General results:

Problem	Method	LDE	PT	Num. Sol	$_{ m rmsd}$	Improv
pdb1a57	quaternionBP	3.139116497086273e-18	2.7274449360000004	1	2.07807988791912e-11	1.337081475730284
pdb1a57	classicBP	1.7968015190364832e-18	2.763913097	1	-	-
pdb1ba5	quaternionBP	4.2565562061067985e-21	0.170793527	1	1.8248664164772802e-10	0.6452820662225855
pdb1ba5	classicBP	1.6682703571436027e-20	0.17189562700000002	1	-	-
pdb1d1n	quaternionBP	4.268492501596864e-11	0.536223609	1	1.119996877351142e-11	0.4199794567419035
pdb1d1n	classicBP	4.268492325113002e-11	0.538475638	1	-	-
pdb1dp3	quaternionBP	2.0483323856148842e-10	0.3614391005	1	8.27941716790074e-11	0.5259707644718503
pdb1dp3	classicBP	2.0483315145496133e-10	0.3633401645	1	-	-
pdb1du1	quaternionBP	2.9207847988293018e-21	0.024465544000000002	1	1.1861845163328228e-12	0.9253503621255987
pdb1du1	classicBP	1.4862131973117249e-21	0.024691936	1	-	-
pdb1eii	quaternionBP	1.087962888232707e-18	1.2937285185	1	5.679145361463853e-11	-0.16818942064621423
pdb1eii	classicBP	9.164306416795705e-19	1.291552604	1	-	-
pdb1fcl	quaternionBP	1.6503122558139677e-10	0.5177888325000001	1	2.5526931938071794e-12	0.7703863524325616
pdb1fcl	classicBP	1.6502855351326824e-10	0.521777807	1	-	-
pdb1fd6	quaternionBP	3.248314586827051e-20	0.35534777700000003	1	1.3999866503837274e-11	0.5743189157477069
pdb1fd6	classicBP	7.49932795743307e-20	0.35738860650000004	1	-	-
pdb1i2u	quaternionBP	4.779084813604124e-22	0.11391551600000001	1	9.10582679457332e-12	1.2961588129926094
pdb1i2u	classicBP	3.5271595061563946e-21	0.11539204200000001	1	-	-
pdb1i2v	quaternionBP	3.178509695929702e-22	0.134612573	1	9.566033317556914e-13	0.3486836255629733
pdb1i2v	classicBP	7.063199270177441e-22	0.135081945	1	-	-
pdb1jlz	quaternionBP	3.8520382360486657e-22	0.0354229905	1	8.655644323252844e-12	0.6237178083538852
pdb1jlz	classicBP	1.65979456814709e-21	0.035643930000000004	1	-	-
pdb1jw3	quaternionBP	7.424760375091941e-22	2.082765515	1	2.046160360397928e-12	-0.9700374744297524
pdb1jw3	classicBP	1.4482623941279345e-21	2.0625619090000002	1	.	-
pdb1k0v	quaternionBP	8.541271727862477e-23	0.284978726	1	3.0991119711078896e-13	-0.3365114348921616
pdb1k0v	classicBP	1.606440032002974e-22	0.28401974	1	-	-
pdb1k37	quaternionBP	6.715722496665788e-22	0.35207783000000004	1	6.547359041608304e-13	0.5643530579587885
pdb1k37	classicBP	7.963217998644766e-22	0.354064792	1	.	· · · - · · · · · · · · · · · ·
pdb1kuw	quaternionBP	8.200812502885925e-24	0.0086844765	1	6.673724742677698e-13	0.7447771895058963
pdb1kuw	classicBP	3.3116078952546554e-23	0.0087491565	1	-	-
pdb1kz0	quaternionBP	2.72194658491024e-24	0.016928508000000002	1	6.911563759648795e-13	0.9086506619484513
pdb1kz0	classicBP	1.5258714912257716e-24	0.017082329	1	4 0 4 6 0 0 0 4 7 7 0 0 0 0 6 - 1 0	
pdb1kz2	quaternionBP classicBP	4.693695320422822e-25	0.019365212500000003	1 1	4.248329647793928e-12	0.6957037006436018
pdb1kz2	quaternionBP	7.77729945323894e-25	0.019499937000000002	1	2.9273222574214085e-12	1.0516214538685675
pdb1kz5 pdb1kz5	classicBP	2.2803466989365198e-24 1.825171237897462e-23	0.0107469755	1	2.9213222514214085e-12	1.0510214558085075
pdb1kz5 pdb1lvz	quaternionBP	2.0037650288428032e-10	0.010859993 0.008832721	1	6.619397292368988e-13	1.50329100171962
pdb1lvz pdb1lvz	classicBP	2.0037650288428032e-10 2.00376503083966e-10	0.008832721	1	0.019397292308988e-13	1.50529100171962
pdb1w2 pdb1m4e	quaternionBP	1.3035797047542093e-10	0.025018007000000002	1	5.982624779899859e-12	0.6285512670933358
pdb1m4e pdb1m4e	classicBP	1.3035797047342093e-10 1.30357966983058e-10	0.025175258000000002	1	5.962024119699659e-12	0.0283312070933338
pdb1m4e pdb1ma2	quaternionBP	8.239332456174382e-10	0.193657835	1	4.84914643200541e-11	0.9555113016728622
pdb1ma2	classicBP	8.239269681328984e-10	0.1955082575	i	4.040140402000416-11	0.9555115010726022
pdb1ma2	quaternionBP	1.6372379338025556e-10	0.06959277400000001	1	5.567945663707319e-13	1.1153492746243776
pdb1ma4	classicBP	1.6372378869871912e-10	0.0703689765	1	-	1.1100402140240110
pdb1ma5	quaternionBP	7.238159762983826e-22	0.019135278000000002	1	4.167455921211496e-12	1.2374630773589912
pdb1ma5	classicBP	2.267906926765571e-22	0.01937207	ī	-	-
pdb1ma6	quaternionBP	3.5689955908587775e-11	0.0178875135	ī	6.099536820773011e-11	0.9911578822847655
pdb1ma6	classicBP	3.5689947994097734e-11	0.018064807000000002	ī	-	-
pdb1nd9	quaternionBP	2.342544906654494e-22	0.38851215800000005	1	1.8713386307550106e-12	0.6545764264087595
pdb1nd9	classicBP	4.573036783930121e-22	0.39105526700000004	1	-	-
pdb1ne5	quaternionBP	3.682459489597174e-21	0.20762489650000002	ī	9.19879217695788e-12	0.9379802388004954
pdb1ne5	classicBP	2.6408928111710663e-20	0.209572377	1	<u>-</u>	-
pdb1nmj	quaternionBP	1.3799602867004394e-25	0.045110050000000006	1	1.6907132435054638e-13	0.6778988274231512
pdb1nmj	classicBP	5.849829824734458e-26	0.0454158505	1	-	-
pdb1o53	quaternionBP	1.0218835734273617e-10	0.0170003965	1	1.187312906666831e-12	0.704774738636238
-	-					

pdb1o53	classicBP	1.0218834362987095e-10	0.017120211	1	-	
pdb1oqp	quaternionBP	2.5078762345729744e-23	2.6524745640000003	1	1.319591740817811e-12	-0.05312984030561019
pdb1oqp	classicBP quaternionBP	7.421226139211143e-23 5.298701333492881e-25	2.6510653085 0.0027926915	1 1	- 4.624176324272228e-13	1.7183602270426368
pdb1plw pdb1plw	classicBP	6.935517110208233e-25	0.0027920915	1	4.0241703242722286-13	1.7183002270420308
pdb1plw pdb1plx	quaternionBP	5.592113965095026e-24	0.0025977540000000000	1	4.7011546502493415e-12	1.7769773427352975
pdb1plx	classicBP	5.513114065887378e-23	0.0026439155000000003	1	-	-
pdb1pv0	quaternionBP	1.2318185736629154e-10	0.1447737195	1	3.3930617215252726e-12	0.6315417626608699
pdb1pv0	classicBP	1.2318182203415926e-10	0.145688026	1	-	-
pdb1r57	quaternionBP	1.7692818297962508e-12	0.7864379290000001	1	2.131572911188102e-12	0.25613324659472525
pdb1r57	classicBP	1.7692818089660747e-12	0.7884522580000001	1	-	-
pdb1ry3	quaternionBP	2.466214648984479e-10	0.25411756150000003	1	3.4230370574881844e-12	0.31144640115712274
pdb1ry3	classicBP	2.466214931294833e-10	0.2549090015	1	-	-
pdb1s4h	quaternionBP	8.706559805853487e-13	0.01140292	1	8.742931790567393e-12	1.2045467301357915
pdb1s4h	classicBP	8.706499673442411e-13	0.0115402735	1	.	
pdb1s4j	quaternionBP	3.4702063383056425e-10	0.012129202	1	9.276228200997332e-13	1.4222947230988492
pdb1s4j	classicBP	3.4702062749986864e-10 1.0958451005358719e-10	$0.012301715000000001 \\ 1.9593135190000002$	1 1	- 1.971353528558558e-12	0.16732886126735735
pdb1s6j	quaternionBP classicBP	1.0958451005358719e-10 1.0958423680812043e-10	1.962592016	1	1.971353528558558e-12	0.16732886126735735
pdb1s6j pdb1sa8	quaternionBP	7.551004875653682e-21	0.569701938	1	2.798914881375975e-12	0.12071786211829139
pdb1sa8	classicBP	9.203686334633368e-21	0.5703896700000001	1	2.796914661373975e-12	0.12071780211829139
pdb1sac	quaternionBP	6.969798778026199e-23	0.040720473	1	2.7850676147011436e-12	0.037357129913506704
pdb1t2y	classicBP	5.709201234178208e-23	0.040735685	1	-	-
pdb1t5q	quaternionBP	1.3716115057317601e-24	0.0457738575	1	1.4824913173909687e-13	0.046960210858348894
pdb1t5q	classicBP	1.909927993028546e-24	0.045795353000000004	1	-	-
pdb1tot	quaternionBP	9.344486719647214e-24	0.135312302	1	2.369678292927337e-13	0.03346406744304531
pdb1tot	classicBP	6.807405425919864e-24	0.135357583	1	-	-
pdb1v6r	quaternionBP	1.3777732304143013e-21	0.0292848295	1	3.730389337370212e-12	0.21587115608783236
pdb1v6r	classicBP	1.1327624370048259e-21	0.029348047000000002	1	-	-
pdb1v92	quaternionBP	2.845776421266189e-23	0.12022935700000001	1	2.4803770407889116e-12	0.6519056739195506
pdb1v92	classicBP	1.866797801130652e-23	0.121013139	1	-	
pdb1vd7	quaternionBP classicBP	2.7038843720364647e-10 2.703884461186263e-10	$0.030142851000000002 \\ 0.030395778000000002$	1 1	2.3012434592328365e-12	0.8390944837965097
pdb1vd7 pdb1vd9	guaternionBP	1.1934482827954317e-9	0.035877800000002	1	3.83554802609916e-11	1.0655915176120079
pdb1vd9	classicBP	1.1934482827954317e-9 1.1934521974563538e-9	0.036259751	1	3.83534802009910e-11	1.0655915176120079
pdb1vdb	quaternionBP	4.943978719392181e-10	0.0315385895	1	1.1209714409538348e-11	0.7197611040912433
pdb1vdb	classicBP	4.943979283591023e-10	0.031765592	1	-	0.7107011040012400
pdb1vpc	quaternionBP	1.104644872290092e-25	0.097879275	ī	1.0206325613776714e-13	0.7212532990257703
pdb1vpc	classicBP	1.0621353256952448e-25	0.09858523250000001	1	-	-
pdb1wnk	quaternionBP	6.73965725937545e-20	0.031160732000000003	1	7.602634708530641e-10	0.8939889473713158
pdb1wnk	classicBP	3.205754342330267e-19	0.0314393055	1	-	-
pdb1wo4	quaternionBP	3.3131730763333625e-21	0.24636655600000001	1	1.3690172371374448e-11	0.9602762397668885
pdb1wo4	classicBP	7.460589222002202e-22	0.2487323555	1	-	-
pdb1wo5	quaternionBP	4.5974850963825957e-11	0.065149652	1	1.6850857534143226e-11	0.9880958381788485
pdb1wo5	classicBP	4.5974834977714614e-11	0.065793393	1	_	
pdb1y5c	quaternionBP	4.250871953238251e-11	0.0084245945	1	9.70075825433811e-12	1.6579492342331692
pdb1y5c	classicBP	4.2508729559197436e-11	0.00856427	1	9 0000051040010509 10	0.5821966020290059
pdb1yx8 pdb1yx8	quaternionBP classicBP	5.857703783376745e-11 5.857703598747301e-11	1.810508334 1.8210490520000002	1 1	3.8893651949616523e-10	0.5821966020290059
pdb1yxs pdb1yxr	quaternionBP	2.2185728711277977e-11	0.589635902	1	2.3743219952292934e-12	0.9666877441937061
pdb1yxr pdb1yxr	classicBP	2.2185723891982057e-11	0.595335840000001	1	2.57452155522525546-12	0.3000017441337001
pdb1yxi pdb2a4j	quaternionBP	4.366096117686307e-24	0.528580153	1	2.9037120012651884e-13	1.003210671059751
pdb2a4j	classicBP	1.1971320328286186e-24	0.5338829255	ī	-	-
pdb2ajj	quaternionBP	3.438163972899142e-10	0.0467348095	1	1.1290044494673194e-12	1.089773351916623
pdb2ajj	classicBP	3.4381641590913174e-10	0.047244113000000004	1	-	-
pdb2ajm	quaternionBP	2.8892998671342377e-10	0.049538781000000004	1	3.0198988516835652e-12	0.8075188608294592
pdb2ajm	classicBP	2.889299441792005e-10	0.049938816000000004	1	-	-
pdb2ajn	quaternionBP	1.8023096111416234e-10	0.047967125000000006	1	4.619322251998628e-13	0.667712521857422
pdb2ajn	classicBP	1.8023095225093148e-10	0.048287407500000004	1	-	-

pdb2ajo	$\begin{array}{c} quaternionBP \\ classicBP \end{array}$	2.8892998671342377e-10 2.889299441792005e-10	0.049584158	1 1	$3.0198988516835652\mathrm{e}\text{-}12$	0.7063657307642579
pdb2ajo pdb2akk	quaternionBP	2.889299441792005e-10 2.4871897689312827e-23	$0.0499344035 \\ 0.719544418$	1	1.1166327612159839e-12	0.6514642991782615
pdb2akk pdb2akk	classicBP	8.362615979032648e-23	0.719344418	1	1.1100327012109839e-12	0.0314042991782013
pdb2c0s	quaternionBP	6.253555168645064e-22	0.20159632300000002	1	1.3871538821281691e-11	0.7180418662695587
pdb2c0s	classicBP	7.694768307162041e-21	0.20304386900000002	1	-	-
pdb2dci	quaternionBP	5.20197097433592e-25	0.022038781	1	1.0732255951927575e-13	0.877795827273764
pdb2dci	classicBP	5.231132546593826e-25	0.022232236500000002	1	-	-
pdb2eem	quaternionBP	1.5530632506809052e-21	0.149279771	1	7.679487354898964e-12	0.6764057803920531
pdb2eem	classicBP	1.9707309867033748e-22	0.15028950800000002	1	-	-
pdb2fxz	quaternionBP	8.122869346805305e-10	0.011341664000000001	1	4.938568031852048e-12	1.5665205740533317
pdb2fxz	classicBP quaternionBP	8.122879245966186e-10	0.011519333500000001	1 1	- 1.9157056722494177e-12	0.8160420619154118
pdb2g9l pdb2g9l	classicBP	5.977422428237824e-24 3.224045757396133e-24	$0.075847806 \\ 0.07646675600000001$	1	1.9157056722494177e-12	0.8160420619154118
pdb2g9i pdb2h5m	quaternionBP	3.715170248893378e-12	0.579691986	1	2.4650015237809485e-11	0.32129355674754834
pdb2h5m	classicBP	3.715161410683595e-12	0.581554499	1	2.40000102010004000-11	-
pdb2hep	quaternionBP	1.788245923717943e-20	0.272487972	ī	1.719684615174632e-11	0.6288150950017002
pdb2hep	classicBP	3.189147203639317e-21	0.27420141750000004	1	-	-
pdb2jmy	quaternionBP	3.342655685926916e-21	0.017076839	1	1.2262187901690759e-12	0.9564592135582028
pdb2jmy	classicBP	2.979722680770414e-21	0.017240172	1	-	-
pdb2jn5	quaternionBP	2.985474498101531e-13	0.013934159500000001	1	1.1243157201554841e-11	1.3474332628387042
pdb2jn5	classicBP	2.9854354070466307e-13	0.014121913000000002	1	<u>-</u>	.
pdb2jnk	quaternionBP	8.533347768218616e-12	1.5805696	1	2.5256292820499e-11	0.45095635143179713
pdb2jnk	classicBP quaternionBP	8.533347937509843e-12 1.655371742913786e-22	$1.5876972790000001 \\ 0.579891457$	1 1	- 4.973139106259666e-12	-0.2062789485101746
pdb2jpn pdb2jpn	classicBP	1.0486578855065648e-23	0.579891457	1	4.973139106259666e-12	-0.2062789485101746
pdb2jpn pdb2jua	quaternionBP	6.900146329234553e-18	0.6259969035	1	2.019961604395927e-11	0.30469679471825106
pdb2jua	classicBP	1.2314179921330559e-17	0.6279042960000001	1	2.0100010040000210-11	-
pdb2jvd	quaternionBP	4.314860264777377e-24	0.133405252	1	3.6251816085484465e-13	0.3687156184825513
pdb2jvd	classicBP	5.269559435470259e-24	0.133897138	1	-	-
pdb2jws	quaternionBP	8.553080616091689e-11	0.1797955705	1	1.084072286330415e-12	0.5196782642651332
pdb2jws	classicBP	8.553080614205863e-11	0.180729929	1	-	-
pdb2jwu	quaternionBP	6.307603314991057e-11	0.513705284	1	6.665180865359863e-12	0.30081343294103835
pdb2jwu	classicBP	6.308079196629333e-11	0.5152505785	1	-	-
pdb2jxf	quaternionBP	2.3490802413293615e-11	0.05317264	1	1.2542163437426709e-12	0.32999772063226906
pdb2jxf	classicBP	2.349080119271583e-11	0.053348108500000005	1	- 0.0070017017007: 10	-
pdb2jz5 pdb2jz5	quaternionBP classicBP	3.9153368239623524e-22 9.033100183907215e-23	$0.8399578615000001 \\ 0.839744212$	1 1	6.3878315815287e-13	-0.02543574026659945
pdb2j23 pdb2k2a	quaternionBP	2.7827008359579248e-24	0.263507901	1	2.828216415039424e-12	0.2607219735699662
pdb2k2a	classicBP	9.67400422980669e-24	0.264194924	1	2.0202104100004240-12	-
pdb2k36	quaternionBP	1.3091873348637108e-11	1.125178983	1	1.809663842480425e-12	1.5065692886302218
pdb2k36	classicBP	1.309187333454815e-11	1.142130584	1	-	-
pdb2k37	quaternionBP	6.702476626952505e-23	0.2079815385	1	2.591426907141696e-12	-0.14396878788355272
pdb2k37	classicBP	8.119007067636214e-23	0.20768211	1	-	-
pdb2k3i	quaternionBP	7.168156850054331e-22	0.9431735135	1	1.8934777949664748e-12	0.40290391381945234
pdb2k3i	classicBP	7.836263356046835e-22	0.9469735965	1	-	-
pdb2k6s	quaternionBP classicBP	1.1145164874053204e-22	2.810607124	1 1	2.3522297186503086e-12	1.9745533278595628
pdb2k6s pdb2kdh	quaternionBP	1.7104485241871e-22 1.9140073502257942e-10	$2.8661040605 \\ 0.401099953$	1	1.2342054163932629e-9	-1.1761731620048455
pdb2kdh	classicBP	1.9140973302237942e-10 1.9140941000662533e-10	0.401099933	1	1.2342034103932029e-9	1.1701731020048433
pdb2kdl	quaternionBP	5.5379601560224984e-11	0.485469482	1	3.8153650157514076e-12	-0.09187436420565742
pdb2kdl	classicBP	5.5379600134130046e-11	0.48502346	1	-	-
pdb2kdm	quaternionBP	6.081403212830075e-11	0.330752995	1	7.393557142348128e-12	0.46247200271007927
pdb2kdm	classicBP	6.081426754303088e-11	0.33228263500000005	1	-	-
pdb2kdp	quaternionBP	2.7249614421658224e-22	0.272919672	1	1.7048776299236185e-12	0.5038610774821706
pdb2kdp	classicBP	1.2853909120815096e-22	0.274294808	1	<u>-</u>	-
pdb2kdr	quaternionBP	3.104162513733105e-11	0.048883081	1	3.3411845462804327e-13	0.6745084255225242
pdb2kdr	classicBP	3.104162464014929e-11	0.0492128015	1 1	- 3.1744260925146267e-13	- 0 599974764407900
pdb2kes	quaternionBP	4.2005836499870455e-24	0.1570242885	1	3.174420U925146267e-13	0.523374764407869

pdb2kes	classicBP	3.820380350214722e-24	0.157846114	1	-	_
pdb2kjn	quaternionBP	7.889602043989169e-14	0.041935595000000006	1	1.3837857176585124e-12	0.7506379723478229
pdb2kjn	classicBP	7.88953141802611e-14 1.2390955810372933e-10	0.042250379500000004	1 1	9.375074704993017e-12	- 0.6397551469400131
pdb2kjo pdb2kjo	quaternionBP classicBP	1.2390955810372933e-10 1.2390961141445714e-10	$0.038195316 \\ 0.0384396725$	1	9.375074704993017e-12	0.6397551469400131
pdb2kl5	quaternionBP	1.2544502666644283e-22	0.667248754	1	3.1368230417247443e-12	0.43006284879476553
pdb2kl5	classicBP	3.622421465044811e-22	0.6701183430000001	i	-	-
pdb2klz	quaternionBP	9.390933564073206e-25	0.1335875635	1	4.631712818470438e-13	-0.2685298620630938
pdb2klz	classicBP	7.719962408380237e-25	0.13322884100000001	1	-	-
pdb2koz	quaternionBP	3.052197396220759e-10	0.06992923300000001	1	1.6248398679638628e-11	0.5460806355476411
pdb2koz	classicBP	3.052194694117852e-10	0.070311103	1	-	-
pdb2kp0	quaternionBP	1.4437105347376573e-11	0.21962782600000003	1	6.207906787878035e-11	0.20804740834614588
pdb2kp0	classicBP	1.4437105052227757e-11	0.22008475600000002	1	.	-
pdb2ksg	quaternionBP	9.981787925806465e-25	0.12212661000000001	1	6.164149051761021e-13	0.3302220539815215
pdb2ksg pdb2kt8	classicBP quaternionBP	1.069383060261906e-24 4.3311729236407237e-20	$0.12252989900000001 \\ 1.024673282$	1 1	- 4.904645474920241e-12	- 0.5161785803252661
pdb2kt8	classicBP	3.759854594269475e-20	1.024673282	1	4.904645474920241e-12	0.5101785803252001
pdb2kuh	quaternionBP	1.308553854127577e-24	0.23467166750000001	1	7.08764792059542e-13	0.6703442374439872
pdb2kuh	classicBP	4.4847284436353714e-24	0.2362447755	1	-	-
pdb2kwh	quaternionBP	1.2743400773879096e-22	0.186667855000000002	1	3.670309278980905e-12	0.5884183969435908
pdb2kwh	classicBP	1.1366517370764783e-23	0.187766243	1	-	-
pdb2kxa	quaternionBP	9.598280894182498e-11	0.0288556025	1	4.155165787008658e-12	0.8274770904540985
pdb2kxa	classicBP	9.598277951020082e-11	0.029094376	1	-	-
pdb2l3m	quaternionBP	2.8406616299871096e-21	0.25457254	1	6.066890623394196e-13	0.5485153661899167
pdb2l3m	classicBP	3.2843838957033104e-21	0.2559689095	1	-	-
pdb2l45 pdb2l45	quaternionBP classicBP	5.244075113072132e-25 2.5669220537994336e-25	0.0300912555 0.030161394	1 1	1.5900438222303643e-13	0.2330859873892699
pdb2l5r	quaternionBP	1.046367572549395e-24	0.034729866500000005	1	6.239391636957459e-13	0.8219899146459486
pdb2l5r pdb2l5r	classicBP	3.0442411725437176e-24	0.035015342500000005	1	0.239391030937439e-13	0.8219899140439480
pdb2l6q	quaternionBP	1.8811939383860744e-10	0.609508471	i	9.81361845728543e-10	0.2970247479956667
pdb2l6q	classicBP	1.8814398780837687e-10	0.6113188620000001	1	-	-
pdb2l6r	quaternionBP	4.110701391669899e-11	0.20660799800000001	1	1.874775136120748e-11	0.2894650767585327
pdb2l6r	classicBP	4.110719034027325e-11	0.207206056	1	-	-
pdb2l98	quaternionBP	5.265785041623191e-22	0.9327745675000001	1	3.2376438368987126e-11	0.15377804562621833
pdb2l98	classicBP	9.739013632079802e-20	0.93420897	1	<u>-</u>	.
pdb2lci	quaternionBP	2.9476459510315687e-22	1.100698841	1	8.26195777110584e-13	0.12545148123763727
pdb2lci	classicBP	6.860553433147958e-22	1.102079684	1 1	9 999709179097917, 19	0 154110441505000
pdb2lde pdb2lde	quaternionBP classicBP	9.21065225903535e-25 8.377812584284727e-25	0.037809557 0.0378678285	1	3.3385981589065917e-13	0.1541184415358332
pdb2le7	quaternionBP	3.8271434077095298e-25	0.0378678285	1	1.0977602186128373e-13	0.7137419055681438
pdb2le7	classicBP	1.152602513045891e-24	0.025943307500000002	1	-	-
pdb2ler	quaternionBP	7.513045672709397e-26	0.0088558125	1	4.8107748683337264e-14	0.6823541035901437
pdb2ler	classicBP	9.731895644314473e-26	0.0089162405	1	-	-
pdb2lgi	quaternionBP	3.8661260816807964e-21	0.34223577	1	5.458896793950659e-12	0.16989515736476335
pdb2lgi	classicBP	8.35974014170768e-21	0.34281721200000004	1	-	-
pdb2lhc	quaternionBP	1.4180058599681725e-10	0.204064134	1	1.2994296477838152e-9	0.9645972378468093
pdb2lhc	classicBP	1.4180992884129067e-10	0.20603253100000002	1	-	
pdb2lhd	quaternionBP	7.37707012988819e-21	2.353310517	1 1	2.5654543601052574e-11	0.15960422446876787
pdb2lhd pdb2lhe	classicBP quaternionBP	8.209848648913255e-21 1.0922308513770161e-17	$2.3570665 \\ 0.6118272690000001$	1	6.321667199665834e-12	0.19894863496185966
pdb2lhe	classicBP	1.1064922275537014e-17	0.613044491	1	0.321007199003834e-12	0.19694603490163900
pdb2lhg	quaternionBP	1.9040820003441288e-23	0.144911173	1	3.223253698477368e-13	0.26401000839320066
pdb2lhg	classicBP	2.1353772201510982e-23	0.145293753	1	-	-
pdb2lix	quaternionBP	5.759153737376175e-24	0.040848616500000004	1	1.4715339745208873e-12	0.6260346663148342
pdb2lix	classicBP	4.386101373318694e-23	0.041104343	1	-	-
pdb2lld	quaternionBP	1.1966430825800705 e-22	0.081288974	1	1.96018127803607e-12	0.20764501222514387
pdb2lld	classicBP	6.260335587133287e-22	0.0814577665	1		
pdb2lm9	quaternionBP	2.575290371553952e-23	0.499415563	1	7.984705413231344e-13	-0.22432981328617263
pdb2lm9	classicBP	1.7582939358547057e-23	0.498295225	1	-	-

pdb2lmf	quaternionBP	4.430122496591272 e-11	0.0303375245	1	$\mathbf{2.324774439826577e\text{-}12}$	0.7848910019009558
pdb2lmf	classicBP	4.4301228249469514e-11	0.030575641	1	-	-
pdb2ln3	quaternionBP	7.449495195280011e-23	0.38066323100000005	1	9.447887099252838e-14	0.45474105693175115
pdb2ln3	classicBP	1.9801111195341633e-22	0.382394263	1	= E 000/2271200201 = 12	0.25076467020261025
pdb2lo2 pdb2lo2	quaternionBP classicBP	5.148195618506491e-25 8.468912356040723e-25	$0.078651834 \\ 0.078934009$	1 1	5.08043271288201e-13	0.35876467928261935
pdb2lqp	quaternionBP	1.6244758377701022e-10	0.266346735	1	1.970236172584261e-11	0.23913827965640344
pdb2lqp	classicBP	1.6244858264708984e-10	0.266983672	1	1.3702301723342016-11	0.23313321303040344
pdb2lr0	quaternionBP	9.050891278097388e-20	1.3334368795	1	1.783701933024433e-11	0.0888341636721579
pdb2lr0	classicBP	1.0288914836901666e-19	1.334621427	î	-	-
pdb2lrh	quaternionBP	2.3347932666150142e-11	1.5372543220000001	1	4.170328869544027e-12	0.11501460589160573
pdb2lrh	classicBP	2.3347933177028843e-11	1.539022389	1	-	-
pdb2ls9	quaternionBP	2.5153821225411906e-23	0.0326867560000000004	1	6.971292417353479e-13	0.6816292812905633
pdb2ls9	classicBP	2.860226729381228e-23	0.032909558500000005	1	-	-
pdb2lsa	quaternionBP	5.35363409842568e-24	0.030418688000000003	1	3.48450695004645e-13	0.6542195376736837
pdb2lsa	classicBP	8.473088370132478e-25	0.030617693	1	-	-
pdb2lss	quaternionBP	3.382062007958243e-23	0.2332566395	1	3.68480438040615e-12	0.5140481756790605
pdb2lss	classicBP	1.966263466120689e-22	0.23445569100000002	1	.	.
pdb2lt3	quaternionBP	7.865984931733466e-23	0.56247374	1	3.4122877555074406e-13	1.008666644597489
pdb2lt3	classicBP	3.839281938021628e-23	0.568147225	1	-	-
pdb2lu6 pdb2lu6	quaternionBP classicBP	6.369687400749886e-26 3.602970837580234e-26	$0.0148167470000000002 \\ 0.015089451500000002$	1 1	1.9323963491154373e-14	1.840515330389314
pdb2lwa	quaternionBP	1.7731506033559633e-10	0.247305878	1	4.680930067286042e-12	-0.16167670709387183
pdb2lwa pdb2lwa	classicBP	1.7731500033339033e-10 1.773150087395255e-10	0.247303878	1	4.0809300072800426-12	-0.10107070709387183
pdb2lwa pdb2lx0	quaternionBP	6.785807869988942e-11	0.0583885665	1	1.947602783217816e-12	0.9199223961081637
pdb2lx0	classicBP	6.78579820793534e-11	0.05892569600000001	1	-	-
pdb2lxb	quaternionBP	2.240113647211788e-22	1.7040931250000002	1	2.443532480706581e-12	0.5862742976561197
pdb2lxb	classicBP	1.6656127813097087e-22	1.7140837850000001	1	-	-
pdb2lxy	quaternionBP	1.8048177304251087e-10	2.5397655985000003	1	3.825753705080231e-11	0.1382148613271017
pdb2lxy	classicBP	1.8048189273029898e-10	2.5432759320000002	1	-	-
pdb2lxz	quaternionBP	1.7970001288560598e-20	0.6825553335000001	1	8.045346345570714e-12	0.6889416534022308
pdb2lxz	classicBP	7.052338016674166e-21	0.6872577415000001	1	-	-
pdb2m1a	quaternionBP	1.7201867975893133e-26	0.052510157	1	1.3767494452416402e-13	0.555690587632407
pdb2m1a	classicBP	4.8814824981351604e-26	0.05280195100000001	1		-
pdb2m1j	quaternionBP	3.2818214786360974e-25	0.0509139885	1	5.465003717867574e-13	0.5916792395865844
pdb2m1j	classicBP	7.377897339225894e-25	0.051215236000000004	1	-	-
pdb2m2y	quaternionBP	1.3151717132444338e-22	0.0214676585	1 1	1.142715912366317e-12	0.9046864612645145
pdb2m2y pdb2m3f	classicBP quaternionBP	3.075891822875334e-23 1.6277525468915171e-24	0.0216618735 0.027876789000000003	1	3.2591966733066444e-13	0.9165797395101594
pdb2m3f	classicBP	4.0285346224450385e-25	0.028132302	1	3.2391900733000444e-13	0.9103797393101394
pdb2m8m	quaternionBP	9.789493810173846e-25	0.03825605	1	1.5744388778838934e-12	0.2225268944389347
pdb2m8m	classicBP	1.870465676721401e-24	0.03834118	1	-	-
pdb2m8o	quaternionBP	2.020234453671637e-25	0.036294466500000004	ī	2.0793277034853773e-13	0.8932890637750379
pdb2m8o	classicBP	1.2771632385078822e-25	0.036618681	1	_	-
pdb2m97	quaternionBP	1.5294032820071725e-23	0.21628721950000002	1	4.257587317315894e-12	0.790723327968057
pdb2m97	classicBP	8.7617579022944e-23	0.217997453	1	-	-
pdb2m9g	quaternionBP	7.823123574218431e-22	2.791190088	1	5.368874018341037e-12	0.5802537802649388
pdb2m9g	classicBP	4.010408220458125e-22	2.807386074	1	-	-
pdb2m9r	quaternionBP	3.184270965390626e-24	0.094303069	1	1.2995479105092582e-12	0.36168812279058216
pdb2m9r	classicBP	4.190203776038421e-24	0.09464415200000001	1	-	-
pdb2mdv	quaternionBP	3.890190146973147e-20	1.7829098790000002	1	3.0055524474079997e-12	0.2766441006410547
pdb2mdv	classicBP	2.3725178085037725e-20	1.7878421940000002	1	4 1 4 4 7 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	-
pdb2me1	quaternionBP	4.659721874233619e-23	0.0459728	1 1	4.164789824405079e-12	0.27930863467093836
pdb2me1 pdb2me2	classicBP quaternionBP	2.8584674281909754e-22 2.3162043193591404e-10	$0.046101206000000006 \ 0.0401405155$	1	- 1.8283198747857824e-12	0.2459098961995254
pdb2me2	classicBP	2.3162043193591404e-10 2.316204462696615e-10	0.0401405155	1	1.02001901410010240-12	-
pdb2me3	quaternionBP	1.7479948027933767e-10	0.040239225	1	2.5262537611960582e-12	0.2395727402597414
pdb2me3	classicBP	1.7479947637175985e-10	0.0379786355	1		-
pdb2me4	quaternionBP	1.4615857813261572e-10	0.0470804825	î	9.337599171311744e-13	0.8097198239206627
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pdb2me4	classicBP	1.461582776437341e-10	0.0474617025	1	-	-
pdb2mg1	quaternionBP	2.1848429804596495e-24	0.035171951	1	1.3041098618960734e-12	0.8134450659276871
pdb2mg1	classicBP	1.1247494698649372e-24	0.0354580555	1	-	-
pdb2mg2	quaternionBP	3.5299268464900037e-25	0.036397231	1	1.4276176722247105e-13	0.9577816510272452
pdb2mg2	classicBP	1.7068450170614242e-25	0.036745837	1	-	-
pdb2mg3	quaternionBP	3.332743839704663e-24	0.040072356	1	8.213076181909183e-13	0.9202665797838128
pdb2mg3	classicBP	6.270129875274045e-24	0.0404411285	1	-	-
pdb2mh8	quaternionBP	5.2091155204457464e-23	0.162588966	1	1.4712878415823763e-12	0.4260375208979372
pdb2mh8	classicBP	2.557777670433981e-23	0.163281656	1	-	-
pdb2mhw	quaternionBP	1.075722345491846e-23	0.0417920855	1	4.04883877201061e-13	0.687121727868778
pdb2mhw	classicBP	8.216652985444039e-24	0.042079248	1	-	-
pdb2mi1	quaternionBP	1.2508396495799117e-10	0.15746555250000002	1	3.256668259109923e-12	1.048315948340517
pdb2mi1	classicBP	1.250839748006101e-10	0.15911628900000002	1	-	-
pdb2mi7	quaternionBP	7.28608209025021e-11	0.22353935500000002	1	1.0261955501914293e-11	0.6416002229227002
pdb2mi7	classicBP	7.286076087855753e-11	0.224973584	1	-	-
pdb2mij	quaternionBP	2.702134458957159e-23	0.0739356115	1	3.583663441974677e-12	0.6822591843985926
pdb2mij	classicBP	2.7702339927355776e-23	0.07444004400000001	1	-	-
pdb2mix	quaternionBP	4.043175434187634e-24	0.02567677	1	2.254333276312768e-13	0.8062637940831285
pdb2mix	classicBP	2.3882325113803497e-24	0.025883792500000002	1	-	-
pdb2mj1	quaternionBP	2.9341503799459225e-23	0.0236367305	1	1.5286017275474824e-12	1.0678909251006674
pdb2mj1	classicBP	8.147708464257724e-24	0.023889145	1	-	-
pdb2mj2	quaternionBP	1.2522984413290332e-23	0.075095097	1	2.8887976078148686e-12	0.5664737339643011
pdb2mj2	classicBP	3.19881131696985e-23	0.07552049100000001	1	-	-
pdb2mjg	quaternionBP	1.0769702253260063e-23	1.2501263875000002	1	2.3581006178684174e-13	0.5128465860816833
pdb2mjg	classicBP	4.8763113402174173e-23	1.256537618	1	-	-
pdb2mji	quaternionBP	1.888391916316195e-11	0.9502635415	1	2.968848723717701e-11	0.5243585365944492
pdb2mji	classicBP	1.88839133585913e-11	0.9552463295000001	1	-	-
pdb2mle	quaternionBP	2.8018205595918246e-22	0.282848419	1	1.1518663648118488e-12	0.24311025051195756
pdb2mle	classicBP	2.7029671721378177e-22	0.2835360525	1	-	-
pdb2mlf	quaternionBP	5.9027099177828e-23	0.2897512365	ī	1.9392378640414637e-12	0.3206272771160368
pdb2mlf	classicBP	5.629638449353748e-23	0.290680258	1	-	-
pdb2mo5	quaternionBP	4.135599400244798e-14	1.6069250810000002	1	6.7951149738969e-11	0.19354978254892963
pdb2mo5	classicBP	4.135615325342054e-14	1.610035281	ī	-	-
pdb2mpu	quaternionBP	4.8446030455686197e-23	0.44423042450000005	1	9.046199940948068e-13	0.29674036880378285
pdb2mpu	classicBP	8.827363216907806e-23	0.4455486355	ī	-	-
pdb2mra	quaternionBP	4.0768398802580017e-22	1.163509377	1	1.2729668724871636e-11	-0.3083958815400245
pdb2mra	classicBP	1.1907735175568202e-20	1.159921162	1	-	-
pdb2msu	quaternionBP	1.121761134794237e-23	0.028573744	ī	8.784856203501941e-13	0.8274414441453715
pdb2msu	classicBP	1.4172121946592304e-23	0.028810175	1	-	-
pdb2mty	quaternionBP	3.669139379291979e-24	0.024416059	1	2.2229083961470215e-12	0.930307794554408
pdb2mty	classicBP	1.0025253111024564e-24	0.024643203500000002	1	-	-
pdb2muh	quaternionBP	9.400973651904422e-11	0.0311208445	i	9.066859920971527e-12	0.9724029179221105
pdb2muh	classicBP	9.400973616543583e-11	0.031423464500000005	1	-	-
pdb2mvj	quaternionBP	6.048581359257156e-23	0.0414284435	1	1.470651341360141e-11	0.7556523334022902
pdb2mvj	classicBP	3.303493563295339e-22	0.0417414985	1	-	-
pdb2mvt	quaternionBP	6.823574178734974e-11	0.1953587525	1	2.7781350276232936e-10	0.32650315987250433
pdb2mvt	classicBP	6.823986532968299e-11	0.19599660500000002	1	2.11010002102020000-10	-
pdb2n00	quaternionBP	4.942520292708914e-11	0.6827303475000001	1	3.078063067777792e-12	0.24575529799486517
pdb2n00	classicBP	4.94252015378427e-11	0.6844081935	1	0.0100000011111020-12	0.24010020100400011
pdb2n0b	quaternionBP	9.255382210917375e-10	0.0070135685	1	8.164066612440974e-13	1.0313294865516687
pdb2n0b	classicBP	9.255382306764167e-10	0.0070859015	i	-	-
pdb2n0c	quaternionBP	8.867752548585699e-10	0.0057347335	1	3.1194028607551117e-13	1.484672304301493
pdb2n0c	classicBP	8.867752455331119e-10	0.0058198755	1	-	1.404012004001400
pdb2n0d	quaternionBP	1.1848120985847436e-9	0.006292993	i	1.1993345731570002e-11	1.4415318752142303
pdb2n0d	classicBP	1.1848110341870683e-9	0.006383708500000001	1	-	-
pdb2n0e	quaternionBP	2.5028199136290067e-20	0.006575265	1	3.990193199943076e-12	1.138364765526556
pdb2n0e	classicBP	1.6305009302240652e-20	0.0066501155000000004	1	-	
pdb2n0f	quaternionBP	2.7978384522973375e-12	0.0071400955000000006	1	1.3315389117746868e-12	1.2853819672299815
pdb2n0f	classicBP	2.7978380568267388e-12	0.007231873000000001	1	00100001111400000-12	
Pubanoi	CIMBBICDI	2	3.337201373333333333	_	_	_

pdb2n0g	quaternionBP	4.723661150581371e-11	0.0073201385	1	$1.1667203360564295\mathrm{e}\text{-}11$	1.290508369479615
pdb2n0g pdb2n0h	classicBP quaternionBP	4.723663976786546e-11 4.8552566108719894e-11	$0.0074146055 \\ 0.00664365$	1 1	- 1.1609419459990784e-11	- 1.4657229083410606
pdb2n0h	classicBP	4.8552433976710044e-11	0.0064365	1	1.16094194599907846-11	1.4657229083410606
pdb2n35	quaternionBP	1.3887862278401277e-24	0.1385788375	1	1.2115960174772069e-12	1.3953425608726366
pdb2n35	classicBP	3.985308450619298e-24	0.14051248700000002	1	-	-
pdb2n41	quaternionBP	1.313569889459136e-22	0.7656463910000001	1	3.566670272302011e-13	0.36554355024707164
pdb2n41	classicBP	4.6283702014585724e-23	0.768445162	1	-	-
pdb2n4e	quaternionBP	7.882167445999888e-23	0.612717391	1	8.828727153549181e-13	0.42265831491634653
pdb2n4e	classicBP	2.2122199917912006e-22	0.615307092	1	-	-
pdb2n5q	quaternionBP	1.3369587983172227e-10	0.101776193	1	5.795010495824257e-12	0.47091366445588534
pdb2n5q	classicBP	1.3369580735256586e-10	0.102255471	1		-
pdb2n67	quaternionBP classicBP	1.1107668626135548e-21 1.0297687463658749e-21	$0.45927046800000004 \\ 0.46115388300000004$	1 1	4.633783062056966e-13	0.4100884187484999
pdb2n67 pdb2n6n	quaternionBP	6.3093612223520026e-12	0.16494233900000002	1	8.319583041132949e-12	0.46100716444914536
pdb2n6n	classicBP	6.309543013898909e-12	0.16570273500000002	1	G.5133G5041132343E-12	0.40100710444314550
pdb2n7i	quaternionBP	1.245260713554165e-11	0.0717497935	ī	1.4499347212609795e-11	0.5880888005622031
pdb2n7i	classicBP	1.2452627296095254e-11	0.07217174600000001	1	-	-
pdb2n7j	quaternionBP	9.10119749009651e-22	0.26501952700000003	1	9.784621222713522e-13	0.6877312100855182
pdb2n7j	classicBP	3.1152016814727277e-22	0.26684214900000003	1	-	-
pdb2na9	quaternionBP	8.60962020463049e-24	0.10185692800000001	1	1.0477949504643867e-12	0.5918684294111021
pdb2na9	classicBP	2.7343495975352924e-23	0.10245978700000001	1	.	-
pdb2ndc	quaternionBP	7.826031466935287e-25	0.0236627165	1	5.787646313490375e-13	0.8074622370597417
pdb2ndc	classicBP quaternionBP	5.632568199816525e-25 8.569658921389604e-24	$0.023853784000000003 \ 0.0183223175$	1 1	- 8.187040163300699e-13	0.8136961931807907
pdb2nde pdb2nde	classicBP	7.158958169501306e-24	0.0183223175	1	8.1870401033000996-13	0.8136961931807907
pdb2ndk	quaternionBP	3.1062064156716694e-10	0.12136477700000001	1	1.5146738315811914e-11	0.3467175653443455
pdb2ndk	classicBP	3.106206498711846e-10	0.12178557000000001	1	-	-
pdb2nvj	quaternionBP	5.5626249032882695e-25	0.0324139275	1	5.867074942784013e-14	0.3890518975215196
pdb2nvj	classicBP	4.3261559384089e-24	0.0325400345	1	-	-
pdb2p6j	quaternionBP	8.387499193494184e-24	0.15153217900000002	1	1.709869637933372e-13	0.31730818046245
pdb2p6j	classicBP	4.017175267102306e-24	0.152013003	1	-	-
pdb2p81	quaternionBP	2.120577994197325e-10	0.097556393	1	8.971861854043987e-12	0.2894817974666175
pdb2p81	classicBP	2.1205783292796826e-10	0.097838801	1		-
pdb2rlg	quaternionBP	1.4600010245975236e-24	0.0216180745	1	6.734563911692263e-13	0.8503393768950263
pdb2rlg pdb2rlh	classicBP quaternionBP	8.366663027931146e-25 3.475860655263986e-24	$0.021801901500000002 \\ 0.023478595$	1 1	1 0799678915776969- 19	0.9202765327311901
pdb2rlh pdb2rlh	classicBP	1.0864915623111197e-23	0.023478395	1	1.0732678215776362e-12	0.9202765327311901
pdb2rmy	quaternionBP	4.8285457949464115e-11	0.07103345100000001	i	1.7484112630780071e-12	0.5957960567057219
pdb2rmy	classicBP	4.8285457373367735e-11	0.0714566655	ī	-	-
pdb2rnd	quaternionBP	7.832826504970844e-23	0.067940002	1	5.111678892314032e-12	0.6781071334086786
pdb2rnd	classicBP	6.754057259779204e-23	0.068400708	1	-	-
pdb2roo	quaternionBP	4.5159194691427756e-20	0.6903075505	1	5.3127370929753114e-12	1.168150774847998
pdb2roo	classicBP	3.6735599803150186e-20	0.6983713835	1	.	.
pdb2rql	quaternionBP	7.43919904417169e-12	2.4026374400000003	1	6.257030031837628e-11	0.48561263575412905
pdb2rql	classicBP	7.439108769153852e-12	2.414304951	1 1	1 0510646055005006 10	0 5000500150000550
pdb2rut pdb2rut	quaternionBP classicBP	3.2265610368197994e-24 1.3048785297508909e-24	$0.07545120350000001 \\ 0.075828956$	1	1.0519646975025026e-12	0.5006580179996556
pdb2ruv	quaternionBP	1.727953418535442e-23	0.073828936	1	1.2232161849714364e-12	1.7403657108695736
pdb2ruv	classicBP	6.722535677730531e-23	0.08248492	1	-	-
pdb2rux	quaternionBP	1.20732424369393e-24	0.081629671	1	9.359110200170622e-14	0.5773795168180884
pdb2rux	classicBP	7.499618835092046e-25	0.082100984	1	-	-
pdb2ruy	quaternionBP	4.030585055886253e-25	0.082370047	1	1.1710502970090598e-12	0.5572596067597413
pdb2ruy	classicBP	6.5846684212202e-25	0.08282906200000001	1	-	
pdb2rv3	quaternionBP	3.083963657657395e-24	0.08271075700000001	1	8.51386815179583e-13	0.8592939126406351
pdb2rv3	classicBP	3.543480555966174e-24	0.0834214855	1	1 0050011000465605 10	0.4059051490905050
pdb2rv5	quaternionBP classicBP	1.0345365949172394e-25 2.4142815182945916e-25	$0.0713397775 \\ 0.071628937$	1 1	1.3358211900467637e-13	0.4053271682827875
pdb2rv5 pdb2y4q	quaternionBP	2.4142815182945916e-25 2.6868916573064497e-11	1.1112611730000002	1	2.2850202811825207e-11	0.639469386014424
pubzyaq	quater monbr	2.00000100100044076-11	1.1112011130000002	1	2.200202011020207e=11	0.00040000014424

pdb2y4q classicBP 2.68689337779516e-11 1.118367348 1 -

Operation results:

D I. I	7.54	4		1.16	D l.	D	T	T
Problem pdb1a57	Mt.	op. nodes [1075505, 1578784, 48788, 121970]	op. virtual path [601804, 750082, 28540, 71350]	op. ddf [70094, 45984, 0, 0]	Branch 10123	Prune 9819	Improv. nop	Improv. total 25.165882195942224
pdb1a57	q c	[1243056, 2097785, 121971, 73183]	[647078, 1105566, 71350, 42810]	[70094, 45984, 0, 0]	10123	9819	[15.5788, 32.8735, 150.002, -39.9992]	25.105882195942224
pdb1ba5	q	[72313, 106219, 3310, 8275]	[38858, 48441, 1838, 4595]	[5212, 3382, 0, 0]	735	637	[15.4426, 32.8228, 150.03, -39.9879]	25.083501212411296
pdb1ba5	c c	[83480, 141083, 8276, 4966]	[41875, 71478, 4595, 2757]	[5212, 3382, 0, 0]	735	637	[10.4420, 02.0220, 100.00, -00.0010]	-
pdb1d1n	q	[112771, 165959, 5310, 13275]	[62720, 78222, 2948, 7370]	[8136, 5214, 0, 0]	1180	831	[15.3887, 33.2305, 150.019, -39.9925]	25.279585624674162
pdb1d1n	c	[130125, 221108, 13276, 7966]	[67954, 115731, 7370, 4422]	[8136, 5214, 0, 0]	1180	831	-	-
pdb1dp3	q	[147039, 215989, 6738, 16845]	[78906, 98399, 3714, 9285]	[10096, 6566, 0, 0]	1511	1271	[15.6047, 32.9883, 150.015, -39.9941]	25.236478010196308
pdb1dp3	c	[169984, 287240, 16846, 10108]	[85389, 145497, 9285, 5571]	[10096, 6566, 0, 0]	1511	1271	-	-
pdb1du1	\mathbf{q}	$[22753,\ 33502,\ 1080,\ 2700]$	[12578, 15689, 590, 1475]	[1444, 930, 0, 0]	244	159	$[15.3298,\ 33.2965,\ 150.093,\ -39.963]$	25.293578745731658
pdb1du1	c	[26241, 44657, 2701, 1621]	[13651, 23232, 1475, 885]	[1444, 930, 0, 0]	244	159		-
pdb1eii	\mathbf{q}	[231172, 339916, 10752, 26880]	[129590, 161585, 6110, 15275]	[16361, 10551, 0, 0]	2320	1836	[15.466, 33.132, 150.009, -39.9963]	25.25824681298463
pdb1eii	C	[266925, 452537, 26881, 16129]	[140035, 238755, 15275, 9165]	[16361, 10551, 0, 0]	2320	1836	[15 0000 00 0155 150 000 00 0055]	- 05 010000045456510
pdb1fcl	q	[358787, 526695, 16286, 40715] [414889, 700070, 40716, 24430]	[197840, 246634, 9356, 23390] [213238, 363957, 23390, 14034]	[25630, 16680, 0, 0]	$\frac{3464}{3464}$	$3255 \\ 3255$	[15.6366, 32.9175, 150.006, -39.9975]	25.212338047476713
pdb1fcl pdb1fd6	c q	[158833, 233386, 7312, 18280]	[88618, 110483, 4186, 10465]	[25630, 16680, 0, 0] [10799, 7015, 0, 0]	1562	1339	[15.522, 33.0294, 150.014, -39.9945]	25.226238658149256
pdb1fd6	c c	[183487, 310472, 18281, 10969]	[95609, 163119, 10465, 6279]	[10799, 7015, 0, 0]	1562	1339	[10.022, 00.0204, 100.014, -00.0040]	25.22025655145256
pdb1i2u	q	[54060, 79562, 2548, 6370]	[30158, 37611, 1418, 3545]	[3796, 2436, 0, 0]	564	396	[15.37, 33.2345, 150.039, -39.9843]	25.275010523361875
pdb1i2u	c	[62369, 106004, 6371, 3823]	[32665, 55638, 3545, 2127]	[3796, 2436, 0, 0]	564	396	[10:01, 00:2010, 100:000, 00:0010]	-
pdb1i2v	q	[60273, 88580, 2780, 6950]	[32674, 40731, 1546, 3865]	[4416, 2854, 0, 0]	616	511	[15.3502, 32.8584, 150.036, -39.9856]	25.065738446113393
pdb1i2v	ć	[69525, 117686, 6951, 4171]	[35201, 60093, 3865, 2319]	[4416, 2854, 0, 0]	616	511	-	-
pdb1jlz	\mathbf{q}	[27214, 40054, 1284, 3210]	[15072, 18798, 708, 1770]	[1778, 1146, 0, 0]	287	198	[15.3671, 33.2426, 150.078, -39.9688]	25.27939578049665
pdb1jlz	c	[31396, 53369, 3211, 1927]	[16338, 27819, 1770, 1062]	$[1778, \ 1146, \ 0, \ 0]$	287	198	-	-
pdb1jw3	\mathbf{q}	[285565, 419767, 13222, 33055]	[159796, 199238, 7540, 18850]	[19714, 12760, 0, 0]	2840	2329	[15.4935, 33.0893, 150.008, -39.997]	25.246504499014776
pdb1jw3	c	[329809, 558665, 33056, 19834]	[172562, 294294, 18850, 11310]	[19714, 12760, 0, 0]	2840	2329	-	
pdb1k0v	\mathbf{q}	[83918, 123529, 3966, 9915]	[46474, 57965, 2182, 5455]	[5864, 3760, 0, 0]	891	604	[15.365, 33.2578, 150.025, -39.9899]	25.28464541314248
pdb1k0v	c	[96812, 164612, 9916, 5950]	[50399, 85800, 5455, 3273]	[5864, 3760, 0, 0]	891 1999	$604 \\ 1825$	[15 500 00 0505 150 01 00 0050]	-
pdb1k37 pdb1k37	q c	$[208553, 306299, 9534, 23835] \ [241008, 407294, 23836, 14302]$	[116942, 145777, 5534, 13835] [125971, 215061, 13835, 8301]	[13455, 8803, 0, 0] [13455, 8803, 0, 0]	1999	1825	[15.562, 32.9727, 150.01, -39.9958]	25.212277530411995
pdb1kuw	q	[10967, 16146, 520, 1300]	[6132, 7648, 288, 720]	[747, 479, 0, 0]	115	77	[15.3278, 33.3086, 150.192, -39.9231]	25.303286904227008
pdb1kuw	c c	[12648, 21524, 1301, 781]	[6648, 11319, 720, 432]	[747, 479, 0, 0]	115	77	[10.0210, 00.0000, 100.102, -00.0201]	-
pdb1kz0	q	[16892, 24881, 806, 2015]	[9456, 11794, 444, 1110]	[1114, 714, 0, 0]	180	114	[15.2557, 33.3266, 150.124, -39.9504]	25.28142799479751
pdb1kz0	c	[19469, 33173, 2016, 1210]	[10254, 17457, 1110, 666]	[1114, 714, 0, 0]	180	114	-	-
pdb1kz2	\mathbf{q}	[18087, 26639, 862, 2155]	[10212, 12736, 480, 1200]	[1258, 804, 0, 0]	190	123	[15.2596, 33.3233, 150.116, -39.9536]	25.2811930544792
pdb1kz2	c	[20847, 35516, 2156, 1294]	[11064, 18843, 1200, 720]	[1258, 804, 0, 0]	190	123	-	-
pdb1kz5	\mathbf{q}	$[13262,\ 19532,\ 632,\ 1580]$	$[7492,\ 9344,\ 352,\ 880]$	[850,546,0,0]	139	90	[15.2767, 33.3453, 150.158, -39.9367]	25.301376906815975
pdb1kz5	c	[15288, 26045, 1581, 949]	$[8120,\ 13827,\ 880,\ 528]$	[850, 546, 0, 0]	139	90		-
pdb1lvz	\mathbf{q}	[11289, 16635, 542, 1355]	[6308, 7868, 296, 740]	[743, 475, 0, 0]	122	73	[15.1829, 33.3574, 150.185, -39.9262]	25.270782334596433
pdb1lvz	c	[13003, 22184, 1356, 814]	[6844, 11649, 740, 444]	[743, 475, 0, 0]	122	73	[15 0410 00 0500 150 100 00 0500]	- 0F 000014046604F0F
pdb1m4e pdb1m4e	q c	[20709, 30494, 984, 2460] $[23886, 40664, 2461, 1477]$	$[11672, 14558, 548, 1370] \ [12658, 21549, 1370, 822]$	[1348, 866, 0, 0] [1348, 866, 0, 0]	$\frac{217}{217}$	$\frac{143}{143}$	[15.3412, 33.3508, 150.102, -39.9593]	25.328014346624705
pdb1m4e pdb1ma2	q	[185593, 272290, 8352, 20880]	[99864, 124506, 4716, 11790]	[13505, 8805, 0, 0]	1817	1755	[15.736, 32.8561, 150.012, -39.9952]	25.219301397000706
pdb1ma2	c c	[214798, 361754, 20881, 12529]	[107766, 183843, 11790, 7074]	[13505, 8805, 0, 0]	1817	1755	[10.700, 02.0001, 100.012, -00.0002]	23.213301337000700
pdb1ma4	q	[54758, 80427, 2506, 6265]	[30240, 37702, 1428, 3570]	[3356, 2204, 0, 0]	538	476	$[15.5831,\ 32.9914,\ 150.04,\ -39.984]$	25.231320681319303
pdb1ma4	c	[63291, 106961, 6266, 3760]	[32634, 55671, 3570, 2142]	[3356, 2204, 0, 0]	538	476	-	-
pdb1ma5	q	[18133, 26693, 858, 2145]	[10098, 12595, 474, 1185]	[1199, 771, 0, 0]	191	129	[15.3698, 33.3009, 150.117, -39.9534]	25.313094566058258
pdb1ma5	c	[20920, 35582, 2146, 1288]	[10953, 18645, 1185, 711]	[1199, 771, 0, 0]	191	129	-	-
pdb1ma6	\mathbf{q}	$[16775,\ 24703,\ 798,\ 1995]$	[9304, 11606, 436, 1090]	[1180, 754, 0, 0]	180	115	$[15.3443,\ 33.3522,\ 150.125,\ -39.9499]$	25.330351697499488
pdb1ma6	c	[19349, 32942, 1996, 1198]	[10106, 17193, 1090, 654]	[1180, 754, 0, 0]	180	115		-
pdb1nd9	\mathbf{q}	[182542, 268151, 8370, 20925]	[102530, 127815, 4850, 12125]	[13437, 8691, 0, 0]	1759	1572	[15.5416, 32.9993, 150.012, -39.9952]	25.21833879180313
pdb1nd9	C	[210912, 356639, 20926, 12556]	[110485, 188595, 12125, 7275]	[13437, 8691, 0, 0]	1759	1572	[15 4000 00 0004 150 000 00 0005]	-
pdb1ne5	q	[92881, 136525, 4298, 10745]	[51636, 64382, 2436, 6090] [55770, 95106, 6090, 2654]	[6676, 4310, 0, 0]	930 930	$761 \\ 761$	[15.4886, 33.0694, 150.023, -39.9907]	25.234302451636136
pdb1ne5 pdb1nmj	c q	$[107267, 181673, 10746, 6448] \ [32225, 47349, 1482, 3705]$	$[55770, 95106, 6090, 3654] \ [17268, 21528, 816, 2040]$	[6676, 4310, 0, 0] [2392, 1546, 0, 0]	930 332	277	[15.4042, 32.856, 150.067, -39.973]	- 25.08700935571784
pdb1nmj	c c	[37189, 62906, 3706, 2224]	[18624, 31779, 2040, 1224]	[2392, 1546, 0, 0]	332	277	[10.1012, 02.000, 100.001, 900.010]	
pdb1o53	q	[17837, 26253, 842, 2105]	[9922, 12375, 466, 1165]	[1209, 777, 0, 0]	187	129	[15.3781, 33.2724, 150.119, -39.9525]	25.3013585050067
-	-							

		[00700 04000 0100 1004]	[10777 10017 1107 000]	[1900 777 0 0]	105	100		
pdb1o53 pdb1oqp	c q	[20580, 34988, 2106, 1264] [402820, 591731, 18466, 46165]	[10757, 18315, 1165, 699] $[225580, 281208, 10672, 26680]$	[1209, 777, 0, 0] [27553, 17923, 0, 0]	$\frac{187}{3896}$	$\frac{129}{3478}$	[15.5318, 32.9815, 150.005, -39.9978]	- 25.20454463916495
pdb1oqp	c c	[465385, 786893, 46166, 27700]	[243056, 414909, 26680, 16008]	[27553, 17923, 0, 0]	3896	3478	[13.3316, 32.3613, 130.003, -33.3316]	20.20404403010400
pdb1plw	q	[5368, 7901, 254, 635]	[2984, 3722, 140, 350]	[318, 206, 0, 0]	56	38	[15.3689, 33.3376, 150.394, -39.8425]	25.342562508828937
pdb1plw	c	[6193, 10535, 636, 382]	[3238, 5511, 350, 210]	[318, 206, 0, 0]	56	38	-	-
pdb1plx	\mathbf{q}	[4962, 7306, 236, 590]	[2732, 3408, 128, 320]	[294, 190, 0, 0]	53	34	$[15.3164,\ 33.3561,\ 150.424,\ -39.8305]$	25.33221322743242
pdb1plx	c	[5722, 9743, 591, 355]	[2968, 5049, 320, 192]	[294, 190, 0, 0]	53	34	·	-
pdb1pv0	\mathbf{q}	[61888, 91108, 2928, 7320]	[34756, 43342, 1636, 4090]	[4104, 2640, 0, 0]	645	444	[15.2954, 33.2287, 150.034, -39.9863]	25.241969076964544
pdb1pv0 pdb1r57	c	[71354, 121382, 7321, 4393] [158136, 232630, 7404, 18510]	[37610, 64086, 4090, 2454] $[89036, 111022, 4196, 10490]$	$[4104, 2640, 0, 0] \ [10868, 7004, 0, 0]$	$645 \\ 1603$	$\frac{444}{1208}$	[15 4045 99 179 150 014 90 0046]	- 25.258231736584435
pdb1r57	q c	[182496, 309812, 18511, 11107]	[96250, 164076, 10490, 6294]	[10868, 7004, 0, 0]	1603	1208	[15.4045, 33.178, 150.014, -39.9946]	25.258231736584435
pdb1ry3	q	[83935, 123545, 3962, 9905]	[46616, 58136, 2192, 5480]	[5516, 3554, 0, 0]	884	611	[15.3333, 33.2138, 150.025, -39.9899]	25.24859157792967
pdb1ry3	c	[96805, 164579, 9906, 5944]	[50488, 85998, 5480, 3288]	[5516, 3554, 0, 0]	884	611	-	-
pdb1s4h	q	[12659, 18641, 602, 1505]	[7000, 8732, 328, 820]	[792, 510, 0, 0]	136	87	[15.3409, 33.3459, 150.166, -39.9336]	25.327027269733883
pdb1s4h	c	[14601, 24857, 1506, 904]	[7604, 12936, 820, 492]	[792, 510, 0, 0]	136	87	-	-
pdb1s4j	\mathbf{q}	$[14540,\ 21404,\ 688,\ 1720]$	$[8046,\ 10035,\ 378,\ 945]$	[959, 617, 0, 0]	154	104	[15.3164, 33.2461, 150.145, -39.9419]	25.2633500208594
pdb1s4j	С	[16767, 28520, 1721, 1033]	[8721, 14850, 945, 567]	[959, 617, 0, 0]	154	104	·	-
pdb1s6j	\mathbf{q}	[394887, 580010, 18072, 45180]	[221362, 275947, 10474, 26185]	[27462, 17852, 0, 0]	3798	3437	[15.5518, 32.9777, 150.006, -39.9978]	25.210639320559956
pdb1s6j	c	[456299, 771284, 45181, 27109]	[238481, 407121, 26185, 15711]	[27462, 17852, 0, 0]	$3798 \\ 1263$	$\frac{3437}{901}$	[15 4096 33 335 150 019 30 003]	- -
pdb1sa8 pdb1sa8	q	$[121121, 178227, 5694, 14235] \ [139784, 237443, 14236, 8542]$	$[67354, 84001, 3166, 7915] \ [72971, 124278, 7915, 4749]$	[8646, 5548, 0, 0] $[8646, 5548, 0, 0]$	1263	901	[15.4086, 33.225, 150.018, -39.993]	25.284627455156496
pdb1t2y	c q	[29441, 43338, 1392, 3480]	[16508, 20588, 776, 1940]	[1956, 1258, 0, 0]	307	211	[15.3493, 33.2733, 150.072, -39.9713]	25.288792159791896
pdb1t2y	c c	[33960, 57758, 3481, 2089]	[17884, 30459, 1940, 1164]	[1956, 1258, 0, 0]	307	211	[10.0400, 00.2100, 100.012, -00.0110]	-
pdb1t5q	q	[29751, 43850, 1432, 3580]	[16746, 20887, 786, 1965]	[2034, 1296, 0, 0]	322	189	[15.1659, 33.3729, 150.07, -39.9721]	25.26808543116279
pdb1t5q	c	[34263, 58484, 3581, 2149]	[18165, 30921, 1965, 1179]	[2034, 1296, 0, 0]	322	189	-	-
pdb1tot	q	[57692, 84825, 2678, 6695]	[31086, 38753, 1470, 3675]	[4369, 2811, 0, 0]	603	474	[15.2673, 32.8653, 150.037, -39.9851]	25.035881229837376
pdb1tot	c	[66500, 112703, 6696, 4018]	[33507, 57189, 3675, 2205]	[4369, 2811, 0, 0]	603	474	-	-
pdb1v6r	\mathbf{q}	$[23891,\ 35182,\ 1136,\ 2840]$	$[13410,\ 16725,\ 630,\ 1575]$	$[1490,\ 960,\ 0,\ 0]$	252	165	$[15.2945,\ 33.3096,\ 150.088,\ -39.9648]$	25.286681787181408
pdb1v6r	c	[27545, 46901, 2841, 1705]	[14535, 24750, 1575, 945]	[1490, 960, 0, 0]	252	165	-	
pdb1v92	\mathbf{q}	[53225, 78384, 2532, 6330]	[29918, 37313, 1406, 3515]	[3727, 2383, 0, 0]	562	367	[15.2823, 33.3002, 150.039, -39.9842]	25.274967786945357
pdb1v92	c	[61359, 104486, 6331, 3799]	$[32419, 55209, 3515, 2109] \ [13924, 17370, 652, 1630]$	[3727, 2383, 0, 0]	$\frac{562}{282}$	$\frac{367}{185}$	[15 2700 22 2522 150 002 20 0072]	-
pdb1vd7 pdb1vd7	q c	$[25761, 37921, 1218, 3045] \ [29723, 50531, 3046, 1828]$	[15134, 25740, 1630, 978]	$[1760, 1130, 0, 0] \ [1760, 1130, 0, 0]$	282 282	185	$[15.3798,\ 33.2533,\ 150.082,\ -39.9672]$	25.289572448303765
pdb1vd9	q	[34573, 50857, 1618, 4045]	[19090, 23807, 898, 2245]	[2345, 1513, 0, 0]	359	265	[15.4195, 33.1655, 150.062, -39.9753]	25.258801444677424
pdb1vd9	c	[39904, 67724, 4046, 2428]	[20669, 35211, 2245, 1347]	[2345, 1513, 0, 0]	359	265	[10/1100, 00/1000, 100/002, 00/0/00]	-
pdb1vdb	q	[24217, 35672, 1156, 2890]	[13320, 16616, 624, 1560]	[1678, 1072, 0, 0]	265	163	$[15.2827,\ 33.3287,\ 150.087,\ -39.9654]$	25.291311488230228
pdb1vdb	c	[27918, 47561, 2891, 1735]	[14472, 24618, 1560, 936]	[1678, 1072, 0, 0]	265	163	· ·	-
pdb1vpc	\mathbf{q}	[50098, 73589, 2294, 5735]	[26676, 33258, 1260, 3150]	[3900, 2516, 0, 0]	516	440	$[15.4637,\ 32.8378,\ 150.044,\ -39.9826]$	25.100215615414978
pdb1vpc	c	[57845, 97754, 5736, 3442]	[28782, 49104, 3150, 1890]	[3900, 2516, 0, 0]	516	440	- ·	-
pdb1wnk	\mathbf{q}	[25548, 37634, 1220, 3050]	[14190, 17699, 666, 1665]	[1752, 1120, 0, 0]	276	172	[15.238, 33.305, 150.082, -39.9672]	25.26092628832355
pdb1wnk	С	[29441, 50168, 3051, 1831]	[15393, 26202, 1665, 999]	[1752, 1120, 0, 0]	276	172	-	-
pdb1wo4 pdb1wo4	q c	[184499, 270849, 8378, 20945] [213327, 360005, 20946, 12568]	[102052, 127218, 4828, 12070] [109958, 187704, 12070, 7242]	[12556, 8202, 0, 0] [12556, 8202, 0, 0]	$1774 \\ 1774$	$1671 \\ 1671$	[15.625, 32.9172, 150.012, -39.9952]	25.20782138811688
pdb1wo5	q	[60630, 89098, 2796, 6990]	[33234, 41441, 1566, 3915]	[4111, 2669, 0, 0]	614	506	[15.5385, 33.049, 150.036, -39.9857]	25.243552290081126
pdb1wo5	c c	[70051, 118544, 6991, 4195]	[35931, 61248, 3915, 2349]	[4111, 2669, 0, 0]	614	506	[10.0000, 00.040, 100.000, -00.0001]	-
pdb1y5c	q	[11134, 16392, 528, 1320]	[6182, 7711, 290, 725]	[673, 435, 0, 0]	118	78	[15.3494, 33.3211, 150.189, -39.9242]	25.318308708381565
pdb1y5c	c	[12843, 21854, 1321, 793]	[6709, 11418, 725, 435]	[673, 435, 0, 0]	118	78	-	-
pdb1yx8	\mathbf{q}	[416113, 610725, 18826, 47065]	[227756, 283904, 10784, 26960]	[31578, 20488, 0, 0]	4020	3853	$[15.614,\ 32.8388,\ 150.005,\ -39.9979]$	25.161041758752624
pdb1yx8	c	[481085, 811280, 47066, 28240]	[245224, 418737, 26960, 16176]	$[31578,\ 20488,\ 0,\ 0]$	4020	3853		-
pdb1yxr	\mathbf{q}	[184400, 271010, 8516, 21290]	[102476, 127776, 4832, 12080]	[13594, 8766, 0, 0]	1841	1524	[15.5347, 33.0818, 150.012, -39.9953]	25.25905988260899
pdb1yxr	c	[213046, 360665, 21291, 12775]	[110728, 188793, 12080, 7248]	[13594, 8766, 0, 0]	1841	1524	[17 0041 00 10 170 017 00 0000]	-
pdb2a4j pdb2a4j	q	$[126900, 186740, 5968, 14920] \ [146397, 248663, 14921, 8953]$	[69102, 86185, 3246, 8115] [74907, 127545, 8115, 4869]	[8068, 5220, 0, 0] [8068, 5220, 0, 0]	$1360 \\ 1360$	$948 \\ 948$	[15.3641, 33.16, 150.017, -39.9933]	25.231370767170457
pdb2a4j pdb2ajj	c q	[30361, 44738, 1456, 3640]	[16986, 21185, 798, 1995]	[1994, 1276, 0, 0]	328	199	[15.1642, 33.3073, 150.069, -39.9725]	25.232246399401447
pdb2ajj pdb2ajj	q c	[34965, 59639, 3641, 2185]	[18411, 31350, 1995, 1197]	[1994, 1276, 0, 0]	328	199	[10.1042, 00.0010, 100.000, 400.0120]	
pdb2ajm	q	[32326, 47620, 1544, 3860]	[18044, 22504, 848, 2120]	[2143, 1373, 0, 0]	347	218	[15.2014, 33.278, 150.065, -39.9741]	25.231400117164625
pdb2ajm	c	[37240, 63467, 3861, 2317]	[19552, 33297, 2120, 1272]	[2143, 1373, 0, 0]	347	218	-	-
pdb2ajn	\mathbf{q}	[32102, 47296, 1536, 3840]	[17994, 22441, 846, 2115]	[2074, 1330, 0, 0]	344	214	$[15.1735,\ 33.284,\ 150.065,\ -39.974]$	25.223535517965413
pdb2ajn	c	[36973,63038,3841,2305]	$[19491,\ 33198,\ 2115,\ 1269]$	$[2074,\ 1330,\ 0,\ 0]$	344	214	-	-

pdb2ajo	\mathbf{q}	[32326, 47620, 1544, 3860]	$[18044,\ 22504,\ 848,\ 2120]$	$[2143,\ 1373,\ 0,\ 0]$	347	218	$[15.2014,\ 33.278,\ 150.065,\ -39.9741]$	25.231400117164625
pdb2ajo	c	[37240, 63467, 3861, 2317]	[19552, 33297, 2120, 1272]	[2143, 1373, 0, 0]	347	218	-	
pdb2akk	q	[237702, 349208, 10912, 27280]	[133324, 166208, 6304, 15760]	[16449, 10683, 0, 0]	2303 2303	$2034 \\ 2034$	[15.5379, 33.0104, 150.009, -39.9963]	25.22260367108089
pdb2akk pdb2c0s	c q	$[274636, 464483, 27281, 16369] \ [75076, 110278, 3436, 8590]$	$[143720, 245289, 15760, 9456] \ [39764, 49572, 1880, 4700]$	[16449, 10683, 0, 0] [5989, 3859, 0, 0]	2303 777	664	[15.4217, 32.7817, 150.029, -39.9884]	25.05269024217245
pdb2c0s	c c	[86654, 146429, 8591, 5155]	[42868, 73161, 4700, 2820]	[5989, 3859, 0, 0]	777	664	[10.4217, 02.7017, 100.020, -00.0004]	-
pdb2dci	q	[19403, 28589, 930, 2325]	[10828, 13506, 508, 1270]	[1332, 850, 0, 0]	210	127	[15.2141, 33.3485, 150.108, -39.957]	25.275625890296016
pdb2dci	c	[22355, 38123, 2326, 1396]	[11750, 19998, 1270, 762]	[1332, 850, 0, 0]	210	127	-	-
pdb2eem	\mathbf{q}	$[83265,\ 122375,\ 3846,\ 9615]$	[46702, 58225, 2206, 5515]	$[5369,\ 3497,\ 0,\ 0]$	819	689	$[15.4915,\ 33.0582,\ 150.026,\ -39.9896]$	25.229916796363327
pdb2eem	c	[96164, 162830, 9616, 5770]	[50387, 85965, 5515, 3309]	[5369, 3497, 0, 0]	819	689	[-	
pdb2fxz pdb2fxz	q	$[14787, 21768, 700, 1750] \ [17059, 29015, 1751, 1051]$	[8146, 10161, 382, 955]	[1050, 672, 0, 0] [1050, 672, 0, 0]	$158 \\ 158$	$\frac{105}{105}$	[15.3648, 33.292, 150.143, -39.9429]	25.307011921548515
pdb2ixz pdb2g9l	c q	[41131, 60598, 1968, 4920]	[8843, 15048, 955, 573] $[23232, 28974, 1092, 2730]$	[2808, 1794, 0, 0]	437	273	[15.2075, 33.3245, 150.051, -39.9797]	25.258477033981784
pdb2g9l	c c	[47386, 80792, 4921, 2953]	[25170, 42867, 2730, 1638]	[2808, 1794, 0, 0]	437	273	[10.2010, 00.0240, 100.001, -00.0101]	-
pdb2h5m	q	[128874, 189674, 6076, 15190]	[72394, 90281, 3406, 8515]	[8722, 5610, 0, 0]	1334	942	[15.3646, 33.2402, 150.016, -39.9934]	25.27529766283909
pdb2h5m	c	[148675, 252722, 15191, 9115]	[78371, 133518, 8515, 5109]	[8722, 5610, 0, 0]	1334	942	-	-
pdb2hep	\mathbf{q}	$[123461,\ 181402,\ 5680,\ 14200]$	$[69134,\ 86191,\ 3266,\ 8165]$	[8803, 5699, 0, 0]	1206	1043	[15.5369, 33.0399, 150.018, -39.993]	25.23811136806644
pdb2hep	c	[142643, 241337, 14201, 8521]	[74581, 127248, 8165, 4899]	[8803, 5699, 0, 0]	1206	1043	-	-
pdb2jmy	q	[17074, 25152, 816, 2040]	[9658, 12045, 454, 1135]	[1194, 762, 0, 0] [1194, 762, 0, 0]	$\frac{180}{180}$	$114 \\ 114$	[15.222, 33.3333, 150.123, -39.951]	25.271727075107584
pdb2jmy pdb2jn5	c q	[19673, 33536, 2041, 1225] [16198, 23835, 762, 1905]	[10463, 17820, 1135, 681] [9016, 11244, 424, 1060]	[1015, 657, 0, 0]	168	120	[15.3784, 33.2243, 150.131, -39.9475]	25.276346604215448
pdb2jn5 pdb2jn5	c c	[18689, 31754, 1906, 1144]	[9764, 16632, 1060, 636]	[1015, 657, 0, 0]	168	120	[10.0704, 00.2240, 100.101, -00.0470]	-
pdb2jnk	q	[319221, 469276, 14796, 36990]	[179272, 223512, 8464, 21160]	[22351, 14447, 0, 0]	3165	2591	[15.4667, 33.0844, 150.007, -39.9973]	25.233165493054123
pdb2jnk	c	[368594, 624533, 36991, 22195]	[193496, 330066, 21160, 12696]	[22351, 14447, 0, 0]	3165	2591	· ·	-
pdb2jpn	\mathbf{q}	$[150332,\ 221045,\ 6990,\ 17475]$	$[83102,\ 103627,\ 3914,\ 9785]$	[9778, 6346, 0, 0]	1537	1198	$[15.4684,\ 33.1114,\ 150.014,\ -39.9943]$	25.24795246588285
pdb2jpn	c	[173586, 294236, 17476, 10486]	[89881, 153186, 9785, 5871]	[9778, 6346, 0, 0]	1537	1198	[17 0474 00 1000 170 014 00 0040]	-
pdb2jua	q	[147158, 216574, 6932, 17330]	[81712, 101902, 3844, 9610]	[10191, 6549, 0, 0]	1543	1086	[15.3454, 33.1928, 150.014, -39.9942]	25.241885183791513
pdb2jua pdb2jvd	c	$[169740, 288461, 17331, 10399] \ [57353, 84449, 2722, 6805]$	$[88466, 150711, 9610, 5766] \ [32526, 40563, 1530, 3825]$	[10191, 6549, 0, 0] [3836, 2462, 0, 0]	$1543 \\ 595$	$\frac{1086}{401}$	[15.307, 33.3006, 150.037, -39.9853]	- 25.285305526369694
pdb2jvd pdb2jvd	q c	[66132, 112571, 6806, 4084]	[35217, 59994, 3825, 2295]	[3836, 2462, 0, 0]	595	401	[13.307, 33.3000, 130.037, -39.9833]	-
pdb2jws	q	[67824, 99880, 3224, 8060]	[37902, 47269, 1782, 4455]	[4527, 2905, 0, 0]	720	472	[15.2586, 33.2569, 150.031, -39.9876]	25.241915659150326
pdb2jws	c	[78173, 133097, 8061, 4837]	[41055, 69927, 4455, 2673]	[4527, 2905, 0, 0]	720	472	-	_
pdb2jwu	\mathbf{q}	[275435, 404468, 12564, 31410]	$[153974,\ 191941,\ 7286,\ 18215]$	$[19412,\ 12622,\ 0,\ 0]$	2638	2437	[15.5855, 32.9588, 150.008, -39.9968]	25.21422838410392
pdb2jwu	c	[318363, 537776, 31411, 18847]	[165871, 283173, 18215, 10929]	[19412, 12622, 0, 0]	2638	2437	-	
pdb2jxf	q	[34139, 50294, 1632, 4080]	[18988, 23682, 892, 2230]	[2334, 1492, 0, 0]	369	$\frac{229}{229}$	[15.1938, 33.2783, 150.061, -39.9755]	25.228243385656434
pdb2jxf pdb2jz5	c	[39326, 67031, 4081, 2449] $[204124, 300054, 9452, 23630]$	[20582, 35046, 2230, 1338] $[115218, 143647, 5442, 13605]$	[2334, 1492, 0, 0] [13559, 8801, 0, 0]	$\frac{369}{2004}$	$\frac{229}{1664}$	[15.4793, 33.0897, 150.011, -39.9958]	- 25.24141011800618
pdb2jz5 pdb2jz5	q c	[235721, 399341, 23631, 14179]	[124317, 212091, 13605, 8163]	[13559, 8801, 0, 0]	2004	1664	[10.4793, 33.0697, 130.011, -39.9936]	25.24141011800018
pdb2k2a	q	[86839, 127568, 3980, 9950]	[46782, 58317, 2214, 5535]	[6501, 4205, 0, 0]	882	761	$[15.4124,\ 32.8154,\ 150.025,\ -39.9899]$	25.067334685136444
pdb2k2a	ć	[100223, 169430, 9951, 5971]	[50391, 86031, 5535, 3321]	[6501, 4205, 0, 0]	882	761	-	-
pdb2k36	\mathbf{q}	$[163617,\ 240991,\ 7798,\ 19495]$	[92588, 115472, 4352, 10880]	[11053, 7077, 0, 0]	1722	1113	[15.271, 33.3228, 150.013, -39.9949]	25.281719653346492
pdb2k36	c	[188603, 321296, 19496, 11698]	[100312, 170841, 10880, 6528]	[11053, 7077, 0, 0]	1722	1113	[-
pdb2k37 pdb2k37	q	[73808, 108677, 3502, 8755]	[41744, 52058, 1964, 4910] [45190, 76989, 4910, 2946]	[5343, 3413, 0, 0]	768 768	$\frac{518}{518}$	[15.2951, 33.2803, 150.029, -39.9886]	25.26933070421378
pdb2k3i	c q	$[85097, 144845, 8756, 5254] \ [180233, 265096, 8420, 21050]$	[101670, 126771, 4794, 11985]	[5343, 3413, 0, 0] [11720, 7590, 0, 0]	1812	1395	[15.42, 33.1627, 150.012, -39.9952]	25.2563716435797
pdb2k3i	c c	[208025, 353009, 21051, 12631]	[109857, 187308, 11985, 7191]	[11720, 7590, 0, 0]	1812	1395	[10.42, 00.1021, 100.012, -00.0002]	-
pdb2k6s	q	[717081, 1052782, 32600, 81500]	[400244, 498906, 18956, 47390]	[47653, 31177, 0, 0]	6821	6463	[15.5934, 32.9152, 150.003, -39.9988]	25.19391304393983
pdb2k6s	c	[828898, 1399307, 81501, 48901]	[430846, 735768, 47390, 28434]	[47653, 31177, 0, 0]	6821	6463	•	-
pdb2kdh	\mathbf{q}	[172384, 253254, 7916, 19790]	[92908, 115862, 4372, 10930]	[12172, 7892, 0, 0]	1771	1472	$[15.5977,\ 33.0174,\ 150.013,\ -39.9949]$	25.249258840968448
pdb2kdh	c	[199272, 336872, 19791, 11875]	[100562, 171336, 10930, 6558]	[12172, 7892, 0, 0]	1771	1472	-	-
pdb2kdl pdb2kdl	q	[181740, 267045, 8366, 20915] [209921, 355220, 20916, 12550]	[101796, 126906, 4812, 12030] [109758, 187308, 12030, 7218]	[12469, 8095, 0, 0] [12469, 8095, 0, 0]	$1776 \\ 1776$	$1534 \\ 1534$	[15.5062, 33.0188, 150.012, -39.9952]	25.21430095426154
pdb2kdn pdb2kdm	c q	[110206, 162000, 5104, 12760]	[61320, 76458, 2892, 7230]	[7858, 5074, 0, 0]	1105	898	[15.491, 33.0846, 150.02, -39.9922]	25.243217154479947
pdb2kdm	c c	[127278, 215597, 12761, 7657]	[66246, 112959, 7230, 4338]	[7858, 5074, 0, 0]	1105	898	-	-
pdb2kdp	\mathbf{q}	[81684, 120248, 3864, 9660]	[45708, 57006, 2148, 5370]	[5364, 3452, 0, 0]	857	584	$[15.3494,\ 33.2712,\ 150.026,\ -39.9896]$	25.285905242833806
pdb2kdp	c	[94222, 160256, 9661, 5797]	[49530,84348,5370,3222]	[5364, 3452, 0, 0]	857	584	-	-
pdb2kdr	\mathbf{q}	[33149, 48834, 1584, 3960]	[18510, 23085, 870, 2175]	[2263, 1447, 0, 0]	356	223	$[15.192,\ 33.276,\ 150.063,\ -39.9747]$	25.22650153666868
pdb2kdr	c	[38185, 65084, 3961, 2377]	[20055, 34155, 2175, 1305]	[2263, 1447, 0, 0]	356 631	223	- [15 908 99 9040 150 094 90 0964]	-
pdb2kes	q	[62046,91353,2942,7355]	[35626, 44425, 1678, 4195]	[4216, 2704, 0, 0]	031	436	[15.308, 33.3049, 150.034, -39.9864]	25.288339360766287

pdb2kes	c	[71544, 121778, 7356, 4414]	[38531, 65670, 4195, 2517]	[4216, 2704, 0, 0]	631	436	_	_
pdb2kin	q	[29467, 43400, 1404, 3510]	[16634, 20745, 782, 1955]	[1896, 1218, 0, 0]	310	201	[15.2577, 33.3111, 150.071, -39.9715]	25.272238721538677
pdb2kjn	c	[33963, 57857, 3511, 2107]	[18019, 30690, 1955, 1173]	[1896, 1218, 0, 0]	310	201	-	-
pdb2kjo	q	[26611, 39202, 1272, 3180]	[14996, 18704, 704, 1760]	[1722, 1104, 0, 0]	283	177	[15.2606, 33.3605, 150.079, -39.9686]	25.299935956735208
pdb2kjo	c	[30672, 52280, 3181, 1909]	[16264, 27687, 1760, 1056]	[1722, 1104, 0, 0]	283	177	-	_
pdb2kl5	\mathbf{q}	[138372, 203667, 6530, 16325]	[77708, 96908, 3656, 9140]	[9031, 5821, 0, 0]	1436	1006	[15.3506, 33.2405, 150.015, -39.9939]	25.26980438154642
pdb2kl5	c	[159613, 271367, 16326, 9796]	[84124, 143319, 9140, 5484]	[9031, 5821, 0, 0]	1436	1006	-	-
pdb2klz	\mathbf{q}	[56727,83531,2694,6735]	$[32414,\ 40421,\ 1526,\ 3815]$	[3735, 2399, 0, 0]	583	395	$[15.289,\ 33.3038,\ 150.037,\ -39.9852]$	25.2800844428708
pdb2klz	c	[65400, 111350, 6736, 4042]	[35071, 59763, 3815, 2289]	[3735, 2399, 0, 0]	583	395	· · · · · · · · · · · · · · · · · · ·	
pdb2koz	\mathbf{q}	[50312, 73991, 2346, 5865]	[27678, 34517, 1302, 3255]	[3509, 2263, 0, 0]	521	394	[15.4595, 33.1419, 150.043, -39.9829]	25.261481805696008
pdb2koz	c	[58090, 98513, 5866, 3520]	[29967, 51051, 3255, 1953]	[3509, 2263, 0, 0]	521	394	[15 6004 22 0688 150 017 20 0022]	-
pdb2kp0	q	[129067, 189540, 5892, 14730]	[71288, 88876, 3368, 8420]	[8972, 5838, 0, 0]	$1261 \\ 1261$	$\frac{1137}{1137}$	[15.6004, 32.9688, 150.017, -39.9932]	25.22543768368859
pdb2kp0 pdb2ksg	c	$[149202, 252029, 14731, 8839] \ [50626, 74595, 2426, 6065]$	[76900, 131208, 8420, 5052] [28532, 35586, 1340, 3350]	[8972, 5838, 0, 0] [3302, 2114, 0, 0]	542	332	[15.2116, 33.3467, 150.041, -39.9835]	- 25.27147899964102
pdb2ksg pdb2ksg	q c	[58327, 99470, 6066, 3640]	[30934, 52668, 3350, 2010]	[3302, 2114, 0, 0]	542 542	332	[13.2110, 33.3407, 130.041, -39.9633]	25.27147899904102
pdb2kt8	q	[378533, 555845, 17258, 43145]	[211816, 264044, 10024, 25060]	[25962, 16920, 0, 0]	3616	3357	[15.5918, 32.9585, 150.006, -39.9977]	25.216504939278096
pdb2kt8	c	[437553, 739043, 43146, 25888]	[228164, 389532, 25060, 15036]	[25962, 16920, 0, 0]	3616	3357	-	-
pdb2kuh	q	[79439, 116704, 3644, 9110]	[42738, 53277, 2022, 5055]	[6213, 4005, 0, 0]	810	693	[15.408, 32.8224, 150.027, -39.989]	25.069292522152065
pdb2kuh	c	[91679, 155009, 9111, 5467]	[46047, 78606, 5055, 3033]	[6213, 4005, 0, 0]	810	693	· · · · · · · · · · · · · · · · · · ·	-
pdb2kwh	\mathbf{q}	[69487, 102330, 3304, 8260]	[39364, 49090, 1852, 4630]	[4706, 3016, 0, 0]	725	481	[15.2705, 33.2913, 150.03, -39.9879]	25.265430987943137
pdb2kwh	c	[80098,136397,8261,4957]	[42614, 72600, 4630, 2778]	[4706, 3016, 0, 0]	725	481	-	-
pdb2kxa	\mathbf{q}	[22783, 33578, 1096, 2740]	[12754, 15909, 598, 1495]	[1765, 1117, 0, 0]	248	145	[15.1955, 33.3879, 150.091, -39.9635]	25.288635646294665
pdb2kxa	c	[26245, 44789, 2741, 1645]	[13847, 23562, 1495, 897]	[1765, 1117, 0, 0]	248	145	·	
pdb2l3m	\mathbf{q}	[76604, 112827, 3650, 9125]	[43202, 53881, 2030, 5075]	[5237, 3351, 0, 0]	809	522	[15.276, 33.3209, 150.027, -39.989]	25.28312710799878
pdb2l3m	c	[88306, 150422, 9126, 5476]	[46819, 79728, 5075, 3045]	[5237, 3351, 0, 0]	809	522	[15 4166 99 1959 150 05 99 0599]	-
pdb2l45 pdb2l45	q c	[30746, 45225, 1438, 3595] [35486, 60233, 3596, 2158]	$[17354, 21639, 818, 2045] \ [18757, 31977, 2045, 1227]$	[1996, 1292, 0, 0] [1996, 1292, 0, 0]	309 309	236 236	[15.4166, 33.1852, 150.07, -39.9722]	25.269122512468513
pdb2l45 pdb2l5r	q	[29646, 43539, 1354, 3385]	[15972, 19910, 756, 1890]	[2254, 1458, 0, 0]	298	264	[15.4523, 32.8097, 150.074, -39.9705]	25.08213130742776
pdb2l5r	c c	[34227, 57824, 3386, 2032]	[17202, 29370, 1890, 1134]	[2254, 1458, 0, 0]	298	264	[13.4323, 32.3037, 130.074, -33.3700]	25.05215150742770
pdb2l6q	q	[181897, 267259, 8366, 20915]	[101136, 126092, 4776, 11940]	[12741, 8261, 0, 0]	1794	1541	[15.5352, 33.0234, 150.012, -39.9952]	25.228190963491535
pdb2l6q	c	[210155, 355517, 20916, 12550]	[109140, 186186, 11940, 7164]	[12741, 8261, 0, 0]	1794	1541	-	-
pdb2l6r	q	[74696, 109958, 3532, 8830]	[41476, 51730, 1948, 4870]	[5006, 3218, 0, 0]	791	536	[15.3529, 33.2582, 150.028, -39.9887]	25.280180289925692
pdb2l6r	c	[86164, 146528, 8831, 5299]	[44966, 76560, 4870, 2922]	[5006, 3218, 0, 0]	791	536	•	-
pdb2l98	\mathbf{q}	$[257620,\ 378461,\ 11822,\ 29555]$	[143814, 179289, 6798, 16995]	[17565, 11423, 0, 0]	2511	2210	[15.5407, 33.001, 150.008, -39.9966]	25.218537532954066
pdb2l98	c	[297656, 503357, 29556, 17734]	[155067, 264627, 16995, 10197]	[17565, 11423, 0, 0]	2511	2210		-
pdb2lci	\mathbf{q}	[190148, 279838, 8956, 22390]	[107584, 134154, 5068, 12670]	[12795, 8237, 0, 0]	1943	1400	[15.3523, 33.2232, 150.011, -39.9955]	25.261303886446495
pdb2lci	c	[219340, 372809, 22391, 13435]	[116342, 198297, 12670, 7602]	[12795, 8237, 0, 0]	1943	1400	[15 0050 00 0116 150 050 00 0600]	- 05 005050100401000
pdb2lde	q	[27066, 39860, 1288, 3220] [31206, 53138, 3221, 1933]	[15084, 18814, 708, 1770]	[1731, 1113, 0, 0]	289 289	186 186	[15.2959, 33.3116, 150.078, -39.9689]	25.287678136461622
pdb2lde pdb2le7	c q	[21426, 31554, 1020, 2550]	$[16362, 27852, 1770, 1062] \ [12176, 15186, 572, 1430]$	$[1731, 1113, 0, 0] \ [1386, 890, 0, 0]$	223	146	[15.3178, 33.3682, 150.098, -39.9608]	25.328028293545547
pdb2le7	c c	[24708, 42083, 2551, 1531]	[13198, 22473, 1430, 858]	[1386, 890, 0, 0]	223	146	[13.3176, 33.3062, 130.036, -33.3006]	20.02002020040041
pdb2ler	q	[11373, 16754, 544, 1360]	[6434, 8025, 302, 755]	[695, 447, 0, 0]	120	75	[15.2642, 33.395, 150.184, -39.9265]	25.323832040225103
pdb2ler	c	[13109, 22349, 1361, 817]	[6979, 11880, 755, 453]	[695, 447, 0, 0]	120	75	-	-
pdb2lgi	q	[144381, 212157, 6650, 16625]	[80822, 100763, 3818, 9545]	[10138, 6568, 0, 0]	1415	1213	[15.5221, 33.0416, 150.015, -39.994]	25.232943580130218
pdb2lgi	c	[166792, 282257, 16626, 9976]	[87193, 148764, 9545, 5727]	[10138, 6568, 0, 0]	1415	1213	<u> </u>	-
pdb2lhc	\mathbf{q}	$[124267,\ 182698,\ 5768,\ 14420]$	[69736, 86946, 3292, 8230]	[7961, 5177, 0, 0]	1237	1001	$[15.4498,\ 33.0896,\ 150.017,\ -39.9931]$	25.229479784687904
pdb2lhc	c	[143466, 243152, 14421, 8653]	[75278, 128403, 8230, 4938]	[7961, 5177, 0, 0]	1237	1001		-
pdb2lhd	\mathbf{q}	[662364, 972145, 29974, 74935]	[366628, 457018, 17356, 43390]	[47622, 31014, 0, 0]	6308	6102	[15.6496, 32.8909, 150.003, -39.9987]	25.203430112830837
pdb2lhd	c	[766021, 1291892, 74936, 44962]	[394814, 674124, 43390, 26034]	[47622, 31014, 0, 0]	6308	6102	[15 5055 00 0050 150 01 00 0000]	-
pdb2lhe	q	[228571, 335675, 10438, 26095]	[126912, 158216, 6000, 15000]	[16111, 10471, 0, 0]	$\frac{2218}{2218}$	$2011 \\ 2011$	[15.5855, 32.9658, 150.01, -39.9962]	25.21775894297238
pdb2lhe	c	[264195, 446333, 26096, 15658] $[63253, 92914, 2896, 7240]$	[136824, 233508, 15000, 9000] [33416, 41658, 1580, 3950]	[16111, 10471, 0, 0]	657	2011 559	[15 4064 22 7701 150 025 20 0862]	- 25 040429226221456
pdb2lhg pdb2lhg	q c	[72998, 123362, 7241, 4345]	[36022, 61479, 3950, 2370]	[5204, 3346, 0, 0] [5204, 3346, 0, 0]	657	559 559	[15.4064, 32.7701, 150.035, -39.9862]	25.040438236231456
pdb2lig pdb2lix	q	[29555, 43507, 1398, 3495]	[16596, 20698, 780, 1950]	[1966, 1264, 0, 0]	308	211	[15.3544, 33.2866, 150.072, -39.9714]	25.297928291963313
pdb2lix	c	[34093, 57989, 3496, 2098]	[17982, 30624, 1950, 1170]	[1966, 1264, 0, 0]	308	211	-	-
pdb2lld	q	[44847, 65908, 2068, 5170]	[24108, 30054, 1140, 2850]	[3406, 2196, 0, 0]	463	381	$[15.3522,\ 32.8473,\ 150.048,\ -39.9807]$	25.060808692041057
pdb2lld	ć	[51732, 87557, 5171, 3103]	[25986, 44352, 2850, 1710]	[3406, 2196, 0, 0]	463	381		-
pdb2lm9	\mathbf{q}	[108714, 160161, 5198, 12995]	[61840, 77122, 2908, 7270]	[7614, 4858, 0, 0]	1144	724	$[15.2244,\ 33.3352,\ 150.019,\ -39.9923]$	25.26997087798013
pdb2lm9	c	[125265, 213551, 12996, 7798]	[66974, 114081, 7270, 4362]	$[7614,\ 4858,\ 0,\ 0]$	1144	724	-	-

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pdb2lmf
                        [23488, 34622, 1132, 2830]
                                                             [13132, 16380, 616, 1540]
                                                                                              [1608, 1024, 0, 0]
                                                                                                                     257
                                                                                                                               148
                                                                                                                                        [15.1482, 33.369, 150.088, -39.9647]
                                                                                                                                                                               25.259376208274254
 pdb2lmf
                        [27046, 46175, 2831, 1699]
                                                             [14252, 24255, 1540, 924]
                                                                                              [1608, 1024, 0, 0]
                                                                                                                     257
                                                                                                                               148
                       [95898, 141198, 4548, 11370]
                                                                                              [6404, 4112, 0, 0]
                                                                                                                     997
                                                                                                                               674
                                                                                                                                        [15.3163, 33.293, 150.022, -39.9912]
                                                                                                                                                                               25.284371615799905
pdb2ln3
                                                            [54260, 67668, 2552, 6380]
pdb2ln3
                      [110586, 188207, 11371, 6823]
                                                            [58756, 100089, 6380, 3828]
                                                                                              [6404, 4112, 0, 0]
                                                                                                                     997
                                                                                                                               674
                                                                                              [2697, 1729, 0, 0]
                                                                                                                                       [15.2848, 33.3372, 150.051, -39.9794]
                                                                                                                                                                               25.296310412464095
 pdb2lo2
                        [40753, 60023, 1942, 4855]
                                                            [23030, 28723, 1082, 2705]
                                                                                                                     429
                                                                                                                               277
                        [46982, 80033, 4856, 2914]
                                                             [24961, 42504, 2705, 1623
                                                                                               [2697, 1729, 0, 0]
                                                                                                                               277
 pdb2lo2
                                                                                                                     429
 pdb2lqp
                       [77789, 114566, 3704, 9260]
                                                             [44172, 55090, 2076, 5190
                                                                                              [5226, 3348, 0, 0]
                                                                                                                     813
                                                                                                                               531
                                                                                                                                       [15.2991, 33.3424, 150.027, -39.9892]
                                                                                                                                                                                25.30403908065011
 pdb2lqp
                       [89690, 152765, 9261, 5557]
                                                            [47862, 81510, 5190, 3114]
                                                                                              [5226, 3348, 0, 0]
                                                                                                                     813
                                                                                                                               531
                      [268956, 395490, 12516, 31290]
                                                           [152092, 189626, 7180, 17950]
 pdb2lr0
                                                                                             [18272, 11816, 0, 0]
                                                                                                                               2132
                                                                                                                                        [15.436, 33.1235, 150.008, -39.9968]
                                                                                                                                                                                25.241863065688474
                                                                                                                     2667
                      310472, 526490, 31291, 18775
                                                           164174, 280038, 17950, 10770]
                                                                                              18272, 11816, 0, 0
                                                                                                                               2132
 pdb2lr0
                                                                                                                     2667
                      [330044, 485135, 15274, 38185]
                                                           [186130, 232051, 8794, 21985]
                                                                                                                                       [15.4731, 33.0737, 150.007, -39.9974]
                                                                                                                                                                               25.230187949410453
 pdb2lrh
                                                                                             [22187, 14393, 0, 0]
                                                                                                                               2702
                                                                                                                     3239
 pdb2lrh
                      [381112, 645587, 38186, 22912]
                                                          [200777, 342573, 21985, 13191]
                                                                                             [22187, 14393, 0, 0]
                                                                                                                     3239
                                                                                                                               2702
                        [23913, 35256, 1156, 2890]
                                                                                                                                       [15.1298, 33.4042, 150.087, -39.9654]
                                                                                                                                                                                25.270900893775217
 pdb2ls9
                                                             [13434, 16757, 630, 1575]
                                                                                               [1557, 993, 0, 0]
                                                                                                                     262
                                                                                                                               147
 pdb2ls9
                        [27531, 47033, 2891, 1735]
                                                             [14583, 24816, 1575, 945]
                                                                                               [1557, 993, 0, 0]
                                                                                                                     262
                                                                                                                               147
                                                                                                                                        [15.2435, 33.3485, 150.087, -39.965]
                                                                                                                                                                                25.286901464186773
 pdb2lsa
                        [23925, 35246, 1144, 2860]
                                                             [13460, 16788, 632, 1580]
                                                                                              [1714, 1092, 0, 0]
                                                                                                                     255
                                                                                                                               159
 pdb2lsa
                        [27572, 47000, 2861, 1717]
                                                             [14596, 24849, 1580, 948]
                                                                                              [1714, 1092, 0, 0]
                                                                                                                     255
                                                                                                                               159
                                                                                                                                       [15.3469,\ 33.2676,\ 150.029,\ -39.9885]
                                                                                                                                                                                25.282812152783162
                                                                                               [5283, 3379, 0, 0]
 pdb2lss
                        [73357, 107994, 3472, 8680]
                                                             [40758, 50835, 1914, 4785
                                                                                                                     778
                                                                                                                               523
                                                                                              [5283, 3379, 0, 0]
 pdb2lss
                       [84615, 143921, 8681, 5209]
                                                             [44193, 75240, 4785, 2871
                                                                                                                     778
                                                                                                                               523
                                                             [66868, 83364, 3160, 7900]
                                                                                                                                       [15.4223, 32.7865, 150.017, -39.9931]
                                                                                                                                                                                25.05497674753956
 pdb2lt3
              \mathbf{q}
                       [126602, 185973, 5798, 14495]
                                                                                              [9841, 6351, 0, 0]
                                                                                                                     1318
                                                                                                                               1116
 pdb2lt3
                      [146127, 246947, 14496, 8698]
                                                            [72116, 123057, 7900, 4740]
                                                                                              9841, 6351, 0, 0
                                                                                                                     1318
                                                                                                                               1116
 pdb2lu6
                        [15698, 23115, 746, 1865]
                                                              [8978, 11197, 422, 1055]
                                                                                               [918, 594, 0, 0]
                                                                                                                     161
                                                                                                                               108
                                                                                                                                       [15.3395, 33.3766, 150.134, -39.9464]
                                                                                                                                                                                25.342796446504433
 pdb2lu6
                        [18106, 30830, 1866, 1120]
                                                              [9727, 16566, 1055, 633]
                                                                                               [918, 594, 0, 0]
                                                                                                                     161
                                                                                                                               108
                                                                                                                                       [15.2448, 33.3861, 150.028, -39.9888]
                                                                                                                                                                                25.305433134360158
 pdb2lwa
                        [74655, 110001, 3578, 8945]
                                                             [42306, 52767, 1986, 4965]
                                                                                              [5212, 3322, 0, 0]
                                                                                                                     795
                                                                                                                               487
                        [86036, 146726, 8946, 5368]
                                                            [45885, 78111, 4965, 2979]
                                                                                              [5212, 3322, 0, 0]
                                                                                                                               487
pdb2lwa
                                                                                                                     795
                        [36572, 53855, 1738, 4345]
 pdb2lx0
                                                             [20436, 25488, 960, 2400]
                                                                                              [2564, 1640, 0, 0]
                                                                                                                     388
                                                                                                                               254
                                                                                                                                        [15.2931, 33.2894, 150.058, -39.977]
                                                                                                                                                                                25.274064863744684
                        [42165, 71783, 4346, 2608]
                                                             [22152, 37719, 2400, 1440]
                                                                                              [2564, 1640, 0, 0]
                                                                                                                     388
                                                                                                                               254
 pdb2lx0
                                                                                                                                       [15.4364, 33.1479, 150.008, -39.9967]
                                                                                                                                                                                25.25480158128579
 pdb2lxb
                      [260456, 383050, 12148, 30370]
                                                           [146314, 182439, 6898, 17245]
                                                                                             [17416, 11264, 0, 0]
                                                                                                                     2624
                                                                                                                               2036
 pdb2lxb
                      [300661, 510023, 30371, 18223]
                                                          [158117, 269577, 17245, 10347]
                                                                                             [17416, 11264, 0, 0]
                                                                                                                     2624
                                                                                                                               2036
pdb2lxy
                      [629330, 923605, 28454, 71135]
                                                           [344044, 428908, 16264, 40660]
                                                                                             [43430, 28386, 0, 0]
                                                                                                                     6094
                                                                                                                               5820
                                                                                                                                       [15.6797, 32.8898, 150.004, -39.9986]
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                                                           370940, 633039, 40660, 24396
                      [728007, 1227377, 71136, 42682]
                                                                                             [43430, 28386, 0, 0]
                                                                                                                     6094
 pdb2lxy
                                                                                                                               5820
                                                                                                                                                                                25.20619762736245
 pdb2lxz
                      [439526, 644996, 19848, 49620]
                                                          [241832, 301462, 11444, 28610]
                                                                                             [29900, 19576, 0, 0]
                                                                                                                     4201
                                                                                                                               4090
                                                                                                                                        [15.6751, 32.8769, 150.005, -39.998]
                      [508422, 857051, 49621, 29773]
                                                          [260506, 444741, 28610, 17166]
                                                                                             [29900, 19576, 0, 0]
                                                                                                                               4090
 pdb2lxz
                                                                                                                     4201
pdb2m1a
                        [35276, 51923, 1666, 4165]
                                                             [20288, 25298, 956, 2390]
                                                                                              [2284, 1472, 0, 0]
                                                                                                                     354
                                                                                                                               254
                                                                                                                                        [15.3504, 33.2916, 150.06, -39.976]
                                                                                                                                                                                 25.2993657959798
                        [40691, 69209, 4166, 2500]
                                                            [21934, 37389, 2390, 1434]
                                                                                              [2284, 1472, 0, 0]
                                                                                                                               254
pdb2m1a
                                                                                                                     354
pdb2m1j
                        [34915, 51390, 1648, 4120]
                                                             [19188, 23934, 900, 2250]
                                                                                              [2278, 1468, 0, 0]
                                                                                                                     373
                                                                                                                               253
                                                                                                                                       [15.3945, 33.2613, 150.061, -39.9757]
                                                                                                                                                                                25.29949062157202
pdb2m1j
                        [40290, 68483, 4121, 2473]
                                                            [20826, 35442, 2250, 1350]
                                                                                              [2278, 1468, 0, 0]
                                                                                                                     373
                                                                                                                               253
pdb2m2v
                        [19335, 28474, 920, 2300]
                                                             [10816, 13490, 508, 1270]
                                                                                               [1248, 802, 0, 0]
                                                                                                                     205
                                                                                                                               133
                                                                                                                                       [15.2832, 33.3076, 150.109, -39.9565]
                                                                                                                                                                                25.281702561288675
                                                             [11726, 19965, 1270, 762]
pdb2m2y
                        [22290, 37958, 2301, 1381]
                                                                                               [1248, 802, 0, 0]
                                                                                                                     205
                                                                                                                               133
                        [22396, 33009, 1078, 2695]
                                                              [12654, 15783, 594, 1485]
                                                                                               [1552, 988, 0, 0]
                                                                                                                                       [15.1724, 33.3879, 150.093, -39.9629]
                                                                                                                                                                                 25.2796647402751
pdb2m3f
                                                                                                                     241
                                                                                                                               142
                        [25794, 44030, 2696, 1618]
                                                             [13725, 23364, 1485, 891]
                                                                                               1552, 988, 0, 0
                                                                                                                               142
pdb2m3f
                                                                                                                     241
pdb2m8m
                        [28697, 42153, 1314, 3285]
                                                             [15114, 18843, 714, 1785]
                                                                                              [2338, 1504, 0, 0]
                                                                                                                     299
                                                                                                                               253
                                                                                                                                       [15.4267, 32.7924, 150.076, -39.9696]
                                                                                                                                                                                25.061962385187343
                        [33124, 55976, 3286, 1972]
                                                                                              [2338, 1504, 0, 0]
                                                                                                                               253
pdb2m8m
                                                            [16305, 27819, 1785, 1071]
                                                                                                                     299
pdb2m8o
                        [27817, 40861, 1274, 3185]
                                                             [14610, 18215, 690, 1725]
                                                                                               [2295, 1475, 0, 0]
                                                                                                                     291
                                                                                                                               245
                                                                                                                                       [15.4258, 32.7917, 150.078, -39.9686]
                                                                                                                                                                                25.06118654032843
pdb2m8o
                        [32108, 54260, 3186, 1912]
                                                            [15765, 26895, 1725, 1035]
                                                                                              [2295, 1475, 0, 0]
                                                                                                                     291
                                                                                                                               245
                                                                                                                                       [15.3607, 32.7752, 150.029, -39.9884]
pdb2m97
                       [74873, 110010, 3440, 8600]
                                                            [39512, 49258, 1868, 4670
                                                                                              [5896, 3798, 0, 0]
                                                                                                                     785
                                                                                                                               651
                                                                                                                                                                                25.02450196269608
                                                                                              [5896, 3798, 0, 0]
pdb2m97
                       [86374, 146066, 8601, 5161]
                                                             [42598, 72699, 4670, 2802]
                                                                                                                     785
                                                                                                                               651
                      [426904, 627485, 19742, 49355]
                                                                                             [29838, 19310, 0, 0]
                                                                                                                                        [15.478, 33.0405, 150.005, -39.998]
                                                                                                                                                                                25.21375433249724
pdb2m9g
                                                           [236142, 294429, 11142, 27855]
                                                                                                                     4299
                                                                                                                               3518
                      [492980, 834809, 49356, 29614]
                                                          [255015, 434907, 27855, 16713]
pdb2m9g
                                                                                             [29838, 19310, 0, 0]
                                                                                                                     4299
                                                                                                                               3518
pdb2m9r
                        [47668, 70153, 2246, 5615]
                                                             [26468, 33010, 1244, 3110]
                                                                                              [2615, 1709, 0, 0]
                                                                                                                     500
                                                                                                                               350
                                                                                                                                       [15.3751, 33.2288, 150.045, -39.9822]
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pdb2m9r
                        [54997, 93464, 5616, 3370]
                                                             [28678, 48840, 3110, 1866]
                                                                                              [2615, 1709, 0, 0]
                                                                                                                     500
                                                                                                                               350
                     [698446, 1025179, 31626, 79065]
                                                                                                                                       [15.5548, 32.7921, 150.003, -39.9987]
                                                                                                                                                                                25.11208537678349
pdb2mdv
                                                          [381618, 475659, 18090, 45225]
                                                                                             [51028, 33204, 0, 0]
                                                                                                                     6767
                                                                                                                               6468
                                                          [410481, 701217, 45225, 27135]
pdb2mdv
                     [807088, 1361357, 79066, 47440]
                                                                                             [51028, 33204, 0, 0]
                                                                                                                     6767
                                                                                                                               6468
pdb2me1
                        [30370, 44732, 1448, 3620]
                                                             [17074, 21295, 802, 2005]
                                                                                              [1991, 1277, 0, 0]
                                                                                                                     322
                                                                                                                               206
                                                                                                                                       [15.2684, 33.3251, 150.069, -39.9724]
                                                                                                                                                                                25.283771984532866
                        [35007, 59639, 3621, 2173]
pdb2me1
                                                            [18509, 31515, 2005, 1203]
                                                                                              [1991, 1277, 0, 0]
                                                                                                                     322
                                                                                                                               206
                                                                                                                                        [15.2391, 33.309, 150.07, -39.9718]
                                                                                                                                                                                25.262889554521696
pdb2me2
                        [29713, 43772, 1420, 3550]
                                                             [16418, 20479, 770, 1925]
                                                                                              [1899, 1219, 0, 0]
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                                                                                                                               199
pdb2me2
                        [34241, 58352, 3551, 2131]
                                                            [17821, 30327, 1925, 1155]
                                                                                              [1899, 1219, 0, 0]
                                                                                                                     324
                                                                                                                               199
pdb2me3
                        [25965, 38279, 1254, 3135]
                                                             [14504, 18092, 680, 1700]
                                                                                              [1666, 1064, 0, 0]
                                                                                                                     286
                                                                                                                               161
                                                                                                                                        [15.1358, 33.3865, 150.08, -39.9681]
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pdb2me3
                        [29895, 51059, 3136, 1882]
                                                            [15748, 26796, 1700, 1020]
                                                                                              [1666, 1064, 0, 0]
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                                                                                                                               161
                                                                                                                                       [15.2904, 33.2821, 150.065, -39.9739]
                        [32236, 47470, 1532, 3830]
                                                             [17930, 22363, 842, 2105]
                                                                                              [2004, 1292, 0, 0]
                                                                                                                                                                                25.26919640757981
pdb2me4
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```

		[07107 00000 0001 0000]	[10441 99000 9107 1969]	[0.04 1000 0 0]	0.4.4	004		
pdb2me4 $pdb2mg1$	c	[37165, 63269, 3831, 2299] [28177, 41389, 1290, 3225]	$[19441, 33099, 2105, 1263] \ [14736, 18372, 696, 1740]$	[2004, 1292, 0, 0] [2304, 1482, 0, 0]	$\frac{344}{296}$	$\frac{224}{249}$	[15 4169 99 779 150 079 90 060]	- 25.046908114091337
	q				296 296	249 249	[15.4168, 32.772, 150.078, -39.969]	25.046908114091337
pdb2mg1	c	[32521, 54953, 3226, 1936]	[15900, 27126, 1740, 1044]	[2304, 1482, 0, 0]			[15 4150 00 500 150 050 00 0000]	05 0500505540
pdb2mg2	q	[28712, 42178, 1316, 3290]	[15076, 18796, 712, 1780]	[2332, 1500, 0, 0] [2332, 1500, 0, 0]	301 301	$252 \\ 252$	[15.4152, 32.792, 150.076, -39.9696]	25.05695665995549
pdb2mg2	c	[33138, 56009, 3291, 1975]	[16268, 27753, 1780, 1068]			262	[15 2022 22 7251 150 072 20 0702]	25 046455200008
pdb2mg3	q	[29880, 43895, 1370, 3425]	$[15744, 19628, 744, 1860] \ [16980, 28974, 1860, 1116]$	[2307, 1489, 0, 0]	$\frac{312}{312}$	262 262	[15.3983, 32.7851, 150.073, -39.9708]	25.046455390098
pdb2mg3 pdb2mh8	c	[34481, 58286, 3426, 2056] [66656, 97917, 3054, 7635]	[35596, 44374, 1684, 4210]	[2307, 1489, 0, 0] [5231, 3373, 0, 0]	684	586	[15 406 22 7041 150 022 20 0860]	25.053348700802225
pdb2mh8	q	[76925, 130028, 7636, 4582]	[38354, 65472, 4210, 2526]	[5231, 3373, 0, 0]	684	586	[15.406, 32.7941, 150.033, -39.9869]	25.053348700802225
pdb2mhw	c	[28424, 41876, 1360, 3400]	[16054, 20023, 754, 1885]	[2038, 1298, 0, 0]	302	188	[15.2371, 33.3556, 150.074, -39.9706]	25.287769784172664
pdb2mhw	q c	[32755, 55844, 3401, 2041]	[17405, 29634, 1885, 1131]	[2038, 1298, 0, 0]	302	188	[13.2371, 33.3330, 130.074, -39.9700]	23.281109184112004
pdb2mi1	q	[194031, 284568, 8684, 21710]	[102506, 127805, 4838, 12095]	[14915, 9703, 0, 0]	1922	1885	[15.7789, 32.7946, 150.012, -39.9954]	25.203293561993977
pdb2mi1	c c	[224647, 377891, 21711, 13027]	[110671, 188760, 12095, 7257]	[14915, 9703, 0, 0]	1922	1885	[10.7760, 02.7040, 100.012, -00.004]	25.205255501555511
pdb2mi7	q	[70231, 103483, 3366, 8415]	[39624, 49422, 1860, 4650]	[4814, 3072, 0, 0]	752	459	[15.2326, 33.3688, 150.03, -39.9881]	25.291247742526757
pdb2mi7	c c	[80929, 138014, 8416, 5050]	[42978, 73161, 4650, 2790]	[4814, 3072, 0, 0]	752	459	[10:2020, 00:0000, 100:00, -00:0001]	20.201241142020101
pdb2mij	q	[39031, 57504, 1868, 4670]	[22224, 27718, 1044, 2610]	[2577, 1649, 0, 0]	411	257	[15.252, 33.382, 150.054, -39.9786]	25.30730647211199
pdb2mij	c	[44984, 76700, 4671, 2803]	[24090, 41019, 2610, 1566]	[2577, 1649, 0, 0]	411	257	[10:202, 00:002, 100:001, 00:01:00]	-
pdb2mix	\mathbf{q}	[21638, 31862, 1028, 2570]	[12100, 15092, 568, 1420]	[1455, 933, 0, 0]	229	150	[15.3249, 33.3218, 150.097, -39.9611]	25.305614907702555
pdb2mix	c	[24954, 42479, 2571, 1543]	[13124, 22341, 1420, 852]	[1455, 933, 0, 0]	229	150		-
pdb2mj1	q	[20997, 30919, 998, 2495]	[11912, 14856, 560, 1400]	[1365, 877, 0, 0]	218	145	[15.3069, 33.3323, 150.1, -39.9599]	25.30455341190059
pdb2mj1	c	[24211, 41225, 2496, 1498]	[12904, 21978, 1400, 840]	[1365, 877, 0, 0]	218	145	-	-
pdb2mj2	\mathbf{q}	[40825, 60126, 1944, 4860]	[23144, 28864, 1088, 2720]	[2644, 1698, 0, 0]	427	279	$[15.2823,\ 33.3283,\ 150.051,\ -39.9794]$	25.290705767713796
pdb2mj2	c	[47064, 80165, 4861, 2917]	[25072, 42702, 2720, 1632]	[2644, 1698, 0, 0]	427	279	-	-
pdb2mjg	\mathbf{q}	[291563, 428292, 13364, 33410]	[161252, 201040, 7616, 19040]	[19122, 12480, 0, 0]	2873	2517	[15.5613, 32.9906, 150.007, -39.997]	25.220934767664673
pdb2mjg	ć	[336934, 569588, 33411, 20047]	[173992, 296835, 19040, 11424]	[19122, 12480, 0, 0]	2873	2517	-	_
pdb2mji	q	[161756, 237986, 7588, 18970]	[89414, 111515, 4202, 10505]	[11820, 7580, 0, 0]	1692	1220	[15.4288, 33.2036, 150.013, -39.9947]	25.28102275392916
pdb2mji	c	[186713, 317006, 18971, 11383]	[96889, 165000, 10505, 6303]	[11820, 7580, 0, 0]	1692	1220	· ·	-
pdb2mle	\mathbf{q}	[81891, 120615, 3902, 9755]	[46162, 57571, 2170, 5425]	[5349, 3433, 0, 0]	865	559	[15.2581, 33.3035, 150.026, -39.9897]	25.26658123730703
pdb2mle	c	[94386, 160784, 9756, 5854]	[50009, 85173, 5425, 3255]	[5349, 3433, 0, 0]	865	559	-	-
pdb2mlf	\mathbf{q}	[83902, 123564, 3992, 9980]	[47460, 59188, 2232, 5580]	[5498, 3530, 0, 0]	879	578	[15.2726, 33.3002, 150.025, -39.99]	25.270730407608454
pdb2mlf	c	[96716, 164711, 9981, 5989]	[51396, 87549, 5580, 3348]	[5498, 3530, 0, 0]	879	578	-	-
pdb2mo5	\mathbf{q}	[269285, 395813, 12458, 31145]	[150082, 187133, 7078, 17695]	[18830, 12180, 0, 0]	2689	2205	[15.5126, 33.0899, 150.008, -39.9968]	25.254373847363
pdb2mo5	c	[311058, 526787, 31146, 18688]	[162143, 276474, 17695, 10617]	[18830, 12180, 0, 0]	2689	2205	-	-
pdb2mpu	\mathbf{q}	[102900, 151495, 4874, 12185]	[57734, 72003, 2714, 6785]	[6910, 4438, 0, 0]	1079	730	[15.3275, 33.273, 150.021, -39.9918]	25.277947644904852
pdb2mpu	c	[118672, 201902, 12186, 7312]	[62545, 106524, 6785, 4071]	[6910,4438,0,0]	1079	730	-	-
pdb2mra	\mathbf{q}	$[242474,\ 356511,\ 11266,\ 28165]$	[136752, 170500, 6456, 16140]	$[15630,\ 10154,\ 0,\ 0]$	2404	1940	[15.4487, 33.1089, 150.009, -39.9964]	25.239185734693372
pdb2mra	c	[279933, 474548, 28166, 16900]	$[147612,\ 251790,\ 16140,\ 9684]$	$[15630,\ 10154,\ 0,\ 0]$	2404	1940	-	-
pdb2msu	\mathbf{q}	$[24403,\ 35918,\ 1152,\ 2880]$	$[13574,\ 16929,\ 638,\ 1595]$	$[1632,\ 1050,\ 0,\ 0]$	256	177	[15.3506, 33.2424, 150.087, -39.9653]	25.27310304103927
pdb2msu	С	[28149, 47858, 2881, 1729]	[14707, 25047, 1595, 957]	[1632, 1050, 0, 0]	256	177	·	-
pdb2mty	\mathbf{q}	[25633, 37635, 1166, 2915]	[13274, 16551, 626, 1565]	[1838, 1196, 0, 0]	269	233	[15.5308, 32.7753, 150.086, -39.9657]	25.09465619385589
pdb2mty	С	[29614, 49970, 2916, 1750]	[14341, 24453, 1565, 939]	[1838, 1196, 0, 0]	269	233		.
pdb2muh	\mathbf{q}	[29005, 42628, 1340, 3350]	[16082, 20053, 758, 1895]	[1934, 1256, 0, 0]	290	239	[15.5353, 33.0933, 150.075, -39.9701]	25.26761264625341
pdb2muh	С	[33511, 56735, 3351, 2011]	[17383, 29634, 1895, 1137]	[1934, 1256, 0, 0]	290	239	-	-
pdb2mvj	q	[28363, 41784, 1356, 3390]	[16042, 20007, 754, 1885]	[1894, 1212, 0, 0]	300	189	[15.2241, 33.3333, 150.074, -39.9705]	25.270719559905473
pdb2mvj	c	[32681, 55712, 3391, 2035]	[17381, 29601, 1885, 1131]	[1894, 1212, 0, 0]	300	189	[15 4000 00 1054 150 005 00 0004]	-
pdb2mvt	q	[80628, 118586, 3764, 9410]	[44376, 55340, 2088, 5220]	[5728, 3688, 0, 0]	837 837	$628 \\ 628$	[15.4363, 33.1354, 150.027, -39.9894]	25.248130779516732
pdb2mvt pdb2n00	c	[93074, 157880, 9411, 5647]	[48036, 81840, 5220, 3132]	[5728, 3688, 0, 0] [12993, 8381, 0, 0]	1897	1463	[15 4017 99 1971 150 011 90 0054]	- 25.229822634571384
pdb2n00 pdb2n00	q	[187687, 276049, 8762, 21905] $[216594, 367496, 21906, 13144]$	[105286, 131277, 4966, 12415] [113735, 193941, 12415, 7449]	[12993, 8381, 0, 0]	1897	$1463 \\ 1463$	[15.4017, 33.1271, 150.011, -39.9954]	25.229822034571384
pdb2n0b	c q	[11022, 16201, 510, 1275]	[5768, 7192, 272, 680]	[727, 473, 0, 0]	118	92	[15.3239, 32.856, 150.196, -39.9216]	25.05860452289024
pdb2n0b	c c	[12711, 21524, 1276, 766]	[6232, 10626, 680, 408]	[727, 473, 0, 0]	118	92	[13.3233, 32.330, 130.130, -33.3210]	25.05000452265024
pdb2n0c	q	[9290, 13676, 440, 1100]	[4884, 6094, 228, 570]	[551, 357, 0, 0]	105	66	[15.3714, 33.2553, 150.227, -39.9091]	25.291765281971767
pdb2n0c	c c	[10718, 18224, 1101, 661]	[5322, 9042, 570, 342]	[551, 357, 0, 0]	105	66	[10.0.11, 00.2000, 100.221, 900.0001]	
pdb2n0d	q	[9785, 14390, 456, 1140]	[5088, 6344, 240, 600]	[659, 427, 0, 0]	107	79	[15.1967, 32.8353, 150.219, -39.9123]	24.997089752046865
pdb2n0d	c c	[11272, 19115, 1141, 685]	[5496, 9372, 600, 360]	[659, 427, 0, 0]	107	79	[10.100., 02.0000, 100.210, 900.0120]	
pdb2n0e	q	[10673, 15684, 492, 1230]	[5592, 6972, 264, 660]	[801, 517, 0, 0]	113	91	[15.3378, 32.8169, 150.203, -39.9187]	25.043626909790227
pdb2n0e	c	[12310, 20831, 1231, 739]	[6036, 10296, 660, 396]	[801, 517, 0, 0]	113	91		_
pdb2n0f	q	[10891, 16029, 514, 1285]	[5854, 7303, 274, 685]	[744, 478, 0, 0]	119	79	[15.398, 33.2522, 150.195, -39.9222]	25.300323827431328
pdb2n0f	c	[12568, 21359, 1286, 772]	[6365, 10824, 685, 411]	[744, 478, 0, 0]	119	79	-	-
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pdb2n0g	\mathbf{q}	[10986, 16172, 520, 1300]	[6018, 7507, 282, 705]	[728, 468, 0, 0]	118	78	[15.3741, 33.2983, 150.192, -39.9231]	25.315756781006282
pdb2n0g	c	$[12675,\ 21557,\ 1301,\ 781]$	$[6537,\ 11121,\ 705,\ 423]$	$[728, \ 468, \ 0, \ 0]$	118	78	-	-
pdb2n0h	\mathbf{q}	$[10783,\ 15839,\ 494,\ 1235]$	[5554, 6925, 262, 655]	[805, 521, 0, 0]	115	95	[15.4039, 32.7672, 150.202, -39.919]	25.043208352439073
pdb2n0h	c	$[12444,\ 21029,\ 1236,\ 742]$	[5999, 10230, 655, 393]	[805, 521, 0, 0]	115	95		-
pdb2n35	\mathbf{q}	[59138,86870,2708,6770]	[31300,39020,1480,3700]	[4642, 2994, 0, 0]	613	522	[15.408, 32.7766, 150.037, -39.9852]	25.044698558069545
pdb2n35	c	[68250, 115343, 6771, 4063]	[33740, 57585, 3700, 2220]	[4642, 2994, 0, 0]	613	522	·	.
pdb2n41	\mathbf{q}	[169430, 249229, 7926, 19815]	[95826, 119485, 4518, 11295]	[11115, 7189, 0, 0]	1703	1300	[15.4129, 33.1795, 150.013, -39.995]	25.26254480286738
pdb2n41	c	[195544, 331922, 19816, 11890]	[103551, 176550, 11295, 6777]	[11115, 7189, 0, 0]	1703	1300		-
pdb2n4e	\mathbf{q}	[122312, 180062, 5788, 14470]	[68980, 86026, 3244, 8110]	[7992, 5144, 0, 0]	1271	872	[15.3411, 33.2785, 150.017, -39.9931]	25.286394406010572
pdb2n4e	c	[141076, 239984, 14471, 8683]	[74702, 127248, 8110, 4866]	[7992, 5144, 0, 0]	1271	872	[15 5555 00 0055 150 00 00 0001]	-
pdb2n5q	q	[73487, 107959, 3374, 8435]	[40768, 50830, 1924, 4810]	[5197, 3369, 0, 0]	724	$627 \\ 627$	[15.5755, 33.0357, 150.03, -39.9881]	25.25161056635017
pdb2n5q	c	[84933, 143624, 8436, 5062]	[44018, 75075, 4810, 2886]	[5197, 3369, 0, 0]	$724 \\ 1087$		[15 9697 99 9807 150 09 90 0010]	25 206147441526506
pdb2n67	q	[104051, 153170, 4920, 12300]	[58388, 72820, 2744, 6860] $[63268, 107745, 6860, 4116]$	[7045, 4525, 0, 0] [7045, 4525, 0, 0]	1087	$745 \\ 745$	[15.3627, 33.2807, 150.02, -39.9919]	25.296147441526596
pdb2n67 pdb2n6n	c	$[120036, 204146, 12301, 7381] \ [86954, 127696, 3968, 9920]$	[47652, 59400, 2256, 5640]	[7045, 4525, 0, 0] $[5944, 3876, 0, 0]$	855	745 774	[15.5047, 32.8632, 150.025, -39.9899]	25.13061285212963
pdb2n6n	q c	[100436, 169661, 9921, 5953]	[51312, 87615, 5640, 3384]	[5944, 3876, 0, 0]	855	774	[13.3047, 32.8032, 130.023, -39.9899]	25.13001285212905
pdb2n0n pdb2n7i	q	[42473, 62396, 1948, 4870]	[22520, 28076, 1064, 2660]	[3291, 2123, 0, 0]	441	371	[15.4192, 32.8146, 150.051, -39.9795]	25.07006186933125
pdb2n7i	c c	[49022, 82871, 4871, 2923]	[24292, 41448, 2660, 1596]	[3291, 2123, 0, 0]	441	371	[10.4102, 02.0140, 100.001, -00.0100]	20.01000100000120
pdb2n7j	q	[106500, 156573, 4942, 12355]	[59760, 74510, 2820, 7050]	[7168, 4644, 0, 0]	1060	858	[15.4676, 33.1028, 150.02, -39.9919]	25.24378499839497
pdb2n7j	c	[122973, 208403, 12356, 7414]	[64530, 110055, 7050, 4230]	[7168, 4644, 0, 0]	1060	858	[10.4010, 00.1020, 100.02, -00.0010]	20.2401040000401
pdb2na9	q	[46617, 68692, 2236, 5590]	[26480, 33026, 1244, 3110]	[3148, 2010, 0, 0]	495	303	[15.2112, 33.3722, 150.045, -39.9821]	25.285256019815638
pdb2na9	c	[53708, 91616, 5591, 3355]	[28702, 48873, 3110, 1866]	[3148, 2010, 0, 0]	495	303		-
pdb2ndc	q	[20462, 30130, 972, 2430]	[11572, 14432, 544, 1360]	[1327, 853, 0, 0]	213	142	[15.3064, 33.319, 150.103, -39.9588]	25.297255250583394
pdb2ndc	ć	[23594, 40169, 2431, 1459]	[12536, 21351, 1360, 816]	[1327, 853, 0, 0]	213	142	· · · · · · · · · · · · · · · · · · ·	-
pdb2nde	q	[17757, 26161, 850, 2125]	[9934, 12391, 466, 1165]	[1157, 741, 0, 0]	191	117	[15.2447, 33.3626, 150.118, -39.9529]	25.29588637963023
pdb2nde	c	[20464, 34889, 2126, 1276]	[10781, 18348, 1165, 699]	[1157, 741, 0, 0]	191	117	-	_
pdb2ndk	\mathbf{q}	[52336, 77111, 2506, 6265]	[29110, 36309, 1366, 3415]	[3711, 2365, 0, 0]	569	346	[15.2132, 33.3182, 150.04, -39.984]	25.256478895657587
pdb2ndk	c	[60298, 102803, 6266, 3760]	[31583, 53757, 3415, 2049]	[3711, 2365, 0, 0]	569	346	<u>-</u>	-
pdb2nvj	\mathbf{q}	$[23109,\ 34068,\ 1116,\ 2790]$	[12930, 16129, 606, 1515]	[1623, 1031, 0, 0]	254	143	[15.1543, 33.4067, 150.09, -39.9642]	25.281993353306163
pdb2nvj	c	$[26611,\ 45449,\ 2791,\ 1675]$	$[14043,\ 23892,\ 1515,\ 909]$	$[1623,\ 1031,\ 0,\ 0]$	254	143	-	-
pdb2p6j	\mathbf{q}	$[58282,\ 85843,\ 2778,\ 6945]$	$[33054,\ 41223,\ 1554,\ 3885]$	[3896, 2496, 0, 0]	611	396	$[15.2671,\ 33.3271,\ 150.036,\ -39.9856]$	25.283396599240817
pdb2p6j	c	[67180, 114452, 6946, 4168]	[35805, 60984, 3885, 2331]	[3896, 2496, 0, 0]	611	396		-
pdb2p81	\mathbf{q}	$[46321,\ 68226,\ 2208,\ 5520]$	[25710, 32069, 1206, 3015]	[3130, 2004, 0, 0]	500	315	[15.2846, 33.3157, 150.045, -39.9819]	25.283991003884676
pdb2p81	c	[53401, 90956, 5521, 3313]	[27903, 47487, 3015, 1809]	[3130, 2004, 0, 0]	500	315	·	.
pdb2rlg	q	[20006, 29467, 954, 2385]	[11232, 14008, 528, 1320]	[1341, 859, 0, 0]	212	136	[15.2304, 33.2949, 150.105, -39.9581]	25.253730212830416
pdb2rlg	c	[23053, 39278, 2386, 1432]	[12168, 20724, 1320, 792]	[1341, 859, 0, 0]	212	136	-	-
pdb2rlh	q	[21713, 31974, 1032, 2580]	[12240, 15264, 576, 1440]	[1516, 970, 0, 0]	227	151	[15.2489, 33.2677, 150.097, -39.9612]	25.246513900766153
pdb2rlh	c	[25024, 42611, 2581, 1549]	[13248, 22572, 1440, 864]	[1516, 970, 0, 0]	227	151	[15 0501 00 0055 150 054 00 0505]	-
pdb2rmy	q	[38989, 57425, 1858, 4645]	[22124, 27592, 1040, 2600]	[2585, 1657, 0, 0]	$\frac{408}{408}$	$\frac{265}{265}$	[15.2761, 33.3357, 150.054, -39.9785]	25.29222577416754
pdb2rmy pdb2rnd	c	$[44945, 76568, 4646, 2788] \ [37175, 54772, 1780, 4450]$	$[23968, 40821, 2600, 1560] \ [20990, 26179, 986, 2465]$	[2585, 1657, 0, 0] [2460, 1574, 0, 0]	396	$\frac{265}{245}$	[15.2199, 33.3473, 150.056, -39.9775]	- 25.27577742241054
pdb2rnd pdb2rnd	q c	[42833, 73037, 4451, 2671]	[22753, 38742, 2465, 1479]	[2460, 1574, 0, 0]	396	245	[13.2133, 33.3473, 130.030, -33.3773]	25.21511142241054
pdb2rnd pdb2roo	q	[447347, 654945, 19498, 48745]	[205348, 256256, 9568, 23920]	[31129, 20621, 0, 0]	4964	4859	[16.1651, 32.6169, 150.005, -39.9979]	25.260927695455493
pdb2roo	c	[519661, 868568, 48746, 29248]	[224120, 380523, 23920, 14352]	[31129, 20621, 0, 0]	4964	4859	[10/1001, 02/0100, 100/000, 00/00/0]	-
pdb2rql	q	[932612, 1368952, 42280, 105700]	[518076, 645800, 24528, 61320]	[65861, 42923, 0, 0]	8875	8516	[15.6314, 32.9044, 150.002, -39.9991]	25.203343969326532
pdb2rql	c	[1078392, 1819397, 105701, 63421]	[557856, 952545, 61320, 36792]	[65861, 42923, 0, 0]	8875	8516	-	-
pdb2rut	q	[39631, 58334, 1872, 4680]	[22300, 27812, 1048, 2620]	[2495, 1611, 0, 0]	411	285	[15.3844, 33.2945, 150.053, -39.9786]	25.313585349751722
pdb2rut	c	[45728, 77756, 4681, 2809]	[24164, 41151, 2620, 1572]	[2495, 1611, 0, 0]	411	285	-	_
pdb2ruv	\mathbf{q}	[41003, 60370, 1944, 4860]	[22980, 28660, 1080, 2700]	[2599, 1675, 0, 0]	431	289	[15.3184, 33.2814, 150.051, -39.9794]	25.279865405770163
pdb2ruv	c	[47284, 80462, 4861, 2917]	[24900, 42405, 2700, 1620]	[2599, 1675, 0, 0]	431	289	· · · · · · · · · · · · · · · · · · ·	-
pdb2rux	\mathbf{q}	[41629, 61288, 1972, 4930]	[23434, 29225, 1102, 2755]	[2615, 1687, 0, 0]	434	295	[15.3211, 33.2773, 150.051, -39.9797]	25.278867955453975
pdb2rux	c	[48007, 81683, 4931, 2959]	[25379, 43230, 2755, 1653]	[2615, 1687, 0, 0]	434	295	<u>-</u>	-
pdb2ruy	\mathbf{q}	[42009, 61834, 1984, 4960]	[23610, 29445, 1110, 2775]	[2578, 1668, 0, 0]	436	303	$[15.3681,\ 33.2746,\ 150.05,\ -39.9798]$	25.29628927581755
pdb2ruy	c	$[48465,\ 82409,\ 4961,\ 2977]$	[25575, 43560, 2775, 1665]	[2578, 1668, 0, 0]	436	303	-	-
pdb2rv3	\mathbf{q}	[42908, 63152, 2024, 5060]	[24190, 30167, 1138, 2845]	[2702, 1746, 0, 0]	442	312	$[15.3701,\ 33.2626,\ 150.049,\ -39.9802]$	25.290779891112216
pdb2rv3	c	[49503, 84158, 5061, 3037]	[26189, 44616, 2845, 1707]	[2702, 1746, 0, 0]	442	312		-
pdb2rv5	\mathbf{q}	[39247, 57787, 1862, 4655]	[22124, 27592, 1040, 2600]	[2505, 1613, 0, 0]	410	275	[15.3184, 33.2999, 150.054, -39.9785]	25.289953742600257
pdb2rv5	c	[45259, 77030, 4656, 2794]	[23968, 40821, 2600, 1560]	[2505, 1613, 0, 0]	410	275	[15 551 00 0045 150 005 00 0051]	-
pdb2y4q	\mathbf{q}	[297633, 437212, 13644, 34110]	[166020, 206972, 7848, 19620]	[21257, 13781, 0, 0]	2897	2567	[15.551, 32.9945, 150.007, -39.9971]	25.219173548650065

pdb2y4q c [343918, 581468, 34111, 20467] [179004, 305481, 19620, 11772] [21257, 13781, 0, 0] 2897 2567