SUPPORTING INFORMATION

Local Protein Structure Refinement via Molecular Dynamics Simulations with locPREFMD

Michael Feig[1,2*]

[1]Department of Biochemistry and Molecular Biology and
[2]Department of Chemistry, Michigan State University,
East Lansing, Michigan 48824, United States
*Email: feig@msu.edu

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Modified CMAP parameters.

Table S1: Bond force field terms that were modified from the standard CHARMM36 force field. Modified values (equilibrium bond distance and/or force constant) are given in bold with the original force field values given in parentheses. CHARMM atom types are given in parentheses below the atom names.

Residue(s)	Atoms	Minimum [Å]	Force constant [kcal/mol/Å^2]
PRO	N-C *(N-C)*	1.329 *(1.30)*	560.0 *(260.0)*
ALA/ARG/ASN/ASP/CYS/GLN/GLU/GLY/HSD/HSE/HSP/ILE/LYS/MET/PHE/SER/THR/TRP/TYR/VAL	N-C *(NH1-C)*	1.329 *(1.345)*	570.0 *(370.0)*

Table S2: Angle force field terms that were modified from the standard CHARMM36 force field. Modified values (equilibrium angle and/or force constant) are given in bold with the original force field values given in parentheses. CHARMM atom types are given in parentheses below the atom names.

Residue(s)	Atoms	Minimum [degrees]	Force constant [kcal/mol/degrees^2]
PHE/TYR	CA-CB-CG *(CT1-CT2-CA)*	110.5 *(107.5)*	151.8 *(51.8)*
ASN/GLN	CA-CB-CG *(CT1-CT2-CC)*	110.0 *(108.0)*	152.0 *(52.0)*
HSD/HSE/HSP	CA-CB-CG *(CT1-CT2-CPH1)*	113.0	158.35 *(58.35)*
ALA/ARG/ASN/ASP/CYS/GLN/GLU/HSD/HSE/HSP/ILE/LYS/MET/PHE/SER/THR/TRP/TYR/VAL	N-C-CA *(NH1-C-CT1)*	116.5	180.0 *(80.0)*
ARG/ASN/CYS/GLN/HSD/HSE/HSP/LYS/MET/PHE/SER/TRP/TYR	N-CA-CB *(NH1-CT1-CT2)*	110.5 *(113.5)*	170.0 *(70.0)*
HSD	NR2-CPH1-CPH1 *(NR1-CPH1-CPH1)*	106.0	230.0 *(130.0)*
HSE	ND1-CG-CD2 *(NR2-CPH1-CPH1)*	108.0 *(110.0)*	230.0 *(130.0)*
HSD/HSE/HSP	NE2-CE1-ND1 *(NR2-CPH2-NR1)*	110.5 *(112.5)*	230.0 *(130.0)*

ASP/GLU	N-CA-CB *(NH1-CT1-CT2A)*	110.5 *(113.5)*	170.0 *(70.0)*
ASP	CA-CB-CG *(CT1-CT2A-CC)*	110.0 *(108.0)*	152.0 *(52.0)*

Table S3: Additional improper torsion terms to maintain sidechain ring planarity.

Residue(s)	Atoms	Minimum	Force constant [kcal/mol/degrees^2]
HIS/HSD/HSE/HSP	CG-CD2-ND1-CB	0	30.0
PHE/TYR	CG-CD1-CD2-CB	0	30.0

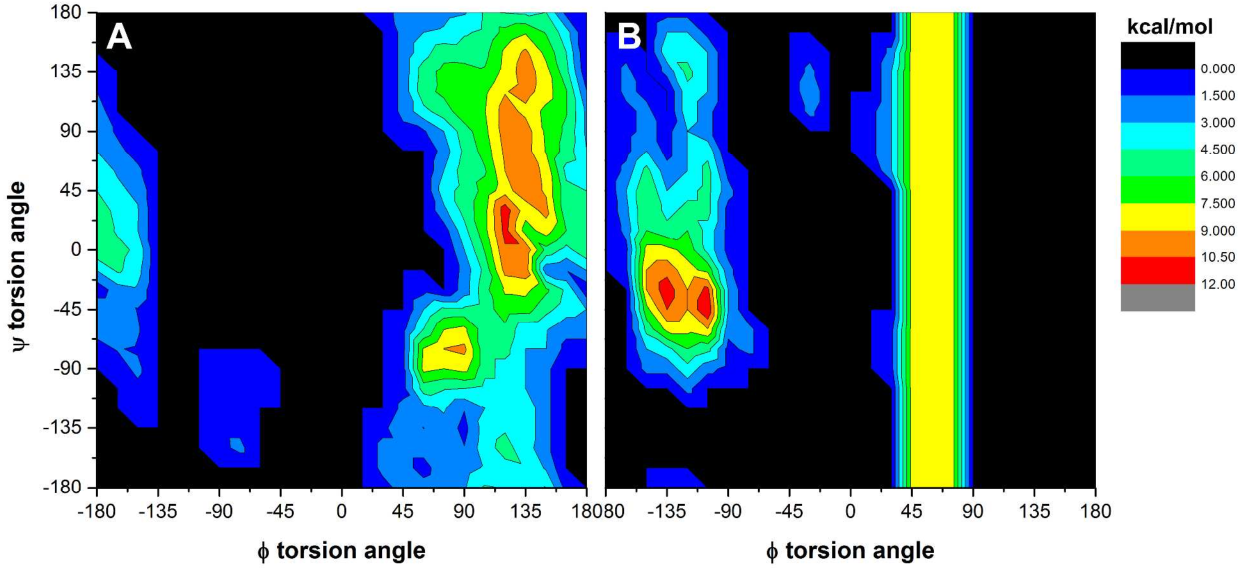

Figure S1: Difference between the CMAP used here as a function of ϕ and ψ backbone torsion angles (in degrees) compared to the standard CHARMM force field for non-proline/non-glycine residues (A; left) and proline residues (B; right).

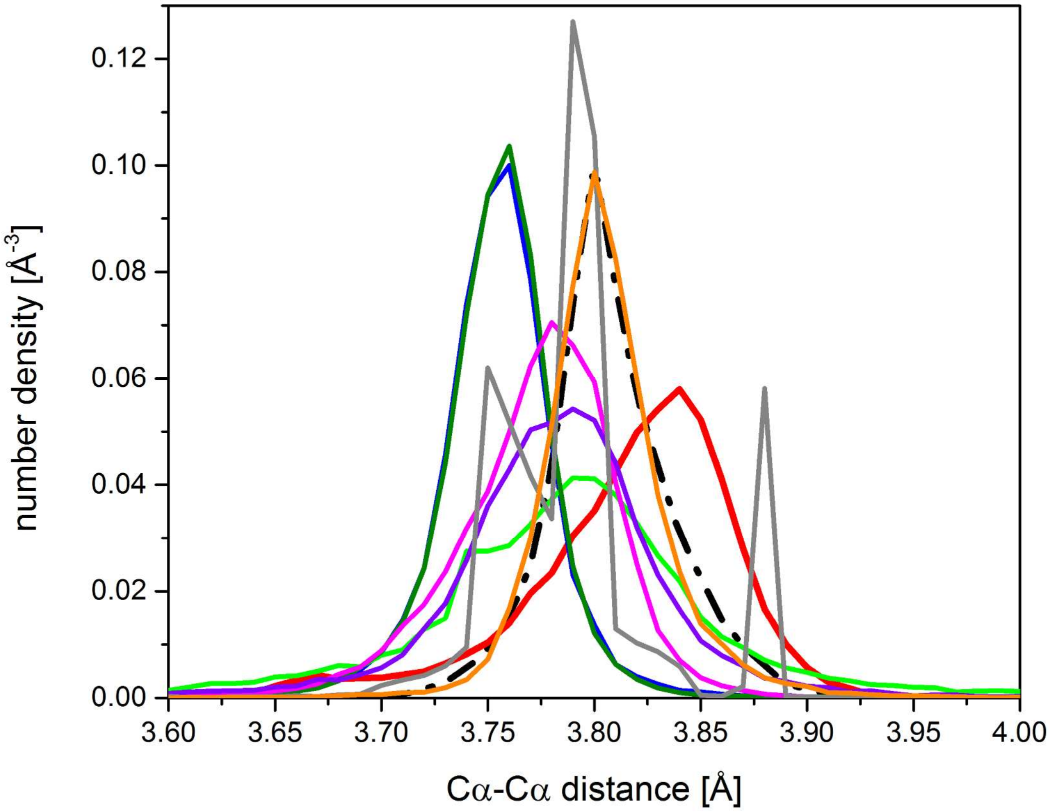

Figure S2: Radial distribution of Cα-Cα distances in subsequent residues normalized by spherical shell volumes as a function of distance for CASP11 server targets. The distribution from the native PDB structures (black dashed line) is compared with model 1 (TS1) server predictions from Zhang-Server (red), Rosetta (orange), TASSER-VMT (grey), RaptorX (violet), HHPredX (green), MULTICOM-CONSTRUCT (dark green), FFAS-3D (blue), and nns (magenta).

Modified CMAP entry to be used in CHARMM parameter file (also available upon request from the author):

```
CMAP
! alanine map
C    NH1  CT1  C    NH1  CT1  C    NH1   24
! phi = -180.0
   0.126790   0.768700   0.971260   1.250970   2.121010
   2.720430   2.089440   2.789790   2.780870   2.288474
   1.501130   0.900520   0.827670   0.821447   0.913223
   0.891106   0.766446   0.204200   0.204589   0.246991
  -0.835350  -1.222656  -0.951542  -0.036650

! phi = -165.0
  -0.127133   1.377090   1.577020   1.872290   2.398990
   2.486630   3.236754   3.529070   3.886456   3.543400
   2.558676   2.000440   1.009477   0.135306   0.420090
   0.602140   0.599128   0.501241   0.101780  -0.861434
  -0.640168  -0.207701  -1.076344  -1.122030

! phi = -150.0
   0.084069   1.420317   1.624350   2.047200   2.853910
   3.816410   4.221416   3.285454   3.257466   3.863293
   2.525720   1.815886   1.583256   0.006154   0.551995
   0.890683   0.554215   0.027243   0.068512  -0.225016
  -0.765479  -1.283444  -1.293226  -0.816303

! phi = -135.0
   0.927992   1.521370   2.242218   2.546305   3.111384
   2.918410   2.460813   2.187970   2.058314   1.852278
   0.115935  -1.183897  -1.995479  -2.278329  -1.959136
  -1.340467  -0.932949   0.021790   0.313725  -0.517358
  -1.152891  -0.983285  -0.566518  -0.442565

! phi = -120.0
   1.357468   1.959160   2.698894   3.037857   3.698960
   3.558453   2.639296   2.773853   2.719664   1.627997
   0.705667  -0.785637  -2.118268  -2.628489  -1.803113
  -0.425969  -0.062320   0.439040   0.910952  -0.546994
  -0.968118  -0.856791  -0.250116   0.449309

! phi = -105.0
   2.045006   2.544424   2.818030   3.088582   3.370620
   3.551568   3.073520   2.903794   2.956634   2.124759
   0.906487  -0.823628  -2.090819  -2.241579  -1.456524
   0.206160   0.082195   0.771710   1.040241  -0.124647
  -0.316550  -0.164333   0.314474   0.733747

! phi = -90.0
   1.451735   2.748481   3.638185   4.156796   4.450028
   4.344157   3.780200   3.898724   3.335030   2.440579
   0.912671  -0.606502  -1.511772  -1.620864  -0.962798
  -0.020653   0.415153   0.908250   0.459433   0.145910
  -0.071054   0.017622   0.280839   0.748823

! phi = -75.0
   1.378160   3.345958   4.352424   4.063543   4.814070
   4.700796   4.980310   4.212293   3.536425   1.693809
   0.095172  -0.682452  -0.123614  -0.427765  -0.598368
   0.226352   0.423308   0.301999   0.551890   0.191719
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  -0.253585  -0.190548  -0.253412   0.468922

! phi = -60.0
   0.237754   1.229980   1.716960   3.168570   4.208190
   5.391860   5.276080   3.673107   2.272295  -0.482789
  -0.406695  -0.038919  -0.357600  -0.823341  -0.173146
   0.139806   0.267796   0.322420   0.309664  -0.666399
  -0.948631  -1.534365  -1.479968  -0.204264

! phi = -45.0
  -1.184837   0.078060   2.347410   4.211350   5.376000
   5.389940   4.380200   2.461506   1.123713   0.107016
   0.007574  -0.149443  -0.797230  -0.582210   0.082910
   0.271580  -0.045570   0.379430   0.247770  -0.890956
  -1.582430  -1.954532  -1.980965  -2.000433

! phi = -30.0
  -1.174720   1.067030   4.180460   6.741610   6.070770
   4.806470   2.783340   1.320806   0.765978  -0.008448
   0.276860  -0.707140   1.314360   1.522590   1.915550
   2.223490   0.194290   0.534000   0.331780  -1.595147
  -2.849141  -3.550465  -3.277369  -2.655135

! phi = -15.0
   0.293590   5.588070   3.732620   3.217620   3.272450
   2.517320   1.588700   1.381760   0.856410   0.655170
   1.616970   0.846920   0.511070   0.740760   1.021020
   1.616580  -0.342400   0.181770  -0.613920  -2.558037
  -3.786839  -3.807325  -3.155346  -1.749204

! phi = 0.0
   2.832310   0.787990   0.323280   0.479230   0.628600
   0.976330   1.238750   1.671950   1.645480   2.520340
   1.606970   0.776350   0.119780   0.070390   0.121170
  -1.569230  -1.213010  -1.846360  -2.744510  -3.792530
  -3.934880  -3.615930  -2.675750  -0.924170

! phi = 15.0
  -0.778340  -1.912680  -2.052140  -1.846280  -1.047430
   0.183400   1.682950   2.223500   1.358370   2.448660
   1.436920   0.678570  -0.237060  -0.535320  -0.790380
  -2.182580  -3.251140  -4.195110  -4.269270  -3.908210
  -3.455620  -2.773970   1.755370   0.313410

! phi = 30.0
  -2.163810  -1.483730  -1.441809  -1.400349  -1.125083
   0.336200   1.428450   1.394630   0.970370   2.462720
   1.522430   0.553620  -0.407380  -1.482950  -3.613920
  -4.159810  -4.709721  -4.496271  -3.764540  -2.959140
  -1.963850  -1.071260  -1.599580  -2.445320

! phi = 45.0
  -1.821496  -1.836549  -1.365327   0.534377   0.984725
   1.362000   1.814380   1.754110   1.502370   1.903420
   0.770220  -0.416420  -3.286310  -3.875270  -4.611550
  -5.287977  -5.146239  -4.038627  -1.865450  -0.368170
  -0.860490  -1.416560  -1.666490  -1.595217

! phi = 60.0
  -1.353683  -1.984416  -0.317412   0.240143   2.257890
   5.922610   8.668070   8.038130   6.895330   4.632470
  -1.041450  -3.218100  -3.915080  -4.568574  -5.096776
  -5.526955  -5.005312  -3.777879  -1.540678   0.508820
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   1.756430   1.640810   0.451845  -0.342810

! phi = 75.0
   0.248733   0.641080   1.010583   2.539656   3.836063
   5.423710   8.017140   9.013120   7.070910   3.692809
  -2.305650  -3.420580  -4.484960  -4.807237  -3.001264
  -1.787739  -1.740525  -1.619378  -0.685150   1.151360
   2.170739   2.725589   1.736732   0.620673

! phi = 90.0
   1.120840   1.177830   1.128430   1.277730   2.407900
   5.303260   8.582510   9.036900   7.086270   3.074070
  -0.593220  -1.828560  -2.211800  -2.294328  -1.617221
  -0.763953   0.272995   0.911450   1.158306   2.473413
   2.099325   2.769822   2.157300   1.651694

! phi = 105.0
   2.850640   2.092420   3.445020   3.828490   4.005520
   4.884820   5.485850   4.818470   4.257670   3.682330
   2.514400   0.481110   0.053510   0.165400   0.171130
   0.728240   1.912230   1.802110   2.034640   2.715990
   2.600554   2.086721   2.274630   2.410940

! phi = 120.0
   2.469230   2.916650   4.540250   4.150330   4.763520
   5.038890   4.758480   5.313530   5.333050   4.872770
   4.366270   4.508260   4.124810   4.034830   4.724320
   4.700200   4.510620   4.185650   4.361620   4.847490
   4.444320   4.004260   4.415720   3.751230

! phi = 135.0
   2.111250   3.168960   3.322790   4.006920   4.316660
   4.086270   3.939170   3.625340   3.166360   4.830310
   4.469470   4.946030   4.112560   4.915580   4.047310
   4.996740   4.996730   4.842690   4.886620   4.300540
   5.094620   5.442210   5.163570   4.183510

! phi = 150.0
   2.757590   2.403620   2.023920   2.362390   2.634520
   3.264920   3.361360   3.948420   3.073680   3.483560
   3.152820   3.835120   3.762860   3.093660   3.744830
   3.390070   3.783930   3.190630   3.115420   3.042280
   4.125570   4.028550   3.026100   2.937910

! phi = 165.0
   0.210590  -0.071500   0.378890   0.543310   1.277880
   1.641310   1.698840   2.519950   2.631950   2.588670
   1.436530   0.835240  -0.563830  -0.408350  -0.889450
  -0.141750  -0.194970   1.666490   1.843450   2.555000
   2.548722   1.746995   1.751289   1.814368
```

```
!proline map
C    N    CP1  C    N    CP1    C    NH1 24
! phi = -180.0
   2.973500   3.348200   3.062900   2.113400   1.040500
   0.770600   0.785200   0.263300  -0.479000  -0.583000
  -0.463800  -0.292600   0.000000   0.259100   0.177100
  -0.151200  -0.173500   0.211700   0.348900  -0.135600
  -0.950000  -1.256600  -0.292800   1.560000

! phi = -165.0
   5.674100   6.011400   5.562700   4.467300   3.390800
   3.008800   2.848600   2.311200   1.661400   1.468400
   1.142700   2.437400   3.113200   4.799500   5.589100
   5.869000   5.016100   4.328500   4.232900   3.547600
   3.647200   3.422700   3.517100   4.339800

! phi = -150.0
   6.752800   6.973200   6.444300   5.389800   4.438600
   4.046000   5.832800   6.442400   8.303500  10.010000
  11.838100  12.162200  11.778300  10.362800  10.603600
  10.546200   9.702100   7.837200   6.549500   5.849600
   4.099200   3.031800   4.060200   5.624800

! phi = -135.0
   8.627800   8.153400   7.342500   5.893500   4.799200
   4.433400   6.551500   8.442800  10.222200  11.276300
  12.190000  12.152300  11.932900  10.274900   9.830800
   8.988600   7.588500   6.211000   5.918000   4.292100
   3.495500   5.449800   8.617700   9.311700

! phi = -120.0
   9.115600   8.477200   7.754300   6.585000   5.537900
   6.964300   8.929000  10.421200  10.336100  10.257800
  10.769300  11.359900  12.018000  12.055500  11.217600
   9.726100   8.512200   8.820200   8.716700   8.872300
   8.066800   9.094600   9.284900   9.931500

! phi = -105.0
   9.249700   9.483000   8.668500   7.525300   7.003200
   6.834600   8.822100  10.287600  12.320600  14.640300
  14.464800  12.100300  10.537600  10.885600  10.842000
  10.248700  10.540200  10.652400   9.196700   8.625400
   8.710100   8.581700   9.651500   9.192800

! phi = -90.0
   9.335600   9.208000   8.564600   8.010200   7.885100
   8.212200   9.737100   9.429100   9.306500   9.474200
   9.651300   9.484700   9.195300   9.295000   8.407200
   8.529900   7.242000   6.227500   6.347300   6.449700
   6.404700   6.579300   7.391700   8.570700

! phi = -75.0
  10.955200  11.455400  11.173300  10.428700  10.062400
  10.044500   9.279600   8.965100   7.361500   5.102700
   6.267600   7.871600   8.009800   7.104500   6.616400
   6.733700   7.504000   8.664700   9.282800   8.795900
   7.872500   7.612400   8.498100   9.894000
```

```
! phi = -60.0
   8.422900   8.529200   8.608500   9.306400  10.239400
  11.025900  11.510800   9.283500   7.566000   6.624600
   7.038700   8.222400   8.786400   8.512000   8.103500
   7.988200   8.192900   8.291000   8.055600   7.436800
   6.651800   6.317000   6.802500   7.746300

! phi = -45.0
   6.913200   7.937400   8.610800   9.316600   9.388500
   9.408400   8.828800   7.297900   5.456400   4.742700
   5.793100   7.118800   7.565400   7.598500   7.438700
   7.512500   7.878100   8.082200   7.642700   6.320500
   4.680400   3.830500   4.215800   5.435200

! phi = -30.0
   5.466700   7.116000   8.908800   8.347200   7.413500
   7.047000   6.031600   4.193100   2.674800   3.023700
   4.485300   5.451700   6.214900   6.422600   6.229300
   6.191100   6.488900   6.646400   5.833400   5.751300
   4.719800   3.064900   2.955800   3.860800

! phi = -15.0
   3.061500   5.603800  12.179500   6.295200   5.323400
   4.826500   3.705600   2.461500   2.291600   3.145900
   3.562100   4.443600   5.337500   5.728800   5.694800
   5.641600   5.943300   6.169000   4.759500   2.569400
   1.357100   1.669800   3.212300   5.031900

! phi = 0.0
   8.085900   8.051100   5.023600   3.450800   2.836100
   2.192500   1.566200   1.456300   2.039300   1.945200
   2.188400   2.921300   3.467500   3.543500   3.374500
   3.472300   4.069900   3.615600   2.082200   0.958600
   0.792600   1.494200   2.794900   4.853100

! phi = 15.0
   6.639500   5.177400   3.252300   1.952700   1.078400
   0.888300   1.505400   2.442300   2.178600   1.578600
   1.777400   2.395400   2.820200   2.795200   2.662400
   2.917100   2.562100   2.557900   2.322300   2.631400
   2.051200   2.555600   3.039100   4.915000

! phi = 30.0
   7.548800   5.095500   2.747000   0.955200   0.444500
   1.318700   3.733300   4.223200   3.565500   2.150900
   2.394400   2.939300   3.266000   3.210000   3.113400
   2.491300   3.978300   3.815300   4.522700   5.055600
   5.199900   5.327600   5.474200   7.977800

! phi = 45.0
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000

! phi = 60.0
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
```

```
   8.000000   8.000000   8.000000   8.000000

! phi = 75.0
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000   8.000000
   8.000000   8.000000   8.000000   8.000000

! phi = 90.0
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000

! phi = 105.0
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000

! phi = 120.0
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000

! phi = 135.0
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000

! phi = 150.0
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000

! phi = 165.0
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000   0.000000
   0.000000   0.000000   0.000000   0.000000
```