

any

analyse y-files

help

- Typing “help” will open a webpage with the manual.
- Typing “help commandname” will open a webpage with the manual entry for the commandname.
Example: “help pk”

Any> rshell

Completeness and Rmerge for Shells

Forbid: EDGEVER EDGEHOR EDGEROT BIGVER BIGROT OVERFLOW

Allow: GOOD WEAK NEGATIVE

Require: NONE

theta from 0.0 to 34.996

Sh	Theta	Reso	Meas	Equi	Obs	Mis	Lost	Total	Perc	Cum	Uni1	Uni2+	Nrsym	Redun	Rsym	Rmeas	Rpim	Chi2
1	15.44	1.335	747	21	768	2	0	770	99.7	99.7	0	64	2320	36.25	0.027	0.027	0.005	54.19
2	19.60	1.060	696	48	744	0	0	744	100.0	99.9	0	48	1773	36.94	0.025	0.026	0.004	5.01
3	22.58	0.926	645	91	736	0	0	736	100.0	99.9	0	47	1273	27.09	0.028	0.028	0.006	3.12
4	25.00	0.841	567	157	724	0	0	724	100.0	99.9	0	42	983	23.40	0.035	0.036	0.008	2.21
5	27.08	0.781	496	304	800	0	0	800	100.0	99.9	0	45	772	17.16	0.034	0.035	0.008	1.88
6	28.93	0.735	395	303	698	0	0	698	100.0	100.0	0	38	546	14.37	0.030	0.031	0.008	2.02
7	30.61	0.698	472	406	878	0	0	878	100.0	100.0	0	52	669	12.87	0.036	0.037	0.010	1.64
8	32.17	0.667	338	324	662	0	0	662	100.0	100.0	0	37	461	12.46	0.038	0.040	0.011	1.42
9	33.62	0.642	357	401	758	0	0	758	100.0	100.0	0	39	483	12.38	0.049	0.051	0.014	1.34
10	35.00	0.620	366	422	788	0	0	788	100.0	100.0	1	42	492	11.71	0.062	0.066	0.020	0.98

=====
35.00 0.620 5079 2477 7556 2 0 7558 100.0 100.0 1 454 9772 21.52 0.028 0.028 0.005 14.96

Resolution 7.288-0.62 (0.642-0.62)

Rsym 0.028 (0.062) Rmeas 0.028 (0.066) Rpim 0.005 (0.02)

Unique 455 (43) Completeness 99.974 (100.0)

Any>

Instability constant (msa)

$$\sigma = kfactor * \sqrt{((sigmafactor * \sigma_{orig})^2 + (msa * intensity)^{msapower})}$$

Defaults:

kfactor: 1.0

sigmafactor: 1.0

msapower: 2.0

msa: 0.02

Any> rshell

Completeness and Rmerge for Shells

Forbid: NONE

Allow: ALL

Require: NONE

theta from 0.0 to 34.996

Sh	Theta	Reso	Meas	Equi	Obs	Mis	Lost	Total	Perc	Cum	Uni1	Uni2+	Nrsym	Redun	Rsym	Rmeas	Rpim	Chi2
1	15.44	1.335	747	21	768	2	0	770	99.7	99.7	0	64	2316	36.19	0.014	0.014	0.002	1.06
2	19.60	1.060	696	48	744	0	0	744	100.0	99.9	0	48	1771	36.90	0.016	0.017	0.003	0.95
3	22.58	0.926	645	91	736	0	0	736	100.0	99.9	0	47	1273	27.09	0.020	0.020	0.004	0.99
4	25.00	0.841	567	157	724	0	0	724	100.0	99.9	0	42	983	23.40	0.027	0.027	0.006	1.01
5	27.08	0.781	496	304	800	0	0	800	100.0	99.9	0	45	772	17.16	0.025	0.026	0.006	0.89
6	28.93	0.735	395	303	698	0	0	698	100.0	100.0	0	38	546	14.37	0.021	0.022	0.005	1.03
7	30.61	0.698	472	406	878	0	0	878	100.0	100.0	0	52	669	12.87	0.029	0.030	0.008	1.00
8	32.17	0.667	338	324	662	0	0	662	100.0	100.0	0	37	461	12.46	0.032	0.034	0.009	1.03
9	33.62	0.642	357	401	758	0	0	758	100.0	100.0	0	39	483	12.38	0.044	0.046	0.013	1.12
10	35.00	0.620	366	422	788	0	0	788	100.0	100.0	1	42	492	11.71	0.058	0.061	0.018	0.97

=====

35.00	0.620	5079	2477	7556	2	0	7558	100.0	100.0	1	454	9766	21.51	0.016	0.017	0.003	1.00
-------	-------	------	------	------	---	---	------	-------	-------	---	-----	------	-------	-------	-------	-------	------

Resolution 7.288-0.62 (0.642-0.62)

Rsym 0.016 (0.058) Rmeas 0.017 (0.061) Rpim 0.003 (0.018)

Unique 455 (43) Completeness 99.974 (100.0)

Any>

Global overview

- rshell
- rint
- rlaue / rpg
- flagall
- icr
- plot
 - plot shifthor
 - plot shiftver
 - plot shiftrot
- listrefl bad

rshell

Any> rshell

Completeness and Rmerge for Shells

Forbid: EDGEVER EDGEHOR EDGEROT BIGVER BIGROT OVERFLOW

Allow: GOOD WEAK NEGATIVE

Require: NONE

theta from 0.0 to 34.996

Sh	Theta	Reso	Meas	Equi	Obs	Mis	Lost	Total	Perc	Cum	Uni1	Uni2+	Nrsym	Redun	Rsym	Rmeas	Rpim	Chi2
1	15.44	1.335	747	21	768	2	0	770	99.7	99.7	0	64	2320	36.25	0.026	0.026	0.005	1.73
2	19.60	1.060	696	48	744	0	0	744	100.0	99.9	0	48	1773	36.94	0.025	0.025	0.004	1.41
3	22.58	0.926	645	91	736	0	0	736	100.0	99.9	0	47	1273	27.09	0.028	0.028	0.006	1.21
4	25.00	0.841	567	157	724	0	0	724	100.0	99.9	0	42	983	23.40	0.035	0.036	0.008	1.20
5	27.08	0.781	496	304	800	0	0	800	100.0	99.9	0	45	772	17.16	0.034	0.035	0.008	1.15
6	28.93	0.735	395	303	698	0	0	698	100.0	100.0	0	38	546	14.37	0.030	0.031	0.008	1.14
7	30.61	0.698	472	406	878	0	0	878	100.0	100.0	0	52	669	12.87	0.036	0.037	0.010	1.13
8	32.17	0.667	338	324	662	0	0	662	100.0	100.0	0	37	461	12.46	0.038	0.040	0.011	1.07
9	33.62	0.642	357	401	758	0	0	758	100.0	100.0	0	39	483	12.38	0.049	0.051	0.014	1.15
10	35.00	0.620	366	422	788	0	0	788	100.0	100.0	1	42	492	11.71	0.062	0.065	0.020	0.90

=====
35.00 0.620 5079 2477 7556 2 0 7558 100.0 100.0 1 454 9772 21.52 0.027 0.027 0.005 1.33

Resolution 7.288-0.62 (0.642-0.62)

Rsym 0.027 (0.062) Rmeas 0.027 (0.065) Rpim 0.005 (0.02)

Unique 455 (43) Completeness 99.974 (100.0)

Any>

rint

Any> rint

Rmerge for different intensities

432 <intensities> from 0.011 to 10169.298

Forbid: EDGEVER EDGEHOR EDGEROT BIGVER BIGROT OVERFLOW

Allow: GOOD WEAK NEGATIVE

Require: NONE

<Int1>	<Int2>	R	Rmeas	Rpim	Chi2	nUni	nRsym	<I>	nMean
0.0	0.4	2.310	2.372	0.508	0.75	43	880	0.18	880
0.4	3.1	0.367	0.378	0.086	0.89	42	766	1.50	767
3.1	9.5	0.140	0.143	0.031	0.95	43	860	5.48	860
9.5	24.2	0.070	0.072	0.017	1.09	43	709	15.69	709
24.2	41.8	0.047	0.049	0.011	1.16	44	869	33.46	869
41.8	66.7	0.038	0.040	0.009	1.31	42	713	52.43	713
66.7	104.2	0.034	0.035	0.007	1.44	43	1054	84.20	1054
104.2	197.5	0.030	0.031	0.006	1.58	44	1085	149.12	1085
197.5	446.3	0.024	0.025	0.004	1.61	42	1208	307.29	1208
446.3	10169.3	0.025	0.025	0.005	2.01	45	1309	1147.00	1309

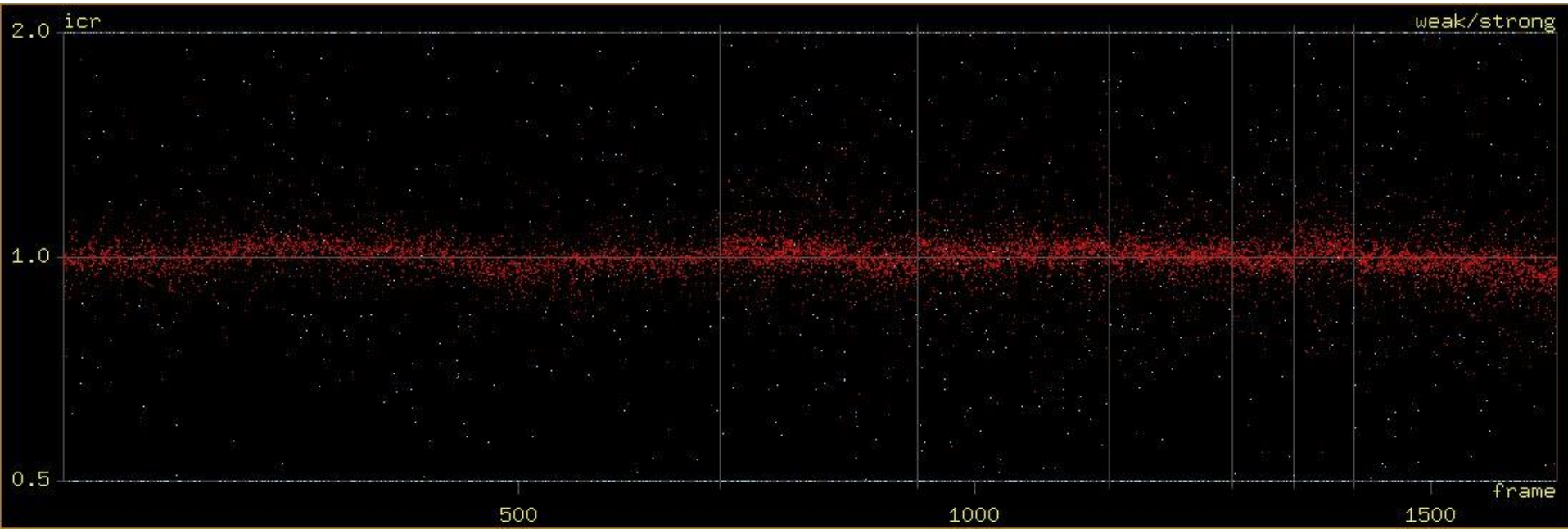
j= 10 a= 0.611 slope= 0.119 abdev= 0.043

Any>

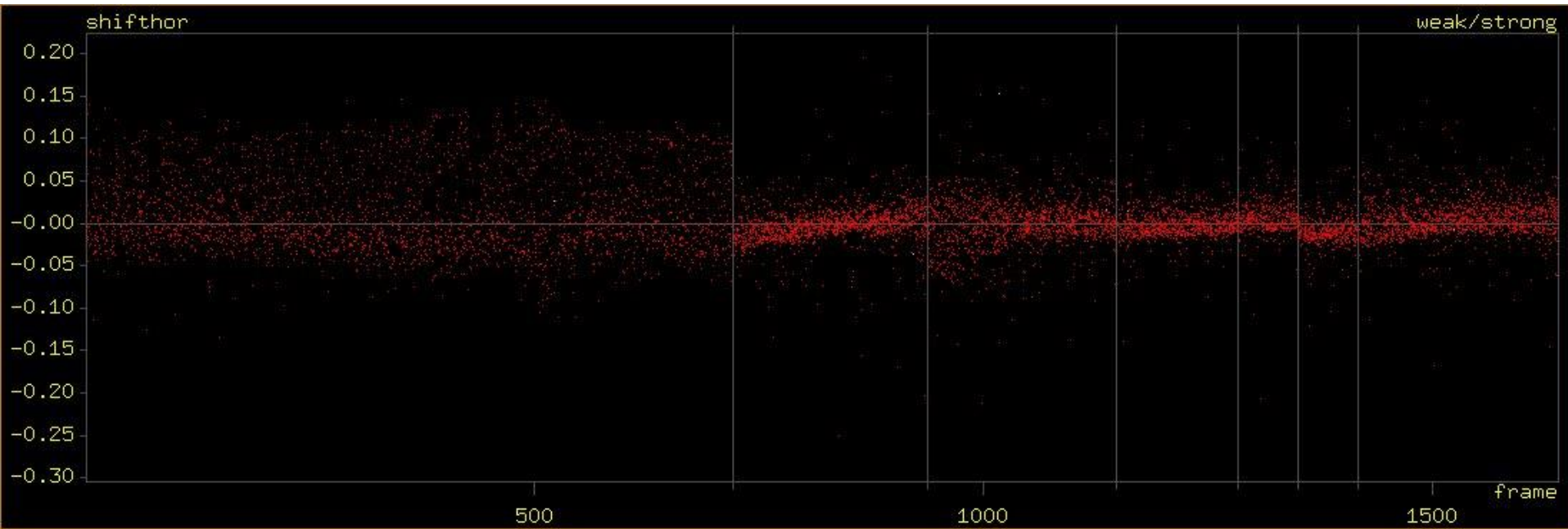
rlaue / rpg

```
Any> rlaue
1...*....10....
pg      R Rmeas  Rpim      Chi2 Uni1 Uni2+ nRsym Redun
-1      0.024 0.027 0.012      1.35 879 2363 8894 3.76 -1 Triclinic
2/m     0.394 0.418 0.136 9448.38 530 1678 9243 5.51 2/m Monoclinic
mmm     0.394 0.408 0.101 8853.67 238 1125 9535 8.48 mmm Orthorhombic
4/m     0.386 0.399 0.098 8869.71 210 1023 9563 9.35 4/m Tetragonal low
4/mmm   0.399 0.409 0.084 8525.73 31 780 9742 12.49 4/mmm Tetragonal high
-3      0.027 0.028 0.008      1.35 1 1273 9772 7.68 -3 Trigonal low
-3m1    0.027 0.028 0.007      1.35 1 788 9772 12.40 -3m1 Trigonal high
-31m    0.027 0.028 0.006      1.33 1 726 9772 13.46 -31m Trigonal high
6/m     0.027 0.028 0.006      1.33 1 667 9772 14.65 6/m Hexagonal low
6/mmm   0.027 0.027 0.005      1.33 1 454 9772 21.52 6/mmm Hexagonal high
R-3     0.577 0.602 0.164 9363.29 642 1736 9131 5.26 R-3 Rhombohedral low
R-3m    0.598 0.613 0.131 9057.66 83 1325 9690 7.31 R-3m Rhombohedral high
m3      0.713 0.735 0.165 11416.21 287 1182 9486 8.03 m3 Cubic low
m3m     0.722 0.732 0.110 10380.81 17 536 9756 18.20 m3m Cubic high
Building 6/mmm
-----
Split intensities into two parts
Forbid: EDGEVER EDGEHOR EDGEROT BIGVER BIGROT OVERFLOW
Allow: GOOD WEAK NEGATIVE
Require: NONE
454 pairs (one nonpair) 9772 daughters accepted 138 daughters rejected
Calculating Extremes 1...*....10....*....20....*....30....*....40....*....50....*....60....*....70.
Cannot calculate half1 for reflection 7709.
.
Cannot calculate half2 for reflection 7709.
..*....80....*....90....*....100....*....
Cannot calculate icr for reflection 2. (total 1230 icr's failed)
...110
Any> 
```

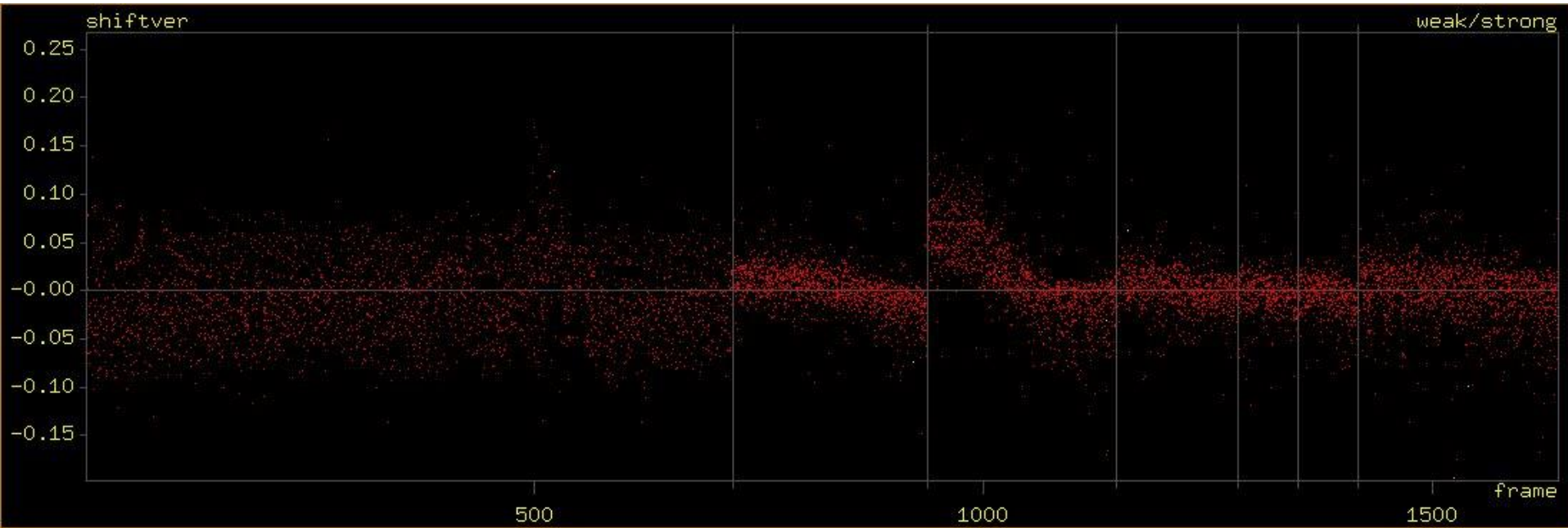
icr



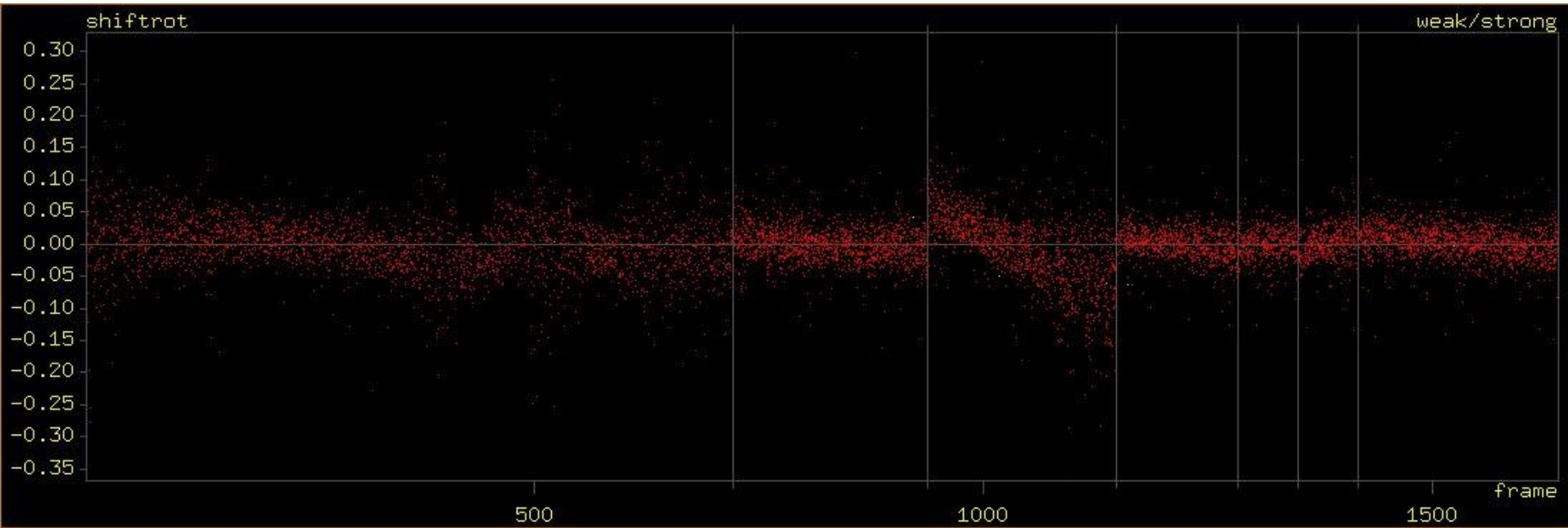
plot shifthor



plot shiftver



plot shiftrtrot



listrefl bad

Any> listrefl bad

```
hkl=0 0 -5 Theta=7.001 Reso=2.915 MaxInt=0.395 Imean=-0.549 Smean=0.563
(mean=-0.549 sigma=0.563 ioversig=-0.975 <ioversig>=-1.543) Rsym=536.227 Rmeas=579.192 Rpim=218.914 Chi2=16.431 n=7
  nr  boxfil  set  refl  h  k  l  intensity  sigma  ioversig  delsig
453 s01f001:  1  453  0  0  -5   -0.39  0.68  -0.57  0.23 +WEAK
576 s01f001:  1  576  0  0   5   -6.05  0.67  -9.08 -8.26 +NEGATIVE
2053 s01f003:  3   46  0  0   5   -1.75  0.67  -2.62 -1.80 +NEGATIVE
2177 s01f003:  3  170  0  0  -5    0.40  0.70   0.56  1.35 +WEAK
4581 s02f002:  6  383  0  0  -5    0.24  0.21   1.13  3.71 +WEAK
5261 s03f001:  7  481  0  0   5   -0.05  0.19  -0.24  2.70 +WEAK
7309 s05f001: 10   17  0  0  -5    0.01  0.27   0.02  2.06 +WEAK
  7 average:
      -1.08  0.48  -1.54  -0.00
More [Y] 
```

go

- With the command “go” you can select a reflection in the graphical window.
- Clicking with the <right mouse button> brings you back to the command line of “any”.

Output files

- pk (peaklist for the program “peakref”)
- hklf4 (SHELXL format)
- hklf5 (SHELXL format)
- sadabs (for the Bruker program “sadabs”)
- twinabs (for the Bruker program “twinabs”)
- jana (JANA format)
- mtz (for CCP4 programs)

Filters

- allow / forbid / require
- limit
- experiment / set
- qvp

Variables

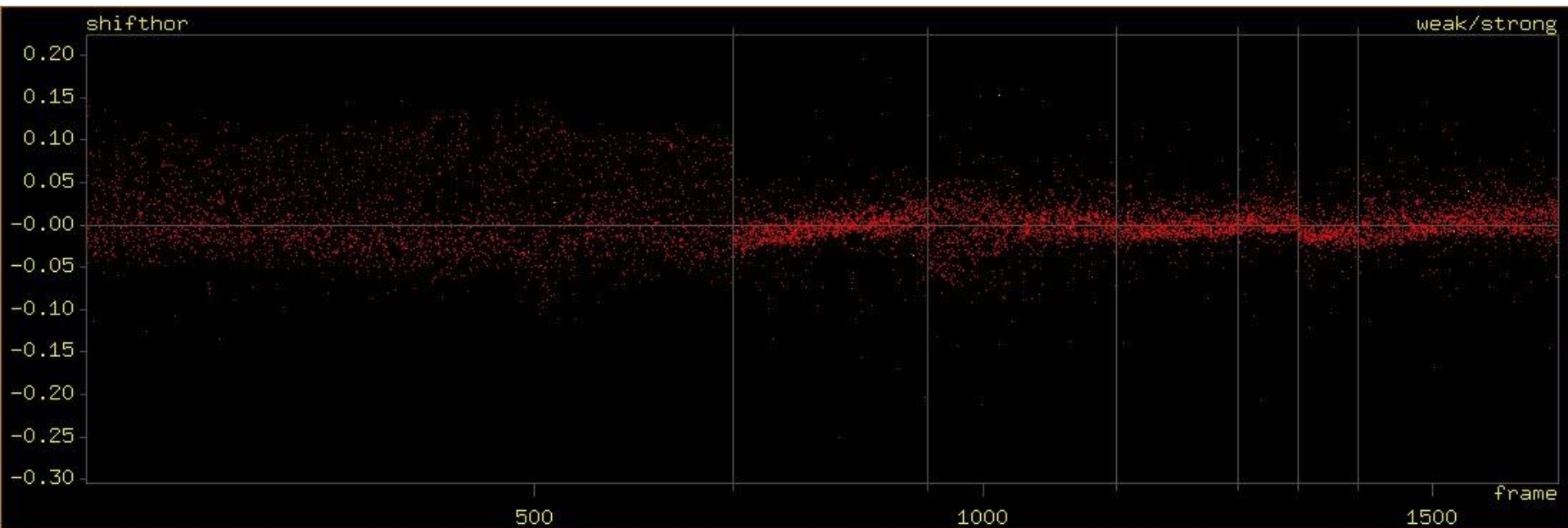
- list var
prints all available variables. (Note: not all values do vary and are then no variables but constants)

Plot

- plot
- plotrefl
- plot2d
- plotc
- plotray

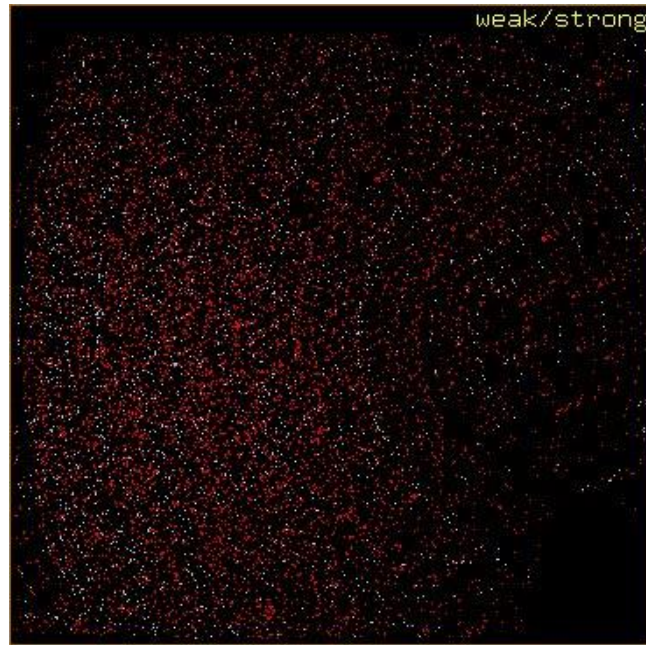
plot

- Create scatterplot of two variables
- Example:
plot shifthor frame



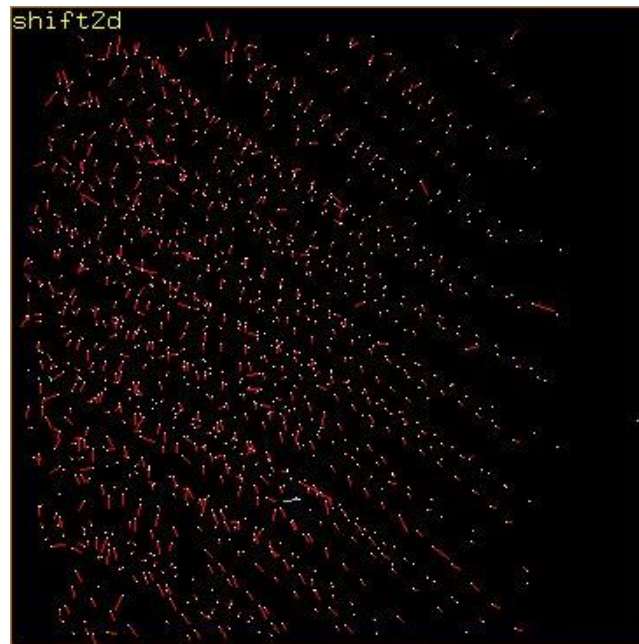
plotrefl

- Plots the 2-dimensional impacts of reflections



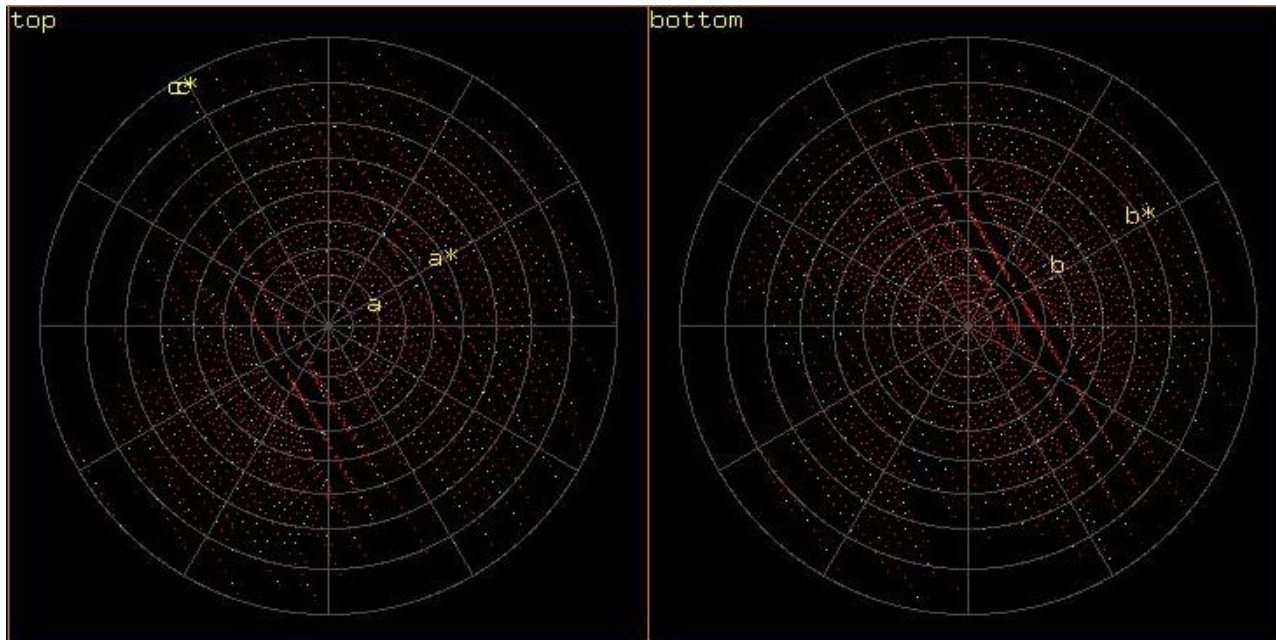
plot2d

- Plots the horizontal and vertical shifts on the detector as a function of the impact position



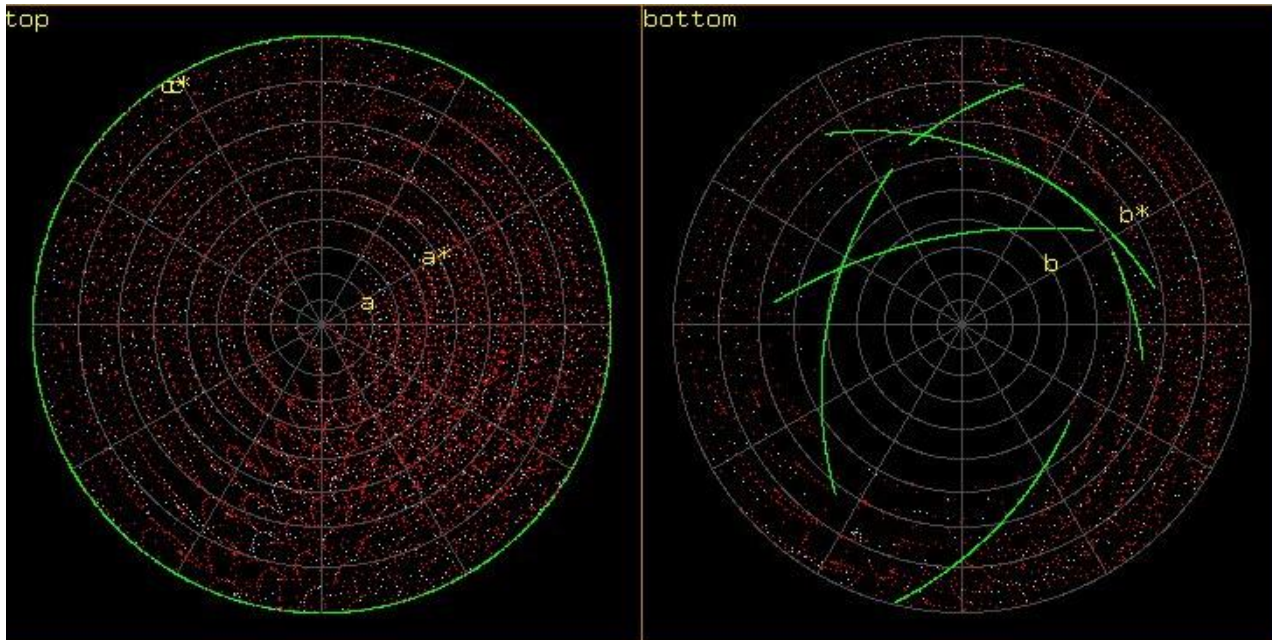
plotc

- Plots the c-vectors a stereographic projections
- Change view direction with the command “wulffvec”



plotray

- Plots InRays and OutRays as stereographic projections



Colourtype

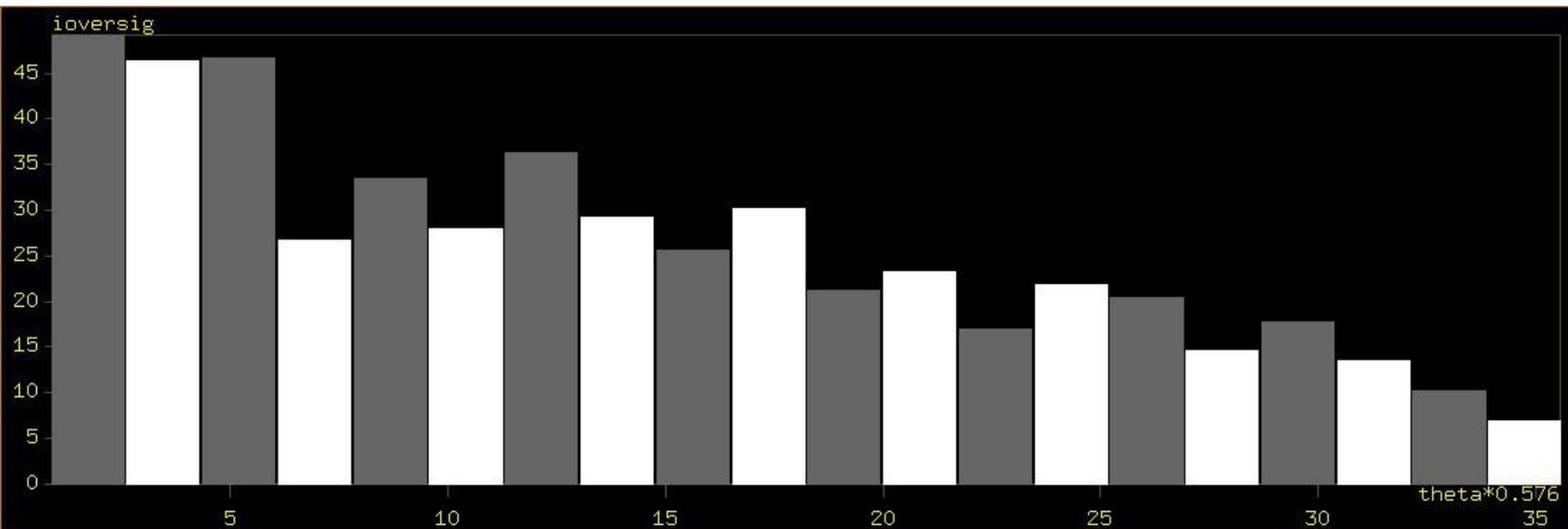
- `colourtype var varname`
the value of `varname` is used to set the colour

Histograms

- histo
- histcount
- Change the number of bins with “histobinfactor”
- “histoline” connects the bins with a line and performs a linear regression

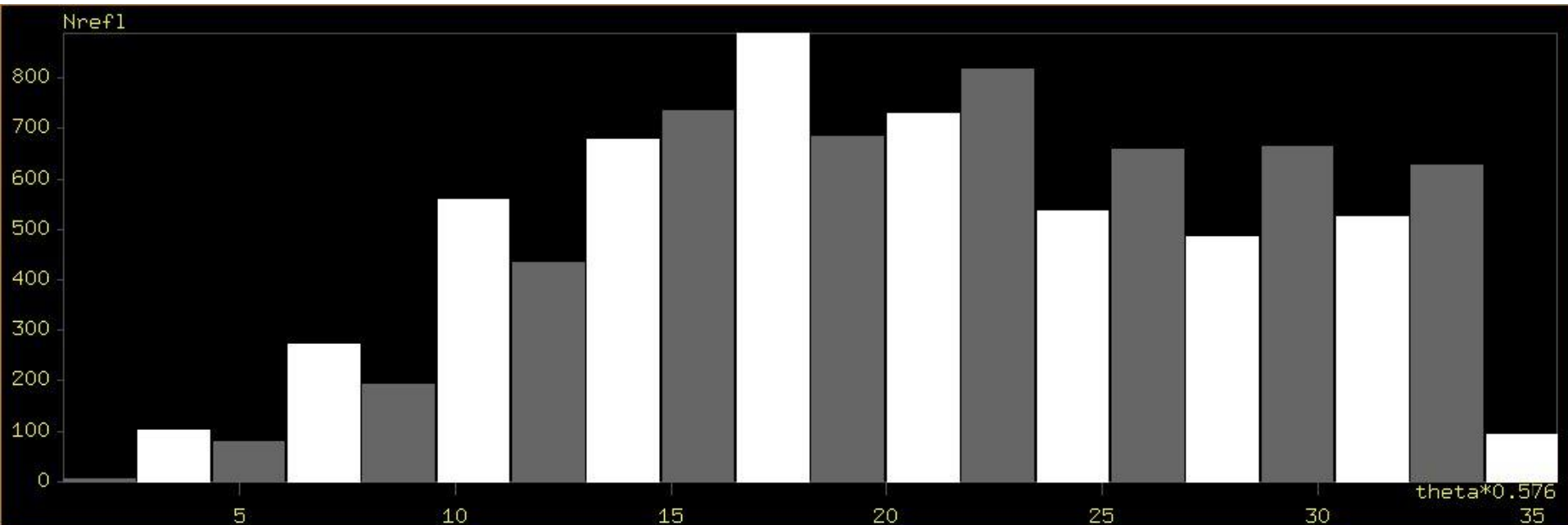
histo

- Creates a histogram of two variables
- Example:
histo ioversig theta



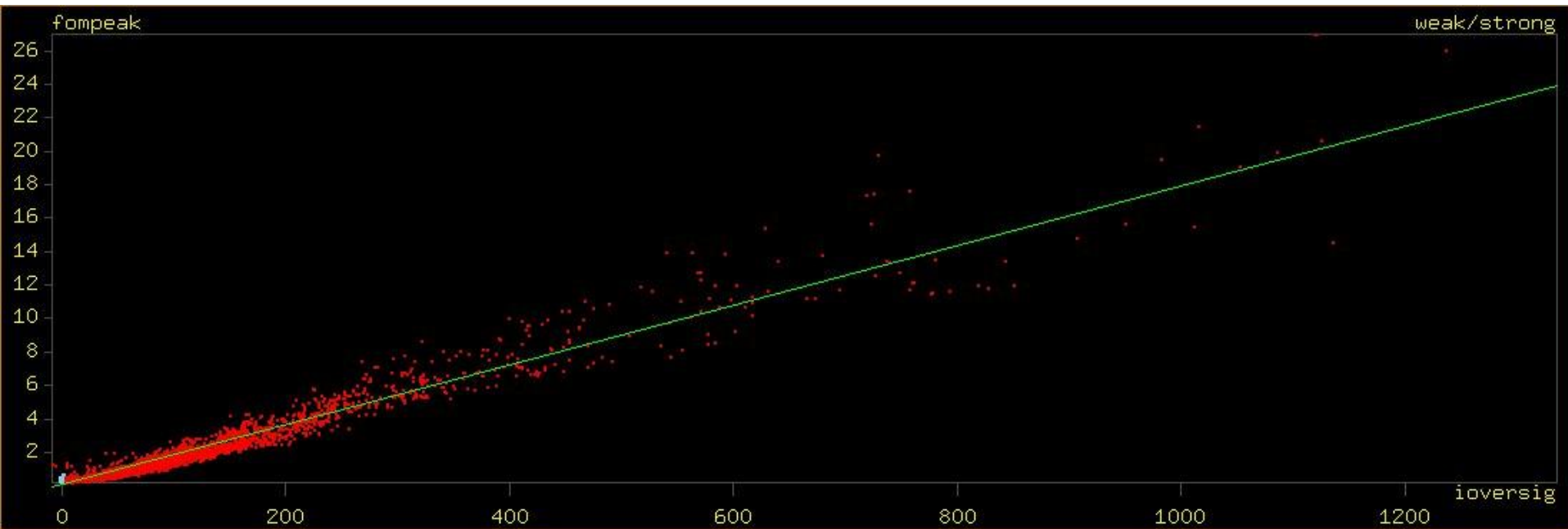
histcount

- Horizontal axis: variable
- Vertical axis: number of reflections per bin
- Example:
histcount intensity



histoline

- Example:
msa 0.0
histoline on
plot fompeak ioversig



$$\text{fompeak} = 0.01782 * \text{ioversig} + 0.07233$$

Renninger

- The command “renninger” creates a variable renningerscore for every reflection
- You may use filters to select reflections based on the renningerscore

Example (Renninger effect)

M. Lutz, A.M.M. Schreurs, A.L. Spek, M.A.H. Moelands, R.J.M. Klein Gebbink
Acta Cryst. (2010) C66, m9-m12.

Table 3

Examples of weak reflections influenced by Renninger effects.

F_{meas}^2 and $\sigma(F_{\text{meas}}^2)$ are taken from the raw data after integration using *EVAl15* (Schreurs *et al.*, 2010) and before the application of *SADABS* (Sheldrick, 2008a). For a definition of the Renninger score, see the *Comment*.

<i>hkl</i>	F_{calc}^2	F_{meas}^2	$\sigma(F_{\text{meas}}^2)$	I/σ	Renninger score
$4\bar{1}\bar{1}$	0.33	17.36	0.57	30.46	1253.46
$4\bar{1}\bar{1}$	0.33	1.30	0.25	5.20	0.00
$4\bar{1}\bar{1}$	0.33	0.51	0.20	2.55	0.00
$4\bar{1}\bar{1}$	0.33	1.15	0.25	4.60	0.00
$4\bar{1}\bar{1}$	0.33	0.50	0.19	2.63	0.00
$\bar{5}12$	0.36	0.80	0.32	2.50	0.00
$\bar{5}12$	0.36	0.71	0.24	2.96	0.00
$\bar{5}12$	0.36	8.90	0.52	17.12	1368.45
$\bar{5}12$	0.36	0.22	0.29	0.76	0.00
$\bar{5}12$	0.36	0.62	0.27	2.30	0.00
$\bar{5}12$	0.36	0.19	0.28	0.68	0.00

expression

- With the command `expression` you can define your own variables.
- Example:
 - `expression 1 sind(theta)`
 - `plot intensity expr1`
- Example:
 - `expression 2 odd(l)`
 - `limit h 0 0 yes`
 - `limit k 0 0 yes`
 - `plot ioversig expr2`

hybrid

- With the command hybrid you can mix Eval15 with Eval14 intensities.
- Example:
hybrid 5 10
 - for reflections with $I/\sigma < 5$: use Eval15
 - for reflections with $I/\sigma > 10$ use Eval14
 - between 5 and 10 mix both intensities

extractsubset

- After “filtering” reflections, you can create a boxfile with a subset of reflections using the command “extractsubset”.
- An instruction file filename.extr is created.
- On the linux commandline, run the program “extractshoe” (in the same directory as the original boxfiles).