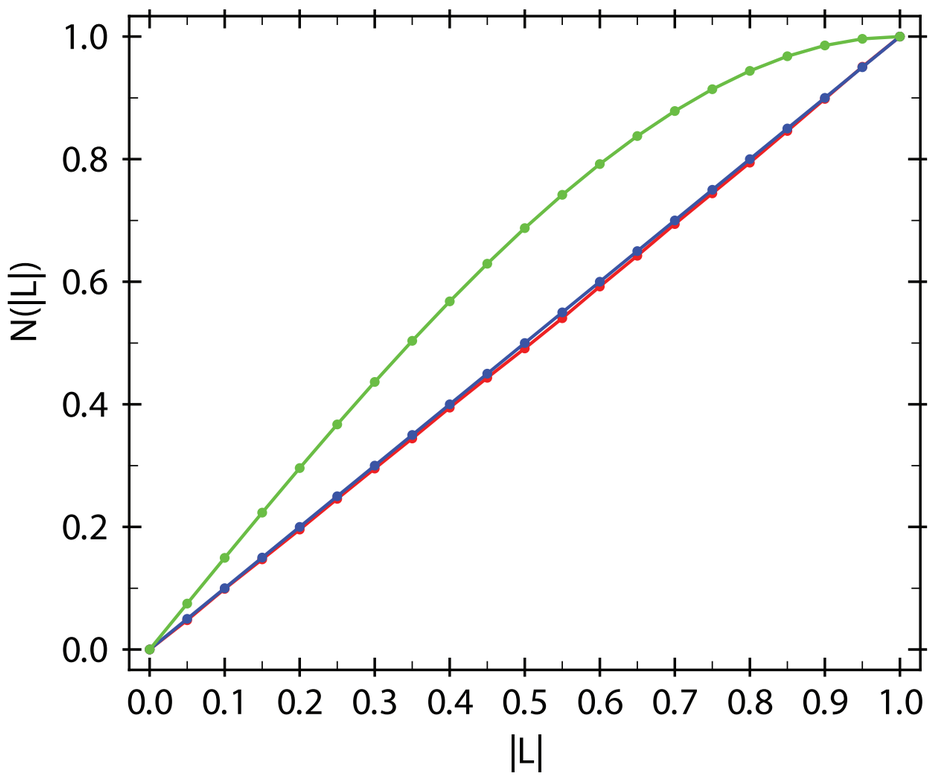
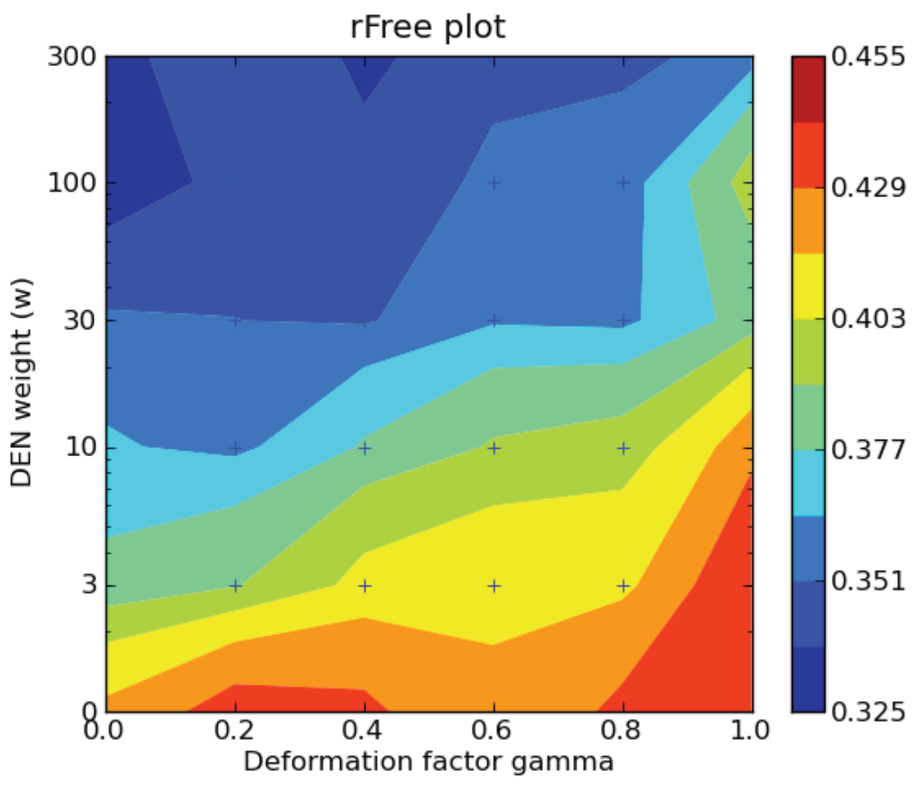
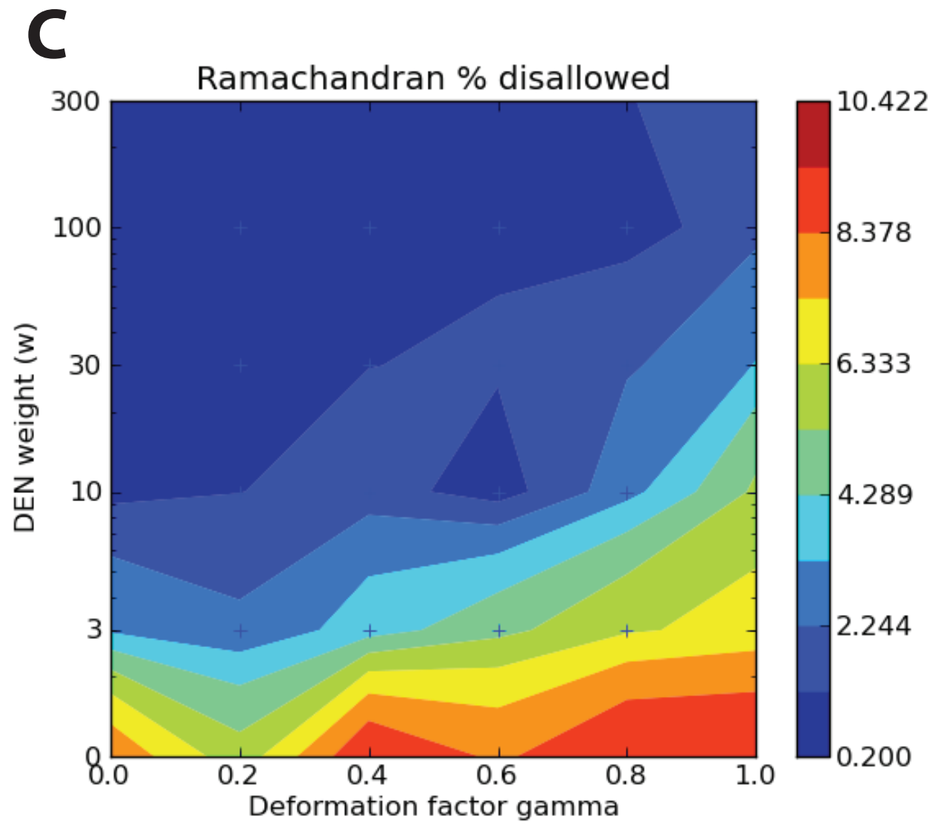
A



B



C



D

Log-file of twinning analysis in CNS

>>>> results of twinning detection
>>>> resolution: 500.0 - 5.9 A
>>>> sg= P3(2)21 a= 146.87 b= 146.87 c= 103.75 alpha= 90 beta= 90 gamma= 120
>>>> reflection file 1 : scaled_new.cns
>>>> reflections with |Fobs|/sigma_F < 0.0 rejected
>>>> reflections with |Fobs| > 10000 * rms(Fobs) rejected
>>>> theoretical total number of refl. in resol. range: 3596 (100.0 %)
>>>> number of unobserved reflections (no entry): 1 (0.0 %)
>>>> number of reflections rejected: 0 (0.0 %)
>>>> total number of reflections used: 3595 (100.0 %)
>>>> number of reflections in working set: 3595 (100.0 %)

==========

testing for perfect twinning

column 1: bin number
columns 2: upper resolution limit
columns 3: lower resolution limit
column 4: number of reflections in bin
column 5: average resolution in bin
column 6: <|I|^2>/(<|I|>)^2
column 7: (<|F|>)^2/<|F|^2>
column 8: fraction of theoretically complete data

<|I|^2>/(<|I|>)^2 is 2.0 for untwinned data, 1.5 for twinned data
(<|F|>)^2/<|F|^2> is 0.785 for untwinned data, 0.865 for twinned data

#bin | resolution range | #refl |

1	11.29	500.01	390	16.2548	6.9180	0.6679	0.7117
2	8.96	11.29	431	9.9532	3.1956	0.6935	0.8225
3	7.83	8.96	423	8.3476	4.0320	0.6877	0.8426
4	7.11	7.83	443	7.4507	4.5658	0.6947	0.8619
5	6.60	7.11	444	6.8389	2.3690	0.8300	0.8792
6	6.21	6.60	434	6.3962	1.9642	0.8926	0.8697
7	5.90	6.21	448	6.0480	1.7855	0.8997	0.8889

----------averages-over-all-bins----------
<|I|^2>/(<|I|>)^2 = 3.4875 (2.0 for untwinned, 1.5 for twinned)
(<|F|>)^2/<|F|^2> = 0.7690 (0.785 for untwinned, 0.865 for twinned)

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testing for partial twinning (using statistical method of Yeates)

>>>> testing for twinning operator= -h,-k,l

<H> = 0.50707: twinning fraction= -.007 (434 reflections used)
<H^2> = 0.34743: twinning fraction= -.010 (434 reflections used)

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Table 2 Source data 1. Diffraction data and refinement analysis. Twinning analysis by L-test in Ctruncate (**A**) and Xtriage indicate no twinning. Blue curve is acentric untwinned data, green curve acentric twinned data, and red curve observed data from Tat:AFF4:P-TEFb-TAR co-crystal. (**B, C**) Optimization of DEN refinement parameters using the web service for low resolution crystal structure refinement (https://portal.sbgrid.org/d/apps/den/).
(**D**) Logfile of twinning analysis in CNS.