.498	235.432	4

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8	-2	-3	2475.10	495.240	5
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8	-2	-1	8823.22	420.074	6
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8	6	-3	362.370	189.314	6
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8	6	-3	1243.56	305.480	5
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-8	-10	-1	37960.2	1848.58	4

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-8	-10	-1	36315.2	1809.19	7
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-8	10	-1	40910.3	2154.99	3
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8	-10	1	35405.6	1847.59	9
8	-10	2	230.186	266.823	9
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8	-10	2	-416.254	276.873	7
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-8	10	-2	405.089	302.273	3
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8	10	3	208.981	240.752	6
-8	-10	-3	470.434	231.668	2
-8	10	-3	1035.50	439.237	3
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-8	-10	-4	-22.0920	237.558	2
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-8	-11	5	485.511	281.926	4
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-8	11	5	-151.919	376.612	3
8	-11	-5	368.454	213.114	5
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-8	-11	4	2221.97	852.283	7
-8	-11	4	2507.93	548.124	4
8	11	-4	1263.24	563.211	6
8	-11	-4	2648.51	591.480	10
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-8	11	0	34739.8	2023.69	3
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-8	-12	0	2143.27	514.979	7
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-9	-2	-4	25946.3	1592.90	1
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9	-2	5	74.7969	181.453	9
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-9	2	-6	17930.6	1594.11	2
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9	-2	6	18965.7	1635.28	9
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-9	-3	5	4426.16	644.987	4
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9	-3	-5	4425.71	685.774	5
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9	-5	-5	1851.24	468.696	5
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9	-5	-1	18320.9	1685.74	5
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9	6	0	3898.73	647.849	5
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-9	6	-5	111.420	158.210	3
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9	7	-6	6123.54	752.791	5
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REM P2(1)/c (#14 with fixed user cell (not necessary: standard = user cell))

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LATT 1
SYMM -x, y+1/2, -z+1/2
SFAC C H N Cl Au
UNIT 48.00 32.00 8.00 12.00 4.00
TREF
HKLF 4
END

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data_4_7phen

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_journal_year 2017
_journal_volume 0000
_journal_issue 0000
_journal_page_first 0000
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loop_

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'Rychlewska, Urszula'

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'War\.zajtis, Beata'

;
Department of Chemistry
Adam Mickiewicz University
Umultowska 89B
61-614 Pozna\ 'n
Poland

;

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The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
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CrysAlisPro (Empirical absorption correction using spherical harmonics,
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2014)
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H1 H 0.2292 0.5382 -0.1709 0.050 Uiso 1 1 calc R U . . .
C2 C 0.0166(16) 0.7582(16) -0.1867(10) 0.055(3) Uani 1 1 d
H2 H 0.0028 0.7783 -0.2746 0.066 Uiso 1 1 calc R U . . .
C3 C -0.0995(16) 0.8745(15) -0.1189(10) 0.055(3) Uani 1 1 d
H3 H -0.1872 0.9730 -0.1638 0.066 Uiso 1 1 calc R U . . .
C5 C 0.0488(15) 0.6868(14) 0.2032(9) 0.048(3) Uani 1 1 d
H5 H -0.0359 0.7680 0.2433 0.058 Uiso 1 1 calc R U . . .
C6 C 0.1752(14) 0.5516(13) 0.2739(9) 0.046(3) Uani 1 1 d
H6 H 0.1786 0.5410 0.3617 0.055 Uiso 1 1 calc R U . . .
C8 C 0.5591(14) 0.1639(12) 0.2366(9) 0.040(2) Uani 1 1 d
H8 H 0.6462 0.0720 0.2885 0.048 Uiso 1 1 calc R U . . .
C9 C 0.5591(15) 0.1725(13) 0.1072(9) 0.043(3) Uani 1 1 d
H9 H 0.6460 0.0872 0.0719 0.052 Uiso 1 1 calc R U . . .
C10 C 0.4313(14) 0.3067(13) 0.0314(9) 0.041(3) Uani 1 1 d
H10 H 0.4297 0.3118 -0.0558 0.049 Uiso 1 1 calc R U . . .
C11 C 0.0393(13) 0.7108(12) 0.0693(9) 0.035(2) Uani 1 1 d
C12 C 0.3050(13) 0.4235(12) 0.2161(8) 0.034(2) Uani 1 1 d
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 C12 0.034(6) 0.037(6) 0.031(5) -0.008(5) 0.002(4) -0.015(5)
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 N4 0.047(6) 0.045(6) 0.042(5) -0.003(4) -0.004(4) -0.001(5)
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 C11 0.0521(18) 0.095(2) 0.0350(13) -0.0007(14) -0.0016(12) -0.0390(17)
 C12 0.068(2) 0.064(2) 0.0254(12) -0.0050(12) -0.0084(12) -0.0181(16)
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used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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C3 H3 0.9300 . ?

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C12 C13 C10 118.0(8) . . ?
C12 C13 C14 118.7(8) . . ?

C10 C13 C14 123.3(8) . . ?
C1 C14 C11 117.1(9) . . ?
C1 C14 C13 123.9(9) . . ?
C11 C14 C13 119.0(8) . . ?
C3 N4 C11 117.2(9) . . ?
C8 N7 C12 121.6(7) . . ?
C8 N7 Au1 116.1(6) . . ?
C12 N7 Au1 122.2(6) . . ?
N7 Au1 C12 179.9(3) . . ?
N7 Au1 C13 88.9(2) . . ?
C12 Au1 C13 91.04(11) . . ?
N7 Au1 C11 89.5(2) . . ?
C12 Au1 C11 90.58(11) . . ?
C13 Au1 C11 176.79(11) . . ?

loop_

_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C14 C1 C2 C3 1.1(17) ?
C1 C2 C3 N4 -2.0(19) ?
C11 C5 C6 C12 -1.1(18) ?
N7 C8 C9 C10 -0.2(17) ?
C8 C9 C10 C13 1.1(17) ?
C6 C5 C11 N4 -179.1(11) ?
C6 C5 C11 C14 1.0(17) ?
C5 C6 C12 N7 179.4(11) ?
C5 C6 C12 C13 0.0(17) ?
N7 C12 C13 C10 1.4(15) ?
C6 C12 C13 C10 -179.2(9) ?
N7 C12 C13 C14 -178.2(9) ?
C6 C12 C13 C14 1.1(15) ?
C9 C10 C13 C12 -1.8(16) ?
C9 C10 C13 C14 177.9(10) ?
C2 C1 C14 C11 0.1(15) ?
C2 C1 C14 C13 179.3(10) ?
N4 C11 C14 C1 -0.5(14) ?
C5 C11 C14 C1 179.4(9) ?
N4 C11 C14 C13 -179.7(10) ?
C5 C11 C14 C13 0.2(14) ?
C12 C13 C14 C1 179.6(9) ?
C10 C13 C14 C1 0.0(15) ?
C12 C13 C14 C11 -1.2(14) ?
C10 C13 C14 C11 179.1(9) ?
C2 C3 N4 C11 1.6(17) ?
C5 C11 N4 C3 179.8(10) ?
C14 C11 N4 C3 -0.3(15) ?

C9 C8 N7 C12 -0.1(15) ?
C9 C8 N7 Au1 -179.4(8) ?
C13 C12 N7 C8 -0.6(15) ?
C6 C12 N7 C8 -179.9(9) ?
C13 C12 N7 Au1 178.7(7) ?
C6 C12 N7 Au1 -0.6(13) ?

_refine_diff_density_max 1.075
_refine_diff_density_min -0.867
_refine_diff_density_rms 0.157

_shelx_res_file
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shelx.res created by SHELXL-2014/7

TITL AuCl3_4_7phen in P-1
CELL 0.71073 7.8420 8.8631 10.7500 78.707 87.300 66.988
ZERR 2.00 0.0012 0.0014 0.0005 0.008 0.008 0.015
LATT 1
SFAC C H N CL AU
UNIT 24 16 4 6 2
MERG 0
FMAP 2
PLAN 10
SIZE 0.030 0.050 0.180
ACTA
BOND \$H
CONF
L.S. 20
TEMP 22.00
WGHT 0.051800
BASF 0.52094
FVAR 1.54065
C1 1 0.149621 0.615743 -0.125686 11.00000 0.03955
0.05865 =
0.02825 -0.00859 0.00729 -0.02058
AFIX 43
H1 2 0.229155 0.538170 -0.170891 11.00000 -1.20000
AFIX 0
C2 1 0.016585 0.758188 -0.186724 11.00000 0.04662
0.07409 =
0.03019 0.00589 -0.00638 -0.01458
AFIX 43
H2 2 0.002780 0.778342 -0.274623 11.00000 -1.20000
AFIX 0
C3 1 -0.099487 0.874497 -0.118888 11.00000 0.04936
0.05302 =
0.04369 0.00427 -0.00789 -0.00609
AFIX 43
H3 2 -0.187192 0.972951 -0.163835 11.00000 -1.20000
AFIX 0
C5 1 0.048758 0.686844 0.203211 11.00000 0.05043
0.04656 =

		0.03674	-0.01565	0.00340	-0.00441	
AFIX	43					
H5	2	-0.035907	0.767955	0.243330	11.00000	-1.20000
AFIX	0					
C6	1	0.175246	0.551578	0.273945	11.00000	0.05379
0.04987	=					
		0.02421	-0.01464	0.00283	-0.00655	
AFIX	43					
H6	2	0.178564	0.541018	0.361684	11.00000	-1.20000
AFIX	0					
C8	1	0.559087	0.163908	0.236569	11.00000	0.04719
0.02994	=					
		0.04171	-0.01084	0.00735	-0.01188	
AFIX	43					
H8	2	0.646227	0.071964	0.288481	11.00000	-1.20000
AFIX	0					
C9	1	0.559122	0.172535	0.107179	11.00000	0.04345
0.03818	=					
		0.04417	-0.01769	0.00583	-0.00836	
AFIX	43					
H9	2	0.645957	0.087168	0.071932	11.00000	-1.20000
AFIX	0					
C10	1	0.431317	0.306724	0.031441	11.00000	0.04714
0.04735	=					
		0.02996	-0.01824	0.00750	-0.01486	
AFIX	43					
H10	2	0.429692	0.311844	-0.055757	11.00000	-1.20000
AFIX	0					
C11	1	0.039293	0.710830	0.069328	11.00000	0.03061
0.04139	=					
		0.03066	-0.00828	0.00113	-0.01095	
C12	1	0.304977	0.423493	0.216071	11.00000	0.03427
0.03666	=					
		0.03101	-0.00848	0.00223	-0.01456	
C13	1	0.301537	0.437878	0.083546	11.00000	0.03441
0.03320	=					
		0.03286	-0.01048	0.00292	-0.01892	
C14	1	0.165830	0.586702	0.007571	11.00000	0.03477
0.03733	=					
		0.03118	-0.00728	0.00260	-0.02180	
N4	3	-0.092265	0.853068	0.006043	11.00000	0.04673
0.04510	=					
		0.04167	-0.00251	-0.00424	-0.00108	
N7	3	0.435332	0.286074	0.288477	11.00000	0.03468
0.03805	=					
		0.02694	-0.00587	0.00299	-0.01397	
CL1	4	0.200130	0.189488	0.500371	11.00000	0.05207
0.09487	=					
		0.03502	-0.00066	-0.00160	-0.03896	
CL2	4	0.477692	0.221452	0.698057	11.00000	0.06803
0.06422	=					
		0.02543	-0.00500	-0.00844	-0.01812	
CL3	4	0.717105	0.308894	0.461286	11.00000	0.05212
0.09488	=					

```
0.05531 -0.03108 0.01186 -0.04020
AU1 5 0.455239 0.255540 0.483529 11.00000 0.03709
0.04340 =
0.02457 -0.00561 -0.00284 -0.00935
HKLF 5
```

```
REM AuCl3_4_7phen in P-1
REM R1 = 0.0362 for 3247 Fo > 4sig(Fo) and 0.0480 for all 4091
data
REM 164 parameters refined using 0 restraints
```

END

```
WGHT 0.0518 0.0000
```

```
REM Highest difference peak 1.075, deepest hole -0.867, 1-sigma level
0.157
```

Q1	1	0.2973	0.4242	0.6609	11.00000	0.05	1.08
Q2	1	0.4794	0.1086	0.5253	11.00000	0.05	1.00
Q3	1	0.5667	0.1036	0.3188	11.00000	0.05	0.89
Q4	1	0.3927	0.2783	0.4854	11.00000	0.05	0.85
Q5	1	0.5546	0.2003	0.4779	11.00000	0.05	0.80
Q6	1	0.4493	0.4022	0.4481	11.00000	0.05	0.80
Q7	1	0.3337	0.3529	0.4835	11.00000	0.05	0.79
Q8	1	0.2273	0.5028	0.4830	11.00000	0.05	0.66
Q9	1	0.3884	0.2402	0.5512	11.00000	0.05	0.62
Q10	1	0.2665	0.2905	0.4312	11.00000	0.05	0.60

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_shelx_res_checksum 63287
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_shelx_hkl_file
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0	0	3	25868.8	70.2948	1
0	0	-4	36084.4	92.7568	1
0	0	5	23944.8	85.8587	1
1	1	6	16491.7	102.439	-2
0	0	-6	16491.7	102.439	1
0	0	-7	5023.89	54.2658	1
0	0	-8	3605.20	65.8141	1
0	0	-9	2174.92	79.1965	1
0	0	-10	3346.00	92.6468	1
2	2	11	750.432	233.295	-2
0	0	-11	750.432	233.295	1
2	2	12	160.879	244.052	-2
0	0	-12	160.879	244.052	1
3	2	12	1683.24	416.830	-2
0	1	-12	1683.24	416.830	1
0	1	-11	1720.05	177.055	1
0	1	-10	2683.99	128.357	1
0	-1	9	5217.61	94.9205	1
0	1	-8	4496.58	89.9596	1
2	1	7	5826.19	101.868	-2
0	1	-7	5826.19	101.868	1

0	-1	6	3545.77	80.9580	1
2	1	6	7569.28	228.462	-2
0	1	-6	7569.28	228.462	1
0	-1	5	3878.36	60.7404	1
0	1	-4	8481.73	70.6327	1
0	1	-3	5140.28	57.7911	1
0	1	-2	52.8603	41.4818	1
-1	0	-1	30818.3	139.233	-2
0	-1	1	30818.3	139.233	1
0	-1	-2	56.5603	29.4183	1
0	-1	-3	5458.26	37.9736	1
0	1	4	6979.78	49.4632	1
0	1	4	14542.5	141.198	-2
0	-1	-4	14542.5	141.198	1
0	1	5	14022.0	95.5269	-2
0	-1	-5	14022.0	95.5269	1
0	-1	-6	6901.86	60.7374	1
0	-1	-7	3567.92	60.1392	1
0	-1	-8	6836.05	74.2810	1
0	-1	-9	6800.16	94.8751	1
1	2	10	5017.25	174.918	-2
0	-1	-10	5017.25	174.918	1
1	2	11	4081.10	276.147	-2
0	-1	-11	4081.10	276.147	1
0	-1	-12	1829.11	200.501	1
0	2	-11	369.998	150.347	1
0	2	-10	1257.03	125.908	1
0	2	-9	1651.15	136.512	1
3	1	8	5668.10	125.937	-2
0	2	-8	5668.10	125.937	1
3	1	7	6065.20	109.328	-2
0	2	-7	6065.20	109.328	1
0	2	-6	5678.52	83.6947	1
0	2	-5	10310.4	95.6335	1
0	2	-4	13489.8	143.396	1
0	2	-3	14162.4	89.0339	1
2	0	2	17755.8	147.504	-2
0	2	-2	17755.8	147.504	1
0	2	-1	30415.6	165.398	1
0	2	0	59653.6	168.089	1
0	-2	-1	33206.7	91.9742	1
0	-2	-2	30475.5	76.6916	1
0	-2	-3	24023.2	94.6210	1
-1	1	3	24229.3	161.368	-2
0	-2	-3	24229.3	161.368	1
-1	1	4	25772.9	115.608	-2
0	-2	-4	25772.9	115.608	1
0	2	5	21652.0	70.8391	1
0	2	6	15322.6	66.0659	1
0	-2	-7	8583.91	67.3066	1
0	-2	-8	2498.66	49.4152	1
0	2	9	7310.43	348.017	-2
0	-2	-9	7310.43	348.017	1
0	2	10	5895.02	269.294	-2

0	-2	-10	5895.02	269.294	1
0	-2	-11	1546.75	182.789	1
0	-2	-12	257.423	194.075	1
0	3	-11	1169.76	177.374	1
0	3	-10	1597.20	167.960	1
4	1	9	11027.8	391.039	-2
0	3	-9	11027.8	391.039	1
4	1	8	5105.93	196.021	-2
0	3	-8	5105.93	196.021	1
0	-3	7	3123.50	80.2372	1
0	-3	6	1721.88	78.5295	1
0	3	-5	1806.83	152.977	1
0	3	-4	3258.21	91.2848	1
-3	0	-3	1936.21	107.764	-2
0	-3	3	1936.21	107.764	1
0	3	-2	3054.06	161.330	1
0	-3	1	60.9936	90.1950	1
0	3	0	93.9779	75.7629	1
0	3	1	504.918	63.5804	1
0	-3	-2	462.034	45.0809	1
2	-1	-3	1197.41	55.0495	-2
0	3	3	1197.41	55.0495	1
0	3	4	3882.92	74.5939	1
0	3	5	4745.88	60.7504	1
0	-3	-6	2805.15	47.1257	1
0	3	7	3466.80	33.1981	1
0	3	8	4032.95	85.6886	1
-1	2	8	8840.99	222.814	-2
0	-3	-8	8840.99	222.814	1
-1	2	9	8081.33	384.776	-2
0	-3	-9	8081.33	384.776	1
0	-3	-10	4887.04	262.009	1
0	-3	-11	2779.06	180.018	1
0	-3	-12	1836.84	186.822	1
5	1	10	1549.57	331.162	-2
0	4	-10	1549.57	331.162	1
5	1	9	3594.00	323.203	-2
0	4	-9	3594.00	323.203	1
0	4	-8	810.613	202.169	1
0	4	-7	727.775	187.932	1
0	4	-6	1314.85	177.764	1
0	4	-5	4402.88	210.840	1
4	0	4	8215.93	159.417	-2
0	4	-4	8215.93	159.417	1
0	-4	3	6957.95	117.327	1
0	4	-2	2068.26	159.054	1
0	4	-1	13646.3	232.292	1
0	4	0	12110.6	216.394	1
0	4	1	17539.5	139.048	1
-3	1	2	27114.8	171.268	-2
0	-4	-2	27114.8	171.268	1
0	4	3	8373.83	83.6653	1
0	-4	-4	8882.22	79.4324	1
0	-4	-5	12718.5	97.8312	1

0	-4	-6	11172.9	89.7921	1
0	-4	-7	7393.45	83.4446	1
-2	2	7	14155.5	160.908	-2
0	-4	-7	14155.5	160.908	1
-2	2	8	924.492	100.543	-2
0	-4	-8	924.492	100.543	1
0	-4	-9	4307.91	178.721	1
0	-4	-10	1881.50	159.753	1
0	-4	-11	1297.80	169.735	1
0	-4	-12	232.106	136.932	1
0	5	-9	1055.07	242.418	1
0	5	-8	1346.17	235.752	1
0	5	-7	1879.09	232.187	1
0	5	-6	427.659	199.831	1
5	0	5	1327.71	270.098	-2
0	5	-5	1327.71	270.098	1
0	-5	4	1620.37	88.1944	1
0	5	-3	1255.46	92.0152	1
0	5	-2	926.963	167.168	1
0	5	-1	165.219	150.402	1
0	5	0	129.608	142.463	1
4	-1	-1	15185.8	339.052	-2
0	5	1	15185.8	339.052	1
0	-5	-2	224.223	70.0790	1
0	5	3	135.753	71.0581	1
0	-5	-4	1008.55	58.4624	1
0	-5	-5	1020.69	76.2855	1
-3	2	6	7484.75	106.265	-2
0	-5	-6	7484.75	106.265	1
3	-2	-7	7897.79	180.321	-2
0	5	7	7897.79	180.321	1
0	-5	-8	2560.66	106.703	1
0	-5	-9	1150.45	152.080	1
0	-5	-10	2709.98	179.308	1
0	-5	-11	1470.54	181.008	1
-2	3	12	1347.45	247.801	-2
0	-5	-12	1347.45	247.801	1
0	6	-8	419.708	257.642	1
0	6	-7	331.441	238.049	1
6	0	6	1282.78	329.371	-2
0	6	-6	1282.78	329.371	1
6	0	5	1916.93	303.871	-2
0	6	-5	1916.93	303.871	1
0	6	-4	2221.70	214.375	1
0	6	-3	2104.75	205.056	1
0	6	-2	1479.38	187.863	1
0	6	-1	2674.95	204.249	1
5	-1	0	11278.8	265.692	-2
0	6	0	11278.8	265.692	1
0	6	1	5344.82	210.318	1
0	-6	-2	4726.77	101.853	1
0	6	3	3744.97	102.675	1
0	6	4	3361.34	90.3776	1
4	-2	-5	12138.9	247.166	-2

0	6	5	12138.9	247.166	1
4	-2	-6	11217.4	274.837	-2
0	6	6	11217.4	274.837	1
0	-6	-7	3089.29	125.539	1
0	6	8	1297.63	115.482	1
0	-6	-9	1313.54	160.594	1
0	-6	-10	1004.52	166.975	1
-3	3	11	760.147	239.011	-2
0	-6	-11	760.147	239.011	1
7	0	6	820.833	347.786	-2
0	7	-6	820.833	347.786	1
0	7	-5	225.824	232.281	1
0	7	-4	1017.48	223.758	1
0	7	-3	524.299	218.612	1
0	7	-2	530.264	205.072	1
6	-1	1	1062.25	292.543	-2
0	7	-1	1062.25	292.543	1
6	-1	0	5145.78	299.501	-2
0	7	0	5145.78	299.501	1
0	7	1	59.8954	171.955	1
0	7	2	65.0973	170.425	1
0	7	3	23.0973	130.542	1
-5	2	4	816.069	151.377	-2
0	-7	-4	816.069	151.377	1
5	-2	-5	2156.77	231.533	-2
0	7	5	2156.77	231.533	1
0	-7	-6	390.249	156.079	1
0	7	7	218.128	153.245	1
0	-7	-8	374.424	252.475	1
0	-7	-9	701.945	262.630	1
-4	3	10	670.457	248.576	-2
0	-7	-10	670.457	248.576	1
0	8	-5	320.835	277.418	1
0	8	-4	558.400	269.266	1
7	-1	3	2161.38	352.764	-2
0	8	-3	2161.38	352.764	1
7	-1	2	1935.80	356.319	-2
0	8	-2	1935.80	356.319	1
7	-1	1	2016.91	326.841	-2
0	8	-1	2016.91	326.841	1
0	8	0	892.949	221.225	1
0	8	1	2328.25	241.389	1
0	8	2	1873.16	223.017	1
6	-2	-3	949.142	268.988	-2
0	8	3	949.142	268.988	1
-6	2	4	1201.08	179.021	-2
0	-8	-4	1201.08	179.021	1
0	-8	-5	1706.21	184.937	1
0	8	6	2335.67	197.277	1
0	8	7	1013.90	185.941	1
0	-8	-8	800.820	300.017	1
-5	3	9	710.055	427.138	-2
0	-8	-9	710.055	427.138	1
8	-1	2	965.393	371.063	-2

0	9	-2	965.393	371.063	1
0	9	-1	188.738	250.131	1
0	9	0	39.9227	240.471	1
0	9	1	-70.3607	238.539	1
7	-2	-2	144.635	322.045	-2
0	9	2	144.635	322.045	1
7	-2	-3	114.951	173.066	-2
0	9	3	114.951	173.066	1
7	-2	-4	154.264	226.892	-2
0	9	4	154.264	226.892	1
0	9	5	-4.46193	175.874	1
0	-9	-6	127.339	189.443	1
-1	9	5	151.441	240.154	1
-1	9	4	107.392	213.709	1
7	-3	-3	1150.12	328.817	-2
-1	9	3	1150.12	328.817	1
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6	1	6	2264.67	301.402	-2

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2	3	0	14275.7	128.749	1

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-4	-3	-6 11479.1	242.138	1
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-7	-3	4	2750.27	122.070	1
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7	3	-3	1992.92	144.550	1
4	8	2	5044.35	172.148	-2
7	3	-2	5044.35	172.148	1
4	8	1	4344.67	144.925	-2
7	3	-1	4344.67	144.925	1
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7	3	1	4104.43	238.244	1
7	3	2	3244.90	231.401	1
3	7	-3	2375.85	273.396	-2
7	3	3	2375.85	273.396	1
3	7	-4	2999.83	317.015	-2
7	3	4	2999.83	317.015	1
3	7	-5	2551.20	301.822	-2
7	3	5	2551.20	301.822	1

7	3	6	1794.23	216.969	1
-7	-3	-7	83.9842	147.191	1
7	3	8	545.737	162.760	1
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-7	-4	6	234.197	207.998	1
-7	-4	5	62.5455	128.152	1
7	4	-4	19.5457	170.093	1
-5	-8	-4	63.2604	295.333	-2
-7	-4	4	63.2604	295.333	1
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-7	-4	3	-65.5912	183.062	1
5	8	2	215.325	151.284	-2
7	4	-2	215.325	151.284	1
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7	4	0	85.7393	197.221	1
7	4	1	350.731	198.120	1
4	7	-2	679.361	282.949	-2
7	4	2	679.361	282.949	1
4	7	-3	2041.50	299.465	-2
7	4	3	2041.50	299.465	1
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7	4	4	1992.43	282.880	1
7	4	5	1779.68	213.718	1
7	4	6	1761.93	220.007	1
7	4	7	2053.20	248.071	1
3	6	-8	2822.66	248.537	-2
7	4	8	2822.66	248.537	1
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-7	-5	5	1971.81	318.271	1
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7	5	-4	2059.61	308.830	1
6	8	3	1626.54	289.740	-2
7	5	-3	1626.54	289.740	1
7	5	-2	1639.00	215.412	1
7	5	-1	1985.93	229.826	1
7	5	0	2253.76	219.276	1
5	7	-1	4177.30	299.598	-2
7	5	1	4177.30	299.598	1
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7	5	2	2830.28	316.913	1
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7	5	3	2483.78	329.603	1
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7	5	6	1078.41	238.746	1
4	6	-7	989.383	289.958	-2
7	5	7	989.383	289.958	1
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7	5	8	1098.48	326.360	1
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7	6	-5	973.592	343.060	1

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7	6	0	4633.11	367.225	1
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7	6	1	2660.89	383.781	1
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7	6	4	807.082	209.172	1
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7	7	-3	576.005	265.069	1
7	7	-2	669.120	257.093	1
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7	7	-1	3757.79	391.837	1
7	7	0	4037.37	418.462	-2
7	7	0	4037.37	418.462	1
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7	7	3	1054.83	275.238	1
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-7	-7	-5	2818.84	283.040	1
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-7	-8	-7	232.628	210.848	1
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7	9	3	205.603	412.563	1
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7	9	4	126.631	419.393	1
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1	10	3	1585.35	200.641	-2
8	-1	-3	1585.35	200.641	1
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8	-1	-2	2208.12	199.844	1
8	-1	-1	1026.35	137.667	1
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8	0	-1	336.212	125.700	1
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-8	0	-1	585.255	197.699	1
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-8	0	-2	1097.44	249.673	1
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8	1	-5	1580.90	243.222	1
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8	1	-4	930.256	223.396	1
8	1	-3	912.905	159.203	1
8	1	-2	1233.10	159.996	1
-8	-1	1	1210.88	224.120	1
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-8	-1	0	2370.10	213.926	1
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-8	-1	-1	934.692	151.029	1
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-8	-1	-2	698.820	196.538	1
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8	2	-3	-2.07723	106.765	1
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8	2	0	806.207	205.591	1
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-8	-2	-1	610.783	194.638	1
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-8	-2	-6	2023.27	396.574	1
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8	3	-3	674.144	111.223	1
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3	8	-4	1884.09	201.860	-2
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3	8	-6	687.606	243.063	-2
8	3	6	687.606	243.063	1
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4	8	-3	1077.95	303.737	-2
8	4	3	1077.95	303.737	1
4	8	-4	2072.38	350.297	-2
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-6	-9	-4	1241.07	216.393	-2
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6	9	2	2049.02	312.193	-2
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8	5	-1	427.028	226.849	1
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8	5	2	746.837	281.599	1
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8	5	3	569.452	282.916	1
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7	9	4	458.041	321.057	-2
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7	9	3	480.687	319.666	-2
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8	6	-1	-23.1774	215.025	1
8	6	0	156.470	232.317	1
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8	6	2	325.573	315.338	1
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8	6	3	684.181	301.286	1
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8	6	5	367.979	216.436	1
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-9	-4	2	259.558	207.925	1
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