

Supplementary information for the article: "Why are diphenylalanine-based peptide nanostructures so rigid? Insights from first principles calculations"

Ido Azuri,¹ Lihi Adler-Abramovich,² Ehud Gazit,²
Oded Hod,³ and Leeor Kronik¹

1. Department of Materials and Interfaces, Weizmann Institute of Science,
Rehovoth 76100, Israel

2. Department of Molecular Microbiology and Biotechnology, George S.
Wise Faculty of Life Sciences, Tel Aviv University, Tel Aviv 69978, Israel

3. Department of Chemical Physics, School of Chemistry, Raymond and
Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv
69978, Israel

**Total energy, followed by geometry, for each of the three theoretical
levels used to study diphenylalanine-based peptide molecular crystals
in this work**

Structure I – Including TS-vdW corrections, using the FHI-AIMS code. See main text for
additional numerical details

Total energy [Ha]: -6194.69919

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C	10.04339253	3.30244592	1.15555358
C	8.98526535	4.34716262	1.59783885
C	18.89254238	18.91750098	1.86048624
C	14.10635064	10.34969358	2.05251964
C	10.91506923	2.74248204	2.25455274
C	18.65698084	20.21723412	2.32266574
C	19.72176408	18.05688563	2.57910488
C	12.67267455	9.95600074	2.49567697
C	12.13026419	3.35649459	2.59141188
C	16.95429224	5.13230472	2.75893797
C	8.09175155	3.81404071	2.72581129
C	10.52485522	1.59835133	2.96804258
C	33.92713753	17.39282390	2.94639495
C	15.02750452	10.82497777	3.15107214
C	15.71071686	5.57794780	3.22095925
C	18.11399940	5.41986027	3.47797742
C	6.23085738	2.36704757	3.34482633
C	9.66195085	15.95424435	3.38970679
C	15.10341427	12.18447746	3.48747945
C	19.22867306	20.67261445	3.52057788
C	12.91629134	2.85860078	3.63436958

C	20.34588753	18.51630975	3.74203782
C	15.97926777	17.24945848	3.65381652
C	12.68782652	8.91611527	3.62420926
C	15.82347702	9.91525088	3.86467179
C	25.79151780	17.38714156	3.84555597
C	11.31157998	1.09569961	4.00671064
C	33.97570761	18.42809462	4.04496478
C	14.97172966	16.39538797	4.11627756
C	20.10306418	19.80834713	4.20367887
C	12.50868894	1.73050487	4.34842089
C	6.92537471	1.29269244	4.18539311
C	5.51147356	3.44524918	4.21069055
C	16.30956839	18.39816418	4.37216867
C	13.01093293	6.58077132	4.24350312
C	26.84964556	16.34242586	4.28783750
C	32.83569581	19.17241684	4.38184969
C	15.60181551	6.30024626	4.41913853
C	15.92800927	12.61657197	4.53000985
C	18.02780905	6.18970392	4.64115664
C	16.94234850	1.77207783	4.55050532
C	10.57010797	15.44792214	4.51831279
C	11.27147228	18.66314813	4.75851523
C	21.72855349	10.33988577	4.74251977
C	16.65257128	10.34558286	4.90288852
C	24.91983912	17.94709928	4.94455646
C	17.17791220	0.47234886	5.01268510
C	16.78729511	6.62516423	5.10264483
C	16.70149527	11.69985144	5.24411536
C	14.28863031	6.64474128	5.08396633
C	11.71750751	6.49698846	5.10944608
C	16.11312384	2.63269348	5.26911841
C	12.75316221	14.55964043	5.13869176
C	23.16223464	10.73357908	5.18566476
C	23.70463960	17.33309045	5.28140675
C	14.29136976	16.66300125	5.31410866
C	32.87296713	20.10187917	0.04500365
C	15.59958354	18.70903822	0.15508157
C	18.88059721	15.55726763	0.06894965
C	27.74315599	16.87554215	0.03581285
C	25.31005679	19.09122152	0.27805770
C	1.90776428	3.29676394	0.25637776
C	35.20251975	19.59561101	0.41737221
C	20.80740605	9.86460267	0.46107629
C	20.12418002	15.11162274	0.53096055
C	14.60233002	17.85257301	0.61700427
C	34.05352264	20.31386403	0.75909310
C	13.33638552	15.69831281	0.59909801
C	12.17817163	13.39789730	0.62458855
C	17.72089691	15.26971152	0.78800018
C	29.60404109	18.32254054	0.65484128
C	26.17295860	4.73534099	0.69968930
C	20.73150148	8.50510072	0.79748421
C	16.60622250	0.01696525	0.83059485
C	22.91861098	17.83097934	0.94436555

C	15.48899910	2.17327178	1.05205250
C	19.85562650	3.44011541	0.96380841
C	23.14708545	11.77346727	0.93419830
C	20.01143159	10.77432518	1.17467945
C	24.52333272	19.59386505	1.31673068
C	1.85918725	2.26149393	1.35494857
C	20.86317678	4.29418630	1.42626117
C	15.73182758	0.88123269	1.51369761
C	23.32621858	18.95906300	1.65843052
C	28.90951709	19.39688457	1.49541003
C	30.32343025	17.24433544	1.52070409
C	19.52531960	2.29142215	1.68217535
C	22.82397045	14.10880806	1.55349113
C	2.99919687	1.51716874	1.69183560
C	20.23308812	14.38932439	1.72914208
C	19.90690726	8.07300284	1.84001441
C	17.80709702	14.49986835	1.95117489
C	25.26478750	5.24166681	1.82830449
C	24.56342112	2.02644259	2.06849661
C	19.18234194	10.34398810	2.21289557
C	19.04761081	14.06440906	2.41265374
C	19.13342043	8.98972084	2.55412015
C	21.54627930	14.04483048	2.39395938
C	24.11740152	14.19259827	2.41943561
C	23.08174015	6.12994133	2.44866885
C	21.54353322	4.02657731	2.62410031
C	2.96192040	0.58770356	2.73498835
C	20.23530557	1.98055679	2.84508709
C	0.63236793	1.09397967	3.10735219
C	21.23256220	2.83701509	3.30700055
C	1.78136137	0.37572110	3.44907486
C	22.49851719	4.99126738	3.28908034
C	23.65673276	7.29168607	3.31457610
H	10.65242434	3.76046860	0.36477355
H	9.48765279	2.48932994	0.67016520
H	8.40168537	4.59088966	0.69984072
H	18.41739614	18.56847889	0.94457369
H	14.01398441	11.10580046	1.26144091
H	14.53244123	9.46161303	1.56740987
H	10.53790529	5.88923543	1.57112268
H	6.75473266	3.00087942	1.37709542
H	12.16951798	9.57187221	1.59809308
H	6.05479726	0.18071142	1.74619463
H	17.01920842	4.54661225	1.84283180
H	12.45197030	4.22810683	2.01609737
H	19.87868610	17.03759388	2.22865603
H	8.96462942	6.39051752	1.98550666
H	33.22592330	17.69050105	2.15537622
H	11.01926148	17.31818061	2.46115630
H	12.11404036	12.07151570	2.46711419
H	12.72413240	7.35141709	2.27582490
H	9.59868178	1.08864781	2.69591559
H	9.74322054	15.32638448	2.49218248
H	14.81696322	5.33527663	2.64411405

H	16.51916902	17.01240832	2.73796708
H	5.40862993	1.91072031	2.77572696
H	14.50931402	12.89867791	2.91202985
H	19.07530607	5.04627953	3.12762019
H	9.83948599	5.56855204	3.11791510
H	10.89298187	10.96052373	2.88276970
H	25.18248702	16.92912084	3.05477278
H	26.34725582	18.20026024	3.36017236
H	31.43980049	16.52706896	3.36235469
H	11.94328894	14.69590598	3.17056362
H	15.80173068	8.85818422	3.59297899
H	27.43322893	16.09870513	3.38983864
H	14.73519556	15.49965851	3.53999470
H	17.41749693	2.12110218	3.63459065
H	13.86150952	3.33870057	3.89106261
H	12.99490139	5.64060186	3.67426612
H	31.92015315	19.01435462	3.80654622
H	17.11356698	19.04389498	4.02151177
H	12.04234129	11.30834490	4.01468476
H	31.79293337	14.91422751	3.77715894
H	21.02093845	17.86845460	4.30025167
H	21.82091261	9.58378224	3.95143864
H	21.30245921	11.22796982	4.25741447
H	11.00230313	0.20061552	4.54884972
H	25.29701080	14.80034873	4.26110953
H	29.08017602	17.68871132	4.06710836
H	12.17639084	18.11655079	4.48643194
H	23.66538386	11.11770508	4.28808054
H	29.78009971	20.50887113	4.43621463
H	7.82284624	1.72559419	4.65088550
H	18.81567665	16.14296063	4.53284443
H	15.98488272	13.67527329	4.78637842
H	13.55957091	14.07513118	4.57020540
H	23.38293162	16.46148214	4.70608351
H	15.95619870	3.65198260	4.91866846
H	32.06658395	16.08323842	4.90935390
H	13.12574671	1.34994409	5.16080876
H	26.87028627	14.29907086	4.67549120
H	20.57468184	20.14471206	5.12969001
H	6.24531082	1.06567163	5.02001617
H	18.92618529	6.45042434	5.19964190
H	2.60897778	2.99908345	4.84536099
H	24.81564142	3.37141194	5.15113794
H	17.27327076	9.63031780	0.06496117
H	23.72086561	8.61806508	5.15710124
H	23.11077873	13.33816466	4.96581346
H	26.23623119	19.60092381	0.00593758
H	26.09168904	5.36320361	5.18216834
H	21.01792623	15.35429149	5.33410957
H	14.36265264	7.63831069	0.16967645
H	19.31573065	3.67716301	0.04795987
H	31.98403221	20.67949865	0.30183429
H	30.42627040	18.77887244	0.08574797
H	21.32560492	7.79090309	0.22203376

H	16.75958817	15.64329593	0.43764935
H	25.99542515	15.12102262	0.42790574
H	17.33987834	12.04436466	0.67611356
H	24.94193516	9.72905704	0.19275129
H	16.73156260	7.20161990	0.64872803
H	14.14515162	5.94210930	0.53842196
H	15.82275870	19.61780389	0.71298714
H	12.24209485	19.77601585	0.95963710
H	4.39510439	4.16251058	0.67234361
H	23.89161467	5.99368275	0.48053945
H	20.03317396	11.83139147	0.90298691
H	21.09971994	5.18990483	0.84996801
H	12.51275842	16.25934211	1.06430326
H	21.97338782	17.35088369	1.20104836
H	22.83999778	15.04897746	0.98425646
H	3.91474076	1.67522853	1.11653523
H	18.72131394	1.64569663	1.33152599
H	23.79257216	9.38123463	1.32466867
H	22.12886272	0.34894438	1.57169632
H	4.04197746	5.77535684	1.08714704
H	14.07503452	18.09298128	1.54285774
H	13.87286468	15.22299400	1.43389102
H	14.81394676	2.82112057	1.61026331
H	24.83261618	20.48893950	1.85888289
H	23.65850322	2.57304245	1.79641052
H	28.01204095	18.96397908	1.96088950
H	19.85003688	7.01430056	2.09637897
H	22.27533496	6.61444915	1.88019085
H	3.76831725	4.60634480	2.21934007
H	22.70916227	19.33961794	2.47082203
H	15.26021174	0.54486970	2.43970895
H	29.58957053	19.62390310	2.33004117
H	16.90872346	14.23914619	2.50966711
H	18.56164040	11.05925296	2.75497190
H	21.47226046	13.05125950	2.85966630
H	3.85085161	0.01008059	2.99181826
H	18.49503710	8.64520390	3.36611858
H	19.10335155	13.48795228	3.33874026
H	21.68975804	14.74745991	3.22841827
H	20.01212252	1.07179112	3.40300370
H	23.59279111	0.91357602	3.64961447
H	23.32214302	4.43024003	3.75429037
H	13.70601641	20.34063826	4.26167417
H	21.75985850	2.59661137	4.23285868
H	21.96203598	5.46659071	4.12387329
N	9.61400162	5.60565370	2.09685002
N	7.11022576	2.96799624	2.34499369
N	11.89744349	11.13031871	2.99378853
N	12.93013117	7.64295153	3.24372305
N	32.14758540	15.86921102	3.88834024
N	11.79379534	15.02081414	4.13821547
N	26.22091546	15.08392457	4.78683685
N	28.72468349	17.72159217	5.03499858
N	23.93745310	9.55925657	0.30378103

N	22.90477848	13.04662717	0.55371566
N	3.68732007	4.82036485	1.19832998
N	24.04112205	5.66876142	1.44821602
O	4.99516331	4.42989979	3.64027361
O	8.33464320	4.10805151	3.90505689
O	10.60660181	6.54280883	4.53910158
O	12.55447935	9.27380809	4.80330624
O	11.58201817	12.45941045	0.05415607
O	5.42323978	3.20046982	0.09144423
O	10.19356018	15.51169817	0.31737066
O	30.83974670	16.25968996	0.95028077
O	11.88542516	6.29767356	0.99011515
O	27.50026276	16.58152347	1.21506032
O	25.22830393	14.14678139	1.84908695
O	12.43519204	13.44294488	1.88516105
O	23.28043629	11.41577247	2.11329492
O	24.25288922	8.23016617	2.74414461
O	30.41165926	17.48910887	2.78145615
O	25.64134131	5.17788273	3.00734538
O	23.94948467	14.39191184	3.68010270
O	23.39970494	7.24663673	4.57514491

Structure II – Including DFT-D2 corrections, using the VASP code. See main text for additional numerical details. Note that the use of pseudopotentials affects the total energy value.

Total energy [Ha]: -61.01633

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C	9.92605	3.25407	1.19459
C	8.88289	4.29388	1.66549
C	18.66831	18.67648	1.80444
C	13.94532	10.22404	2.09900
C	10.80177	2.69254	2.28612
C	18.47098	19.97192	2.29672
C	19.44138	17.76398	2.52166
C	12.52343	9.84025	2.57026
C	12.03463	3.28579	2.59141
C	16.76202	5.06536	2.70839
C	8.00104	3.73721	2.78657
C	10.39787	1.56913	3.02336
C	33.52172	17.18867	3.00382
C	14.86981	10.70130	3.19040
C	15.54136	5.54224	3.20037
C	17.93866	5.27870	3.42581
C	6.15714	2.28604	3.40385
C	9.54097	15.76553	3.47539
C	14.97255	12.06551	3.49615
C	19.02979	20.36799	3.52012
C	12.83538	2.77863	3.61889
C	20.05980	18.16762	3.70868
C	15.79463	17.04887	3.61336
C	12.56483	8.79782	3.69099
C	15.64093	9.78955	3.92715
C	25.47685	17.18610	3.90809
C	11.19824	1.05615	4.04657
C	33.57045	18.22818	4.09498
C	14.77142	16.23039	4.10589
C	19.85795	19.45626	4.19764
C	12.42038	1.66374	4.35119
C	6.90513	1.22792	4.21329
C	5.44455	3.34791	4.28889
C	16.19846	18.17472	4.33035
C	12.89956	6.47518	4.30760
C	26.52002	16.14629	4.37898
C	32.44031	18.99921	4.40057
C	15.47757	6.22437	4.42367
C	15.81234	12.50505	4.52360
C	17.89812	6.01633	4.61267
C	16.73456	1.76367	4.51795
C	10.46407	15.28058	4.59659
C	11.14359	18.44036	4.83170
C	21.45759	10.21613	4.81250

C	16.48557	10.22585	4.95034
C	24.60113	17.74762	4.99962
C	16.93190	0.46823	5.01024
C	16.68111	6.48589	5.10132
C	16.57050	11.58794	5.25544
C	14.19001	6.59381	5.11689
C	11.62385	6.38870	5.19290
C	15.96151	2.67618	5.23518
C	12.64299	14.40943	5.21362
C	22.87947	10.59992	5.28376
C	23.36827	17.15438	5.30491
C	14.14914	16.51656	5.32930
C	32.47950	19.94649	0.00082
C	15.53979	18.50875	0.09034
C	18.64088	15.37479	5.42190
C	27.40186	16.70296	0.07307
C	25.00504	18.87102	0.30988
C	1.88119	3.25152	0.29029
C	34.79000	19.39021	0.42768
C	20.53310	9.73885	0.47690
C	19.86155	14.89792	0.48687
C	14.52473	17.68976	0.57954
C	33.65281	20.14480	0.73259
C	13.18539	15.58642	0.59580
C	12.08008	13.26131	0.67179
C	17.46424	15.16144	0.71233
C	29.24575	18.15412	0.69037
C	25.86194	4.67464	0.76188
C	20.43036	8.37464	0.78264
C	16.37309	0.07217	0.80665
C	22.56752	17.66153	0.90539
C	15.34310	2.27254	0.99521
C	19.60826	3.39129	0.89986
C	22.83809	11.64235	0.97749
C	19.76198	10.65060	1.21366
C	24.20466	19.38400	1.33309
C	1.83245	2.21199	1.38145
C	20.63147	4.20977	1.39237
C	15.54494	0.98391	1.48417
C	22.98252	18.77642	1.63770
C	28.49776	19.21223	1.49982
C	29.95834	17.09225	1.57540
C	19.20443	2.26544	1.61686
C	22.50335	13.96498	1.59409
C	2.96259	1.44096	1.68704
C	19.92534	14.21578	1.71018
C	19.59057	7.93509	1.81009
C	17.50479	14.42383	1.89920
C	24.93884	5.15959	1.88309
C	24.25930	1.99982	2.11816
C	18.91734	10.21429	2.23685
C	18.72180	13.95426	2.38784
C	18.83241	8.85220	2.54194
C	21.21291	13.84634	2.40339

C	23.77907	14.05146	2.47939
C	22.75991	6.03074	2.50009
C	21.25376	3.92361	2.61578
C	2.92340	0.49368	2.71429
C	19.86311	1.93143	2.80385
C	0.61289	1.04997	3.14115
C	20.87818	2.75041	3.29303
C	1.75008	0.29538	3.44606
C	22.21752	4.85374	3.30927
C	23.32281	7.17886	3.38527
H	10.53024	3.72938	0.40942
H	9.35894	2.44916	0.70763
H	8.28967	4.56597	0.78259
H	18.20308	18.37157	0.86763
H	13.83538	10.98528	1.31421
H	14.35872	9.33073	1.61143
H	10.45609	5.79570	1.63724
H	6.66988	2.92283	1.42713
H	11.99087	9.46293	1.68739
H	6.04763	0.22629	1.72976
H	16.79366	4.50983	1.77169
H	12.36186	4.14738	2.00498
H	19.55914	16.74653	2.15242
H	8.90488	6.32321	2.10557
H	32.80776	17.47389	2.21874
H	10.90019	17.09983	2.51660
H	12.00935	11.95357	2.54303
H	12.60428	7.23810	2.33111
H	9.45053	1.08348	2.78163
H	9.60198	15.11536	2.59279
H	14.62899	5.35034	2.63328
H	16.29122	16.79821	2.67656
H	5.33102	1.81430	2.85088
H	14.38987	12.77991	2.91012
H	18.87873	4.87183	3.05686
H	9.79548	5.46802	3.19455
H	10.77715	10.87372	3.01165
H	24.87266	16.71079	3.12293
H	26.04395	17.99101	3.42113
H	31.05577	16.37689	3.44685
H	11.83480	14.53492	3.23707
H	15.58782	8.72639	3.68505
H	27.11325	15.87422	3.49607
H	14.48123	15.34417	3.53913
H	17.19979	2.06857	3.58114
H	13.79710	3.24295	3.84423
H	12.89499	5.52402	3.75436
H	31.53029	18.85158	3.81458
H	17.02075	18.78530	3.96097
H	11.96364	11.21701	4.10007
H	31.37460	14.76998	3.91599
H	20.69336	17.47744	4.26632
H	21.56753	9.45488	4.02772
H	21.04417	11.10943	4.32493

H	10.88013	0.17295	4.60401
H	24.94683	14.64447	4.35071
H	28.73303	17.51735	4.14065
H	12.03778	17.86276	4.58973
H	23.41203	10.97725	4.40089
H	29.35523	20.21385	4.44328
H	7.82524	1.67776	4.61443
H	18.60923	15.93031	4.48520
H	15.89116	13.57000	4.74930
H	13.46451	13.92991	4.66047
H	23.04104	16.29279	4.71847
H	15.84376	3.69363	4.86594
H	31.66971	15.96941	5.00434
H	13.05069	1.26740	5.14726
H	26.49804	14.11696	4.81903
H	20.31787	19.75328	5.14211
H	6.28720	0.99151	5.09223
H	18.81252	6.22004	5.17045
H	2.59515	2.96630	4.93222
H	24.50272	3.34036	5.23007
H	17.09151	9.50856	0.08039
H	23.39354	8.48661	5.25651
H	22.79861	13.20205	5.04461
H	25.95239	19.35666	0.06817
H	25.80093	5.32483	5.30629
H	20.77391	15.08982	5.34678
H	14.26046	7.61548	0.09124
H	19.11165	3.64194	5.39007
H	19.79558	0.10726	0.22640
H	30.07188	18.62587	0.13741
H	21.01303	7.66024	0.19659
H	16.52416	15.56831	0.34338
H	25.60745	14.97214	0.48103
H	17.22903	11.93534	0.62453
H	24.62577	9.56643	0.29810
H	16.65363	7.03284	0.61871
H	14.08590	5.94028	0.56869
H	15.82079	19.40264	0.64776
H	12.11215	19.55651	0.98469
H	4.34714	4.06327	0.73333
H	23.56812	5.90525	0.52355
H	19.81510	11.71376	0.97158
H	20.92165	5.09599	0.82561
H	12.33581	16.15838	0.99696
H	21.60579	17.19722	1.13071
H	22.50791	14.91614	1.04086
H	3.87261	1.58859	1.10105
H	18.38214	1.65486	1.24749
H	23.43929	9.22314	1.38655
H	21.88017	0.44909	1.52847
H	4.02832	5.67018	1.20247
H	14.03761	17.93976	1.52400
H	13.69926	15.16969	1.47473
H	14.70955	2.96273	1.55286

H	24.52277	20.26721	1.89052
H	23.36512	2.57742	1.87619
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H	19.51176	6.87014	2.03578
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H	3.73322	4.47075	2.29083
H	22.35222	19.17274	2.43378
H	15.08501	0.68689	2.42864
H	29.11569	19.44865	2.37875
H	16.59040	14.22013	2.45699
H	18.31140	10.93158	2.79390
H	21.14246	12.82467	2.80473
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H	18.17389	8.50480	3.33803
H	18.74930	13.40732	3.33223
H	21.31702	14.49987	3.28220
H	19.58210	1.03755	3.36130
H	23.29074	0.88368	3.69816
H	23.06711	4.28179	3.71041
H	13.52271	19.99109	4.24195
H	21.36529	2.50043	4.23750
H	21.70367	5.27046	4.18821
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N	25.86076	14.91412	4.89408
N	28.39162	17.53025	5.11331
N	23.61673	9.41310	0.37264
N	22.61680	12.91307	0.59034
N	3.65666	4.71964	1.27700
N	23.72757	5.60320	1.49625
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O	8.25757	3.99921	3.97581
O	10.50174	6.42593	4.63663
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O	11.48739	12.30789	0.11533
O	5.36993	3.09720	0.12291
O	10.10901	15.37199	0.35885
O	30.48713	16.10200	1.01885
O	11.80399	6.19844	1.02686
O	27.14532	16.44095	1.26231
O	24.90117	14.01424	1.92310
O	12.33437	13.32235	1.93285
O	22.93643	11.28952	2.16687
O	23.91549	8.13229	2.82881
O	30.03298	17.34295	2.83643
O	25.29389	5.06817	3.07234
O	23.59894	14.24169	3.74035
O	23.06853	7.11781	4.64633

Structure III – No vdW corrections, using the FHI-AIMS code. See main text for additional numerical details

Total energy [Ha]: -6194.17373

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C	10.25005931	3.67586062	1.34842674
C	9.23432519	4.73664596	1.84447376
C	19.54141165	20.47478379	1.88847448
C	14.47528708	10.71373922	2.27780920
C	11.18553449	3.05887843	2.36637711
C	6.75261741	0.02403833	2.45674845
C	20.43336120	19.59058152	2.50037696
C	13.04843011	10.36611955	2.77419154
C	12.47271674	3.58020483	2.57535164
C	17.09697092	5.45554161	2.81452005
C	8.33436892	4.21750945	2.98415801
C	10.80942942	1.90902611	3.08009796
C	10.49160101	17.89380958	3.20791380
C	15.47728978	11.21573466	3.29568872
C	15.88343193	5.85938013	3.38470682
C	18.30967138	5.78499857	3.42495087
C	6.38707944	2.84348721	3.58632310
C	10.08054449	16.48337339	3.70257969
C	15.66923707	12.59124718	3.50413303
C	7.36620709	0.41910510	3.65556396
C	13.35055256	2.97821183	3.48418897
C	21.07346039	19.97928791	3.68247617
C	16.36300649	17.53207200	3.74382010
C	13.04711019	9.32746594	3.91411821
C	16.28491274	10.31544822	4.01005801
C	27.34305050	18.02876661	4.13593046
C	11.68389353	1.30601647	3.98798249
C	35.61768967	19.01164032	4.22693481
C	15.40448629	16.68455178	4.31285684
C	20.80571012	21.22734659	4.24895632
C	12.95875863	1.84114664	4.19627746
C	7.04892028	1.71253075	4.38221129
C	5.68906680	3.92231233	4.48348824
C	16.68507763	18.74667945	4.35440526
C	13.26158765	6.95397722	4.51667345
C	28.35877984	16.96797644	4.63196677
C	34.52165034	19.86484444	4.43425778
C	15.85014281	6.58778218	4.58392866
C	16.62923986	13.05089462	4.41301465
C	18.29509636	6.53290581	4.60761461
C	18.05168662	1.22982824	4.67597917
C	10.97969498	15.96297776	4.84223703
C	11.73772988	19.26078803	4.94374584
C	23.11780257	10.99090507	5.06527714
C	17.24414887	10.77171832	4.91796083
C	26.40756807	18.64574410	5.15388060
C	30.84047600	21.68056734	5.24425443

C	17.08136113	6.92535386	5.17604565
C	17.41795653	12.14343739	5.12573342
C	14.57236570	6.96077605	5.31183987
C	11.97864894	6.89017696	5.41424468
C	17.15974280	2.11403540	5.28789327
C	13.14307816	14.96325873	5.44413974
C	24.54466328	11.33851468	5.56165482
C	25.12038366	18.12441750	5.36283939
C	14.75585352	17.02117742	5.51107751
C	34.60132656	20.92510046	5.34442383
C	16.02862382	19.10945046	5.53578731
C	20.49612989	16.24908796	0.02701097
C	29.25872352	17.48709413	0.19667352
C	26.78367302	19.79558457	0.29261603
C	27.10149781	3.81079972	0.42037792
C	11.81993799	20.31864104	0.27800947
C	22.11580567	10.48890303	0.50816366
C	21.70967034	15.84523675	0.59719350
C	15.07969212	18.25616438	0.52797810
C	35.78006572	21.15422054	0.48465053
C	13.79275076	16.10215011	0.66376687
C	12.55717377	13.82037936	0.76716931
C	19.28342744	15.91964323	0.63745729
C	31.20602528	18.86112552	0.79883352
C	27.51255732	5.22124594	0.91505062
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C	30.22688582	21.28550938	0.86807477
C	24.24254317	18.72640137	0.69667774
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C	21.23007804	4.17255101	0.95628387
C	24.54599337	12.37716100	1.12659053
C	21.30819394	11.38918664	1.22255158
C	25.90920756	20.39858632	1.20050433
C	1.97541530	2.69298008	1.43941094
C	22.18859706	5.02007334	1.52531132
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C	24.63433848	19.86345868	1.40878515
C	30.54417371	19.99207811	1.59471678
C	31.90403745	17.78230348	1.69599253
C	20.90801148	2.95794627	1.56687059
C	24.33152004	14.75064805	1.72915012
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C	21.74295301	15.11684148	1.79641571
C	20.96385949	8.65373637	1.62548390
C	19.29800777	15.17173630	1.82012612
C	26.61339502	5.74164582	2.05470468
C	25.85537319	2.44383167	2.15622542
C	20.34896722	10.93291214	2.13046216
C	20.51174238	14.77928156	2.38854395
C	20.17515676	9.56119082	2.33822284
C	23.02073333	14.74383924	2.52431760
C	25.61445262	14.81444768	2.62671824
C	24.45001627	6.74136734	2.65658505
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O	5.63262361	3.69270634	0.17310534
O	10.62634595	16.09014269	0.44741775
O	32.44226061	16.81041466	1.11855608
O	12.14965594	6.72619056	1.10381447
O	28.97178053	17.24472069	1.37671199
O	26.72540201	14.79348330	2.04969655
O	12.78510903	13.88638990	2.03160864
O	24.61202825	12.00724869	2.30669158
O	25.60985625	8.83586628	2.97776436
O	31.96047933	18.01191346	2.96061382
O	26.96674285	5.61448626	3.23487439
O	25.44344708	14.97843922	3.89129042
O	24.80797780	7.81824630	4.81905634