

## Supplementary Text 10

Call:

```
pca.xyz(xyz = xyz96, rm.gaps = TRUE)
```

Class:

```
pca
```

Number of eigenvalues:

```
1089
```

	Eigenvalue	Variance	Cumulative
PC 1	1451.111	72.530	72.530
PC 2	128.498	6.423	78.952
PC 3	99.560	4.976	83.929
PC 4	67.942	3.396	87.324
PC 5	46.299	2.314	89.639
PC 6	44.221	2.210	91.849

(Obtained from 96 conformers with 1089 xyz input values).

+ attr: L, U, z, au, sdev, mean, call

```
[,1]      [,2]      [,3]      [,4]      [,5]      [,6]
E:\\R-3.1.2\\scripts\\40.1ns_data\\NAT0.pdb
-26.174766 -49.19484841 -13.655031 -8.4493930 1.648399e+00 -4.410633
E:\\R-3.1.2\\scripts\\40.1ns_data\\LJP6.pdb
-7.137154 -43.56926318 -12.301589 15.2993715 1.291078e+01 10.959699
E:\\R-3.1.2\\scripts\\40.1ns_data\\3WY9.pdb
-9.109342 -41.94685048 1.522348 -34.4764359 -1.993688e+01 11.397632
E:\\R-3.1.2\\scripts\\40.1ns_data\\ZSP9.pdb
-19.659492 -40.28741188 -26.246999 12.7487217 9.812384e+00 -12.332311
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\013d855ad26c877c.final.pdb
52.364186 -7.89376335 10.028222 3.1244011 -2.053072e+00 -9.113038
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\0a2a705342ca0d54.final.pdb
-24.106361 0.06297032 -15.802606 7.3011151 1.205262e+01 -2.752591
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\0a59fceedb4194d9.final.pdb
51.814984 6.72738105 -4.898246 -3.8622086 1.459474e+00 3.485965
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\0dba59f3306825e8.final.pdb
52.321256 -5.67851580 10.586261 3.2141411 1.090832e+00 -4.835424
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\126f26a78b57339c.final.pdb
51.837928 -1.75043352 10.253150 2.5403043 6.869624e+00 2.897134
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\12f06f3e342df706.final.pdb
-24.134824 1.31338096 -17.286996 7.0723233 1.152521e+01 -2.362576
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-40.739549 8.82544584 -2.865992 -4.7330800 1.223670e+00 -2.312585
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\1f305f598641eeb2.final.pdb
-32.005064 -9.71362521 13.466948 -0.5339163 -5.491641e+00 -9.002533
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-40.739549 8.82544584 -2.865992 -4.7330800 1.223670e+00 -2.312585
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52.299583 2.79894692 -4.531414 -3.1529005 -4.293366e+00 -4.249328
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52.342705 0.62283021 -5.059441 -3.2313690 -7.361823e+00 -8.448938
E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\2b3027889e2fdc42.final.pdb
```

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52.532401 4.27560457 -4.147460 -2.9836572 -4.734571e+00 -5.132649  
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-32.505208 -3.41648142 13.458951 -1.0404743 3.628293e+00 3.215256  
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-28.902894 -6.40891637 10.824239 -1.2267218 4.192342e+00 6.727459  
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-33.307115 0.17342018 16.643395 14.9074755 -2.255632e+00 9.848612  
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-3.018193 10.44977856 -6.042500 -2.3170632 5.685494e+00 -4.742247  
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-25.012963 2.20198344 -5.412306 -6.2897189 -7.419569e-04 6.369788  
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-32.901658 -3.17807128 16.589663 1.8450382 7.905855e+00 4.046966  
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51.814984 6.72738105 -4.898246 -3.8622086 1.459474e+00 3.485965  
E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b669942ef97459a2.final.pdb  
-31.978950 -9.55981126 13.234022 -0.4563775 -5.294403e+00 -8.794916  
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51.814984 6.72738105 -4.898246 -3.8622086 1.459474e+00 3.485965  
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51.814984 6.72738105 -4.898246 -3.8622086 1.459474e+00 3.485965  
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-31.978950 -9.55981126 13.234022 -0.4563775 -5.294403e+00 -8.794916  
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 8.504919 -7.45048531 -8.031510 -5.2420083 -5.277923e+00 4.798081  
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 -20.704482 14.82002266 -2.915211 -0.1741302 9.318393e+00 -9.899160  
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 13.943274 6.69178313 -4.886790 -5.3947333 2.084602e+00 2.168631  
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 -31.170422 1.01758054 -2.245144 -6.2688814 -1.007595e+01 -10.498153  
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 -40.739549 8.82544584 -2.865992 -4.7330800 1.223670e+00 -2.312585  
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 52.364186 -7.89376335 10.028222 3.1244011 -2.053072e+00 -9.113038  
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 -33.131949 7.59861551 -1.733757 -6.8126959 -1.489380e+00 1.008771  
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 -25.012963 2.20198344 -5.412306 -6.2897189 -7.419569e-04 6.369788  
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 -32.505208 -3.41648142 13.458951 -1.0404743 3.628293e+00 3.215256  
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 51.814984 6.72738105 -4.898246 -3.8622086 1.459474e+00 3.485965  
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 51.922946 4.87625360 -3.779175 -4.1070775 2.059351e+00 3.214305  
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 -40.794879 8.90289420 -2.113708 -4.8426400 1.268972e+00 -2.592993  
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 -20.704482 14.82002266 -2.915211 -0.1741302 9.318393e+00 -9.899160  
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 -4.055341 -8.07198586 -16.918572 1.4175543 5.514134e+00 12.329708  
 E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\f83584e22003fb92.final.pdb  
 51.409674 9.88838643 -4.823055 9.2992846 -8.643122e+00 9.160267  
 E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\f8e2bf87e52caa29.final.pdb  
 52.364186 -7.89376335 10.028222 3.1244011 -2.053072e+00 -9.113038

[,7] [,8] [,9] [,10] [,11] [,12]  
 E:\\R-3.1.2\\scripts\\40.1ns\_data\\NAT0.pdb  
 17.06345632 -24.6291789 16.7251184 -1.12762224 15.97285860 -5.31095965  
 E:\\R-3.1.2\\scripts\\40.1ns\_data\\LJP6.pdb  
 0.02495566 -22.5977242 -14.5192516 -7.59201751 -19.30663541 3.29050749  
 E:\\R-3.1.2\\scripts\\40.1ns\_data\\3WY9.pdb  
 21.41368785 21.8273251 -12.9965379 -11.96713478 1.62777178 0.96118231  
 E:\\R-3.1.2\\scripts\\40.1ns\_data\\ZSP9.pdb  
 13.66185423 21.2789629 13.0804015 17.81886777 -11.24871290 2.03112756  
 E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\013d855ad26c877c.final.pdb

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-3.64246511 0.7569109 -0.6655648 -1.08306161 0.47400424 0.63188736  
E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\0a2a705342ca0d54.final.pdb  
-5.79142728 6.1537747 0.6867361 -6.72779820 5.18515905 3.77263176  
E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\0a59fceadb4194d9.final.pdb  
1.52248558 -0.5869192 1.5805519 -0.26987727 -0.50029384 1.40808310  
E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\0dba59f3306825e8.final.pdb  
-2.79492795 1.8929649 1.0360744 -1.41074777 -0.62236801 -2.16266062  
E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\126f26a78b57339c.final.pdb  
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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\83c0eefcfe12d3f9.final.pdb  
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-2.660868e-15

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3.917238e-15

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4.573013e-15

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[,205]	[,206]	[,207]	[,208]	[,209]	[,210]
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-2.682001e-15					
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-1.407602e-15					
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-3.336047e-15					
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-1.315339e-14					
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-2.033992e-14					
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-4.309338e-15					
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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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-7.043393e-16

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-2.361771e-15

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1.874222e-15

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3.160064e-15

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-2.530945e-15  
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9.000060e-15

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-2.058795e-15					
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-2.856312e-15					
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-2.024548e-15					
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-2.332850e-15					
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3.294822e-15	1.584917e-15	-3.782031e-15	3.129152e-16	3.158248e-15	
-3.242812e-15					
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb					
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-1.038002e-15					
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb					
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-5.217986e-16					
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb					
6.233557e-15	9.091531e-16	-5.824906e-15	4.827363e-15	1.974426e-15	
-3.549960e-18					
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb					
2.002751e-15	8.466833e-16	-3.417956e-15	1.459480e-16	2.953334e-15	
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[,235] [,236] [,237] [,238] [,239] [,240]  
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3.656495e-15 1.604185e-15 -5.232470e-15 1.231794e-16 1.216334e-14  
6.576017e-15



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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\12f06f3e342df706.final.pdb  
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-1.481313e-15

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6.576017e-15

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-3.981575e-15					
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-2.756152e-15					
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-2.870898e-15					
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-2.979867e-15					

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Supplementary Text 10

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-2.929992e-15

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-5.658506e-15

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2.889771e-15

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Supplementary Text 10

9.896963e-15

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-4.622689e-15					
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-6.498951e-15					
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-7.019918e-15					
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-3.557135e-15					
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-4.588619e-15					
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3.312211e-15					
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7.002307e-16	-2.554813e-15	-2.630688e-17	2.512856e-16	8.413158e-16	
-3.444970e-15					
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-1.672541e-16

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-4.692945e-15

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1.397611e-15

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-5.304229e-15

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-1.920950e-15

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-4.366698e-15

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-6.498951e-15

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-3.398898e-15

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-5.169344e-15

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Supplementary Text 10

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Supplementary Text 10

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2.039792e-15  
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2.711535e-15  
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-5.924479e-16  
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4.488545e-15

E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\8b6ef9ac3fe74395.final.pdb  
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[,361] [,362] [,363] [,364] [,365] [,366]  
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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

4.376700e-15

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6.483088e-15

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 -3.922824e-15

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 -6.596505e-15

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 -5.866279e-15

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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\ef8e88d4ad93a0ad.final.pdb  
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-3.270396e-15 5.542160e-16 3.923942e-15 8.280113e-15 -1.753970e-14  
-5.624007e-15

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-9.614941e-16

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-7.171178e-16

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4.504225e-16

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-7.627906e-16

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-2.343340e-15

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-6.148651e-16

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-2.238985e-15

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4.504225e-16

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-3.093222e-16

E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b4dd239fcabff1df.final.pdb  
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4.504225e-16

E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b669942ef97459a2.final.pdb  
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-9.098137e-15

E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b99f4d9d87c1017b.final.pdb  
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1.919487e-16

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-9.098137e-15

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-1.917308e-15

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-6.240189e-15

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2.163816e-15 -3.023845e-15 -1.413422e-15 6.044539e-16 -3.448988e-15  
3.882197e-17



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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\d678141e4018054a.final.pdb  
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-1.914905e-15

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5.408135e-15

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-3.335547e-15

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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\e5d589d996d0a960.final.pdb  
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-7.627906e-16

E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\eba517be32db050e.final.pdb  
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4.504225e-16

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-4.597282e-16

E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\ef8e88d4ad93a0ad.final.pdb  
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3.882197e-17

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-6.148651e-16

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[,529]	[,530]	[,531]	[,532]	[,533]	[,534]
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1.116414e-15	5.000557e-15	7.109770e-15	8.416845e-16	-7.196333e-15	
-4.367595e-15					
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-4.795255e-15					
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-2.961415e-15					
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-4.482954e-15					
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-9.535260e-15					
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-5.635871e-15					
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-7.677538e-16  
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-5.580153e-16  
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6.081813e-16

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-1.441561e-14

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-4.913043e-17					
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-6.005848e-16					
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-1.210599e-15					
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7.371180e-16					
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-5.503058e-16					
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1.468859e-15					
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-4.091698e-16					
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Supplementary Text 10

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-4.243959e-15  
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Supplementary Text 10

-1.176686e-14

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3.303541e-15					
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7.498758e-16					
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2.635823e-16					
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3.079328e-15					
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5.304333e-16					
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7.718563e-16					
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5.764035e-16

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-7.297213e-15



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-1.001685e-15

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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[,841] [,842] [,843] [,844] [,845] [,846]

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-4.080231e-15

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-9.395412e-15

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-9.395412e-15

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-7.801859e-15

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-6.773389e-15

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-3.686769e-15

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-1.021002e-15					
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5.930426e-16					
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-2.744435e-15					
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-1.151907e-14					
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-2.649825e-15					
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-2.784348e-15					
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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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-1.837077e-15  
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-4.967482e-15  
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-1.670080e-15  
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-1.031381e-15

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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\59b091fe385e05fc.final.pdb  
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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\8b34852716dad62.final.pdb  
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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b4dd239fcabff1df.final.pdb  
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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b669942ef97459a2.final.pdb  
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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b99f4d9d87c1017b.final.pdb  
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5.867063e-15 -1.032851e-15 7.231057e-15 -1.039071e-14 -5.703530e-15  
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-5.403751e-15  
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-6.981170e-15

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[,979] [,980] [,981] [,982] [,983] [,984]

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Supplementary Text 10

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Supplementary Text 10

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[,1021] [,1022] [,1023] [,1024] [,1025] [,1026]  
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Supplementary Text 10

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Supplementary Text 10

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1.701756e-15 2.696644e-17 4.247143e-15 -6.071126e-15 -1.371066e-14  
-1.507987e-15

[,1027] [,1028] [,1029] [,1030] [,1031] [,1032]  
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-2.087521e-15  
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3.691267e-15  
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Supplementary Text 10

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Supplementary Text 10

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[,1075] [,1076] [,1077] [,1078] [,1079] [,1080]  
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-2.376021e-14

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E:\\R-3.1.2\\scripts\\mPDBS\\summary\_pdb\_93\\b42c4924e3cd1aec.final.pdb  
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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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STANDARD DEVIATION

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