Table 1: Results

Problem	Method	LDE	RMSD	Time	Improv time
pdb1ba5	Classic	1.668×10^{-20}		1.4413×10^{-1}	
	Quaternion	4.257×10^{-21}	1.8249×10^{-10}	1.4349×10^{-1}	0.446 49
pdb1d1n	Classic	4.268×10^{-11}		4.4043×10^{-1}	
	Quaternion	4.268×10^{-11}	1.1200×10^{-11}	4.3901×10^{-1}	0.324 44
pdb1dp3	Classic	2.048×10^{-10}		2.9882×10^{-1}	
	Quaternion	2.048×10^{-10}	8.2794×10^{-11}	2.9610×10^{-1}	0.917 71
pdb1du1	Classic	1.486×10^{-21}		2.0292×10^{-2}	
	Quaternion	2.921×10^{-21}	1.1862×10^{-12}	2.0271×10^{-2}	0.104 44
pdb1fcl	Classic	1.650×10^{-10}		4.4086×10^{-1}	
	Quaternion	1.650×10^{-10}	2.5527×10^{-12}	4.3771×10^{-1}	0.720 93
pdb1fd6	Classic	7.499×10^{-20}		3.0047×10^{-1}	
	Quaternion	3.248×10^{-20}	1.4000×10^{-11}	2.9859×10^{-1}	0.631 64
pdb1i2u	Classic	3.527×10^{-21}		9.7327×10^{-2}	
	Quaternion	4.779×10^{-22}	9.1058×10^{-12}	9.6471×10^{-2}	0.887 48
pdb1i2v	Classic	7.063×10^{-22}		1.1454×10^{-1}	
	Quaternion	3.179×10^{-22}	9.5660×10^{-13}	1.1369×10^{-1}	0.748 27
pdb1jlz	Classic	1.660×10^{-21}		3.0144×10^{-2}	
	Quaternion	3.852×10^{-22}	8.6556×10^{-12}	2.9886×10^{-2}	0.862 10
pdb1k0v	Classic	1.606×10^{-22}		2.3926×10^{-1}	
	Quaternion	8.541×10^{-23}	3.0991×10^{-13}	2.3946×10^{-1}	$-0.081 85$
pdb1k37	Classic	7.963×10^{-22}		2.9570×10^{-1}	
	Quaternion	6.716×10^{-22}	6.5474×10^{-13}	2.9406×10^{-1}	0.556 86
pdb1kuw	Classic	3.312×10^{-23}		7.4052×10^{-3}	
	Quaternion	8.201×10^{-24}	6.6737×10^{-13}	7.3113×10^{-3}	1.283 74
pdb1kz0	Classic	1.526×10^{-24}		1.4565×10^{-2}	
	Quaternion	2.722×10^{-24}	6.9116×10^{-13}	1.4381×10^{-2}	1.276 29
pdb1kz2	Classic	7.777×10^{-25}		1.6620×10^{-2}	
	Quaternion	4.694×10^{-25}	4.2483×10^{-12}	1.6437×10^{-2}	1.108 78
pdb1kz5	Classic	1.825×10^{-23}		9.2964×10^{-3}	
	Quaternion	2.280×10^{-24}	2.9273×10^{-12}	9.1759×10^{-3}	1.313 70
pdb1lvz	Classic	2.004×10^{-10}		7.6495×10^{-3}	
	Quaternion	2.004×10^{-10}	6.6194×10^{-13}	7.5425×10^{-3}	1.418 22
pdb1m4e	Classic	1.304×10^{-10}		2.1458×10^{-2}	
	Quaternion	1.304×10^{-10}	5.9826×10^{-12}	2.1240×10^{-2}	1.030 08
pdb1ma2	Classic	8.239×10^{-10}		1.6603×10^{-1}	
	Quaternion	8.239×10^{-10}	4.8491×10^{-11}	1.6443×10^{-1}	0.976 79
pdb1ma4	Classic	1.637×10^{-10}		5.9359×10^{-2}	
	Quaternion	1.637×10^{-10}	5.5679×10^{-13}	5.8936×10^{-2}	0.717 77
pdb1ma5	Classic	2.268×10^{-22}		1.6428×10^{-2}	
	Quaternion	7.238×10^{-22}	4.1675×10^{-12}	1.6354×10^{-2}	0.452 90
pdb1ma6	Classic	3.569×10^{-11}		1.5277×10^{-2}	
	Quaternion	3.569×10^{-11}	6.0995×10^{-11}	1.5208×10^{-2}	0.450 95
pdb1nd9	Classic	4.573×10^{-22}		3.3095×10^{-1}	
	Quaternion	2.343×10^{-22}	1.8713×10^{-12}	3.3016×10^{-1}	0.240 16
pdb1ne5	Classic	2.641×10^{-20}		1.7650×10^{-1}	
	Quaternion	3.682×10^{-21}	9.1988×10^{-12}	1.7643×10^{-1}	0.040 45

Table 2: Results - continued

Problem	Method	LDE	RMSD	Time	Improv time
pdb1nmj	Classic	5.850×10^{-26}		3.8740×10^{-2}	
	Quaternion	1.380×10^{-25}	1.6907×10^{-13}	3.8519×10^{-2}	0.575 07
pdb1o53	Classic	1.022×10^{-10}		1.4653×10^{-2}	
	Quaternion	1.022×10^{-10}	1.1873×10^{-12}	1.4545×10^{-2}	0.747 34
pdb1plw	Classic	6.936×10^{-25}		2.4240×10^{-3}	
	Quaternion	5.299×10^{-25}	4.6242×10^{-13}	2.3922×10^{-3}	1.329 36
pdb1plx	Classic	5.513×10^{-23}		2.2514×10^{-3}	
	Quaternion	5.592×10^{-24}	4.7012×10^{-12}	2.2188×10^{-3}	1.470 79
pdb1pv0	Classic	1.232×10^{-10}		1.2315×10^{-1}	
	Quaternion	1.232×10^{-10}	3.3931×10^{-12}	1.2260×10^{-1}	0.450 33
pdb1r57	Classic	1.769×10^{-12}		6.6138×10^{-1}	
	Quaternion	1.769×10^{-12}	2.1316×10^{-12}	6.5990×10^{-1}	0.223 55
pdb1ry3	Classic	2.466×10^{-10}		2.1507×10^{-1}	
	Quaternion	2.466×10^{-10}	3.4230×10^{-12}	2.1416×10^{-1}	0.424 70
pdb1s4h	Classic	8.706×10^{-13}		9.9728×10^{-3}	
	Quaternion	8.707×10^{-13}	8.7429×10^{-12}	9.9124×10^{-3}	0.609 58
pdb1s4j	Classic	3.470×10^{-10}		1.0673×10^{-2}	
	Quaternion	3.470×10^{-10}	9.2762×10^{-13}	1.0524×10^{-2}	1.417 84
pdb1sa8	Classic	9.204×10^{-21}		4.9189×10^{-1}	
	Quaternion	7.551×10^{-21}	2.7989×10^{-12}	4.8932×10^{-1}	0.526 37
pdb1t2y	Classic	5.709×10^{-23}		3.5555×10^{-2}	
	Quaternion	6.970×10^{-23}	2.7851×10^{-12}	3.5177×10^{-2}	1.073 18
pdb1t5q	Classic	1.910×10^{-24}		3.9906×10^{-2}	
	Quaternion	1.372×10^{-24}	1.4825×10^{-13}	3.9586×10^{-2}	0.808 47
pdb1tot	Classic	6.807×10^{-24}		1.1682×10^{-1}	
	Quaternion	9.344×10^{-24}	2.3697×10^{-13}	1.1597×10^{-1}	0.735 30
pdb1v6r	Classic	1.133×10^{-21}		2.5292×10^{-2}	
	Quaternion	1.378×10^{-21}	3.7304×10^{-12}	2.5302×10^{-2}	$-0.040 87$
pdb1v92	Classic	1.867×10^{-23}		1.0239×10^{-1}	
	Quaternion	2.846×10^{-23}	2.4804×10^{-12}	1.0186×10^{-1}	0.522 24
pdb1vd7	Classic	2.704×10^{-10}		2.5956×10^{-2}	
	Quaternion	2.704×10^{-10}	2.3012×10^{-12}	2.5745×10^{-2}	0.819 55
pdb1vd9	Classic	1.193×10^{-9}		3.1137×10^{-2}	
	Quaternion	1.193×10^{-9}	3.8355×10^{-11}	3.0860×10^{-2}	0.898 38
pdb1vdb	Classic	4.944×10^{-10}		2.7120×10^{-2}	
	Quaternion	4.944×10^{-10}	1.1210×10^{-11}	2.6924×10^{-2}	0.729 43
pdb1vpc	Classic	1.062×10^{-25}		8.3528×10^{-2}	
	Quaternion	1.105×10^{-25}	1.0206×10^{-13}	8.3257×10^{-2}	0.325 13
pdb1wnk	Classic	3.206×10^{-19}		2.6900×10^{-2}	
	Quaternion	6.740×10^{-20}	7.6026×10^{-10}	2.6695×10^{-2}	0.766 78
pdb1wo4	Classic	7.461×10^{-22}		2.1281×10^{-1}	
	Quaternion	3.313×10^{-21}	1.3690×10^{-11}	2.1081×10^{-1}	0.951 04
pdb1wo5	Classic	4.597×10^{-11}		5.6402×10^{-2}	
	Quaternion	4.597×10^{-11}	1.6851×10^{-11}	5.5896×10^{-2}	0.905 59
pdb1y5c	Classic	4.251×10^{-11}		7.3340×10^{-3}	

2

Table 2: Results - continued

Problem	Method	LDE	RMSD	Time	Improv time
	Quaternion	4.251×10^{-11}	9.7008×10^{-12}	7.2662×10^{-3}	0.933 77
pdb1yxr	Classic	2.219×10^{-11}		5.0028×10^{-1}	
	Quaternion	2.219×10^{-11}	2.3743×10^{-12}	4.9826×10^{-1}	0.404 86
pdb2a4j	Classic	1.197×10^{-24}		4.5177×10^{-1}	
	Quaternion	4.366×10^{-24}	2.9037×10^{-13}	4.5070×10^{-1}	0.238 20
pdb2ajj	Classic	3.438×10^{-10}		4.0839×10^{-2}	
	Quaternion	3.438×10^{-10}	1.1290×10^{-12}	4.0565×10^{-2}	0.675 87
pdb2ajm	Classic	2.889×10^{-10}		4.3200×10^{-2}	
	Quaternion	2.889×10^{-10}	3.0199×10^{-12}	4.2870×10^{-2}	0.771 18
pdb2ajn	Classic	1.802×10^{-10}		4.1825×10^{-2}	
	Quaternion	1.802×10^{-10}	4.6193×10^{-13}	4.1507×10^{-2}	0.765 02
pdb2ajo	Classic	2.889×10^{-10}		4.3132×10^{-2}	
	Quaternion	2.889×10^{-10}	3.0199×10^{-12}	4.2863×10^{-2}	0.628 78
pdb2akk	Classic	8.363×10^{-23}		6.2126×10^{-1}	
	Quaternion	2.487×10^{-23}	1.1166×10^{-12}	6.1873×10^{-1}	0.408 58
pdb2c0s	Classic	7.695×10^{-21}		1.7448×10^{-1}	
	Quaternion	6.254×10^{-22}	1.3872×10^{-11}	1.7263×10^{-1}	1.066 82
pdb2dci	Classic	5.231×10^{-25}		1.9252×10^{-2}	
	Quaternion	5.202×10^{-25}	1.0732×10^{-13}	1.9080×10^{-2}	0.898 60
pdb2eem	Classic	1.971×10^{-22}		1.2915×10^{-1}	
	Quaternion	1.553×10^{-21}	7.6795×10^{-12}	1.2805×10^{-1}	0.858 13
pdb2fxz	Classic	8.123×10^{-10}		1.0055×10^{-2}	
	Quaternion	8.123×10^{-10}	4.9386×10^{-12}	9.9432×10^{-3}	1.122 97
pdb2g9l	Classic	3.224×10^{-24}		6.6193×10^{-2}	
	Quaternion	5.977×10^{-24}	1.9157×10^{-12}	6.5694×10^{-2}	0.758 26
pdb2h5m	Classic	3.715×10^{-12}		4.9788×10^{-1}	
	Quaternion	3.715×10^{-12}	2.4650×10^{-11}	4.9684×10^{-1}	0.208 12
pdb2hep	Classic	3.189×10^{-21}		2.3597×10^{-1}	
	Quaternion	1.788×10^{-20}	1.7197×10^{-11}	2.3431×10^{-1}	0.710 53
pdb2jmy	Classic	2.980×10^{-21}		1.4922×10^{-2}	
	Quaternion	3.343×10^{-21}	1.2262×10^{-12}	1.4788×10^{-2}	0.905 44
pdb2jn5	Classic	2.985×10^{-13}		1.2230×10^{-2}	
	Quaternion	2.985×10^{-13}	1.1243×10^{-11}	1.2114×10^{-2}	0.957 76
pdb2jpn	Classic	1.049×10^{-23}		4.9439×10^{-1}	
	Quaternion	1.655×10^{-22}	4.9731×10^{-12}	4.9119×10^{-1}	0.651 16
pdb2jua	Classic	1.231×10^{-17}		5.3358×10^{-1}	
	Quaternion	6.900×10^{-18}	2.0200×10^{-11}	5.3087×10^{-1}	0.509 91
pdb2jvd	Classic	5.270×10^{-24}		1.1403×10^{-1}	
	Quaternion	4.315×10^{-24}	3.6252×10^{-13}	1.1327×10^{-1}	0.669 95
pdb2jws	Classic	8.553×10^{-11}		1.5524×10^{-1}	
	Quaternion	8.553×10^{-11}	1.0841×10^{-12}	1.5374×10^{-1}	0.975 22
pdb2jwu	Classic	6.308×10^{-11}		4.4432×10^{-1}	
	Quaternion	6.308×10^{-11}	6.6652×10^{-12}	4.4120×10^{-1}	0.708 61
pdb2jxf	Classic	2.349×10^{-11}		4.5784×10^{-2}	
	Quaternion	2.349×10^{-11}	1.2542×10^{-12}	4.5361×10^{-2}	0.933 89

Problem	Method	LDE	RMSD	Time	Improv time
pdb2jz5	Classic	9.033×10^{-23}		7.1518×10^{-1}	
	Quaternion	3.915×10^{-22}	6.3878×10^{-13}	7.1144×10^{-1}	0.526 08
pdb2k2a	Classic	9.674×10^{-24}		2.2462×10^{-1}	
	Quaternion	2.783×10^{-24}	2.8282×10^{-12}	2.2392×10^{-1}	0.310 73
pdb2k36	Classic	1.309×10^{-11}		9.5795×10^{-1}	
	Quaternion	1.309×10^{-11}	1.8097×10^{-12}	9.5117×10^{-1}	0.712 06
pdb2k37	Classic	8.119×10^{-23}		1.7820×10^{-1}	
	Quaternion	6.702×10^{-23}	2.5914×10^{-12}	1.7650×10^{-1}	0.958 72
pdb2k3i	Classic	7.836×10^{-22}		8.0314×10^{-1}	
	Quaternion	7.168×10^{-22}	1.8935×10^{-12}	7.9830×10^{-1}	0.607 26
pdb2kdh	Classic	1.914×10^{-10}		3.4888×10^{-1}	
	Quaternion	1.914×10^{-10}	1.2342×10^{-9}	3.4531×10^{-1}	1.034 71
pdb2kdl	Classic	5.538×10^{-11}		4.1603×10^{-1}	
	Quaternion	5.538×10^{-11}	3.8154×10^{-12}	4.1312×10^{-1}	0.705 99
pdb2kdm	Classic	6.081×10^{-11}		2.8322×10^{-1}	
	Quaternion	6.081×10^{-11}	7.3936×10^{-12}	2.8103×10^{-1}	0.777 87
pdb2kdp	Classic	1.285×10^{-22}		2.3389×10^{-1}	
	Quaternion	2.725×10^{-22}	1.7049×10^{-12}	2.3269×10^{-1}	0.513 95
pdb2kdr	Classic	3.104×10^{-11}		4.2004×10^{-2}	
	Quaternion	3.104×10^{-11}	3.3412×10^{-13}	4.1603×10^{-2}	0.963 95
pdb2kes	Classic	3.820×10^{-24}		1.3388×10^{-1}	
	Quaternion	4.201×10^{-24}	3.1744×10^{-13}	1.3295×10^{-1}	0.699 37
pdb2kjn	Classic	7.890×10^{-14}		3.6111×10^{-2}	
	Quaternion	7.890×10^{-14}	1.3838×10^{-12}	3.6017×10^{-2}	0.262 16
pdb2kjo	Classic	1.239×10^{-10}		3.3074×10^{-2}	
	Quaternion	1.239×10^{-10}	9.3751×10^{-12}	3.2755×10^{-2}	0.974 33
pdb2kl5	Classic	3.622×10^{-22}		5.6996×10^{-1}	
	Quaternion	1.254×10^{-22}	3.1368×10^{-12}	5.6571×10^{-1}	0.751 22
pdb2klz	Classic	7.720×10^{-25}		1.1474×10^{-1}	
	Quaternion	9.391×10^{-25}	4.6317×10^{-13}	1.1414×10^{-1}	0.525 60
pdb2koz	Classic	3.052×10^{-10}		6.1232×10^{-2}	
	Quaternion	3.052×10^{-10}	1.6248×10^{-11}	6.0651×10^{-2}	0.957 22
pdb2kp0	Classic	1.444×10^{-11}		1.9142×10^{-1}	
	Quaternion	1.444×10^{-11}	6.2079×10^{-11}	1.8952×10^{-1}	1.003 82
pdb2ksg	Classic	1.069×10^{-24}		1.0602×10^{-1}	
	Quaternion	9.982×10^{-25}	6.1641×10^{-13}	1.0521×10^{-1}	0.769 81
pdb2kt8	Classic	3.760×10^{-20}		8.8593×10^{-1}	
	Quaternion	4.331×10^{-20}	4.9046×10^{-12}	8.7856×10^{-1}	0.839 78
pdb2kuh	Classic	4.485×10^{-24}		2.0172×10^{-1}	
	Quaternion	1.309×10^{-24}	7.0876×10^{-13}	2.0076×10^{-1}	0.474 61
pdb2kwh	Classic	1.137×10^{-23}		1.6084×10^{-1}	
	Quaternion	1.274×10^{-22}	3.6703×10^{-12}	1.5920×10^{-1}	1.031 90
pdb2kxa	Classic	9.598×10^{-11}		2.4971×10^{-2}	
	Quaternion	9.598×10^{-11}	4.1552×10^{-12}	2.4736×10^{-2}	0.947 74
pdb2l3m	Classic	3.284×10^{-21}		2.1724×10^{-1}	

Table 2: Results - continued

Problem	Method	LDE	RMSD	Time	Improv time
	Quaternion	2.841×10^{-21}	6.0669×10^{-13}	2.1761×10^{-1}	$-0.172\,15$
pdb2l45	Classic	2.567×10^{-25}		2.6002×10^{-2}	
	Quaternion	5.244×10^{-25}	1.5900×10^{-13}	2.5860×10^{-2}	$0.549\,72$
pdb2l5r	Classic	3.044×10^{-24}		3.0131×10^{-2}	
	Quaternion	1.046×10^{-24}	6.2394×10^{-13}	2.9900×10^{-2}	$0.771\,47$
pdb2l6q	Classic	1.881×10^{-10}		5.2458×10^{-1}	
	Quaternion	1.881×10^{-10}	9.8136×10^{-10}	5.2225×10^{-1}	$0.446\,43$
pdb2l6r	Classic	4.111×10^{-11}		1.7773×10^{-1}	
	Quaternion	4.111×10^{-11}	1.8748×10^{-11}	1.7736×10^{-1}	$0.206\,90$
pdb2l98	Classic	9.739×10^{-20}		8.0137×10^{-1}	
	Quaternion	5.266×10^{-22}	3.2376×10^{-11}	7.9837×10^{-1}	$0.375\,57$
pdb2lci	Classic	6.861×10^{-22}		9.4134×10^{-1}	
	Quaternion	2.948×10^{-22}	8.2620×10^{-13}	9.3921×10^{-1}	$0.227\,38$
pdb2lde	Classic	8.378×10^{-25}		3.2788×10^{-2}	
	Quaternion	9.211×10^{-25}	3.3386×10^{-13}	3.2598×10^{-2}	$0.582\,30$
pdb2le7	Classic	1.153×10^{-24}		2.2337×10^{-2}	
	Quaternion	3.827×10^{-25}	1.0978×10^{-13}	2.2132×10^{-2}	$0.926\,90$
pdb2ler	Classic	9.732×10^{-26}		7.7418×10^{-3}	
	Quaternion	7.513×10^{-26}	4.8108×10^{-14}	7.6680×10^{-3}	$0.962\,11$
pdb2lgi	Classic	8.360×10^{-21}		2.9400×10^{-1}	
	Quaternion	3.866×10^{-21}	5.4589×10^{-12}	2.9234×10^{-1}	$0.567\,15$
pdb2lhc	Classic	1.418×10^{-10}		1.7750×10^{-1}	
	Quaternion	1.418×10^{-10}	1.2994×10^{-9}	1.7624×10^{-1}	$0.717\,30$
pdb2lhe	Classic	1.106×10^{-17}		5.2633×10^{-1}	
	Quaternion	1.092×10^{-17}	6.3217×10^{-12}	5.2365×10^{-1}	$0.511\,61$
pdb2lhg	Classic	2.135×10^{-23}		1.2483×10^{-1}	
	Quaternion	1.904×10^{-23}	3.2233×10^{-13}	1.2435×10^{-1}	$0.385\,66$
pdb2lix	Classic	4.386×10^{-23}		3.5660×10^{-2}	
	Quaternion	5.759×10^{-24}	1.4715×10^{-12}	3.5353×10^{-2}	$0.867\,66$
pdb2lld	Classic	6.260×10^{-22}		7.0179×10^{-2}	
	Quaternion	1.197×10^{-22}	1.9602×10^{-12}	6.9871×10^{-2}	$0.441\,38$
pdb2lm9	Classic	1.758×10^{-23}		4.2582×10^{-1}	
	Quaternion	2.575×10^{-23}	7.9847×10^{-13}	4.2422×10^{-1}	$0.375\,95$
pdb2lmf	Classic	4.430×10^{-11}		2.6360×10^{-2}	
	Quaternion	4.430×10^{-11}	2.3248×10^{-12}	2.6084×10^{-2}	$1.056\,23$
pdb2ln3	Classic	1.980×10^{-22}		3.2482×10^{-1}	
	Quaternion	7.449×10^{-23}	9.4479×10^{-14}	3.2283×10^{-1}	$0.616\,10$
pdb2lo2	Classic	8.469×10^{-25}		6.8230×10^{-2}	
	Quaternion	5.148×10^{-25}	5.0804×10^{-13}	6.7595×10^{-2}	$0.939\,23$
pdb2lqp	Classic	1.624×10^{-10}		2.2855×10^{-1}	
	Quaternion	1.624×10^{-10}	1.9702×10^{-11}	2.2887×10^{-1}	$-0.139\,82$
pdb2ls9	Classic	2.860×10^{-23}		2.8447×10^{-2}	
	Quaternion	2.515×10^{-23}	6.9713×10^{-13}	2.8362×10^{-2}	$0.301\,57$
pdb2lsa	Classic	8.473×10^{-25}		2.6515×10^{-2}	
	Quaternion	5.354×10^{-24}	3.4845×10^{-13}	2.6428×10^{-2}	$0.331\,68$

Table 2: Results - continued

Problem	Method	LDE	RMSD	Time	Improv time
pdb2lss	Classic	1.966×10^{-22}		2.0018×10^{-1}	
	Quaternion	3.382×10^{-23}	3.6848×10^{-12}	2.0076×10^{-1}	$-0.290\,62$
pdb2lt3	Classic	3.839×10^{-23}		4.8177×10^{-1}	
	Quaternion	7.866×10^{-23}	3.4123×10^{-13}	4.8275×10^{-1}	$-0.202\,78$
pdb2lu6	Classic	3.603×10^{-26}		1.3044×10^{-2}	
	Quaternion	6.370×10^{-26}	1.9324×10^{-14}	1.2950×10^{-2}	$0.722\,82$
pdb2lwa	Classic	1.773×10^{-10}		2.1130×10^{-1}	
	Quaternion	1.773×10^{-10}	4.6809×10^{-12}	2.0978×10^{-1}	$0.723\,98$
pdb2lx0	Classic	6.786×10^{-11}		5.1191×10^{-2}	
	Quaternion	6.786×10^{-11}	1.9476×10^{-12}	5.0853×10^{-2}	$0.664\,92$
pdb2lxz	Classic	7.052×10^{-21}		5.9028×10^{-1}	
	Quaternion	1.797×10^{-20}	8.0453×10^{-12}	5.8716×10^{-1}	$0.532\,12$
pdb2m1a	Classic	4.881×10^{-26}		4.5472×10^{-2}	
	Quaternion	1.720×10^{-26}	1.3767×10^{-13}	4.5154×10^{-2}	$0.705\,01$
pdb2m1j	Classic	7.378×10^{-25}		4.4061×10^{-2}	
	Quaternion	3.282×10^{-25}	5.4650×10^{-13}	4.3734×10^{-2}	$0.747\,14$
pdb2m2y	Classic	3.076×10^{-23}		1.8689×10^{-2}	
	Quaternion	1.315×10^{-22}	1.1427×10^{-12}	1.8605×10^{-2}	$0.455\,32$
pdb2m3f	Classic	4.029×10^{-25}		2.4177×10^{-2}	
	Quaternion	1.628×10^{-24}	3.2592×10^{-13}	2.4088×10^{-2}	$0.367\,99$
pdb2m8m	Classic	1.870×10^{-24}		3.3201×10^{-2}	
	Quaternion	9.789×10^{-25}	1.5744×10^{-12}	3.3081×10^{-2}	$0.363\,02$
pdb2m8o	Classic	1.277×10^{-25}		3.1695×10^{-2}	
	Quaternion	2.020×10^{-25}	2.0793×10^{-13}	3.1571×10^{-2}	$0.392\,82$
pdb2m97	Classic	8.762×10^{-23}		1.8591×10^{-1}	
	Quaternion	1.529×10^{-23}	4.2576×10^{-12}	1.8452×10^{-1}	$0.755\,44$
pdb2m9r	Classic	4.190×10^{-24}		8.1743×10^{-2}	
	Quaternion	3.184×10^{-24}	1.2995×10^{-12}	8.1254×10^{-2}	$0.602\,29$
pdb2me1	Classic	2.858×10^{-22}		4.0207×10^{-2}	
	Quaternion	4.660×10^{-23}	4.1648×10^{-12}	3.9749×10^{-2}	$1.151\,68$
pdb2me2	Classic	2.316×10^{-10}		3.5160×10^{-2}	
	Quaternion	2.316×10^{-10}	1.8283×10^{-12}	3.4713×10^{-2}	$1.289\,29$
pdb2me3	Classic	1.748×10^{-10}		3.3134×10^{-2}	
	Quaternion	1.748×10^{-10}	2.5263×10^{-12}	3.2719×10^{-2}	$1.268\,17$
pdb2me4	Classic	1.462×10^{-10}		4.1246×10^{-2}	
	Quaternion	1.462×10^{-10}	9.3376×10^{-13}	4.0764×10^{-2}	$1.181\,00$
pdb2mg1	Classic	1.125×10^{-24}		3.0880×10^{-2}	
	Quaternion	2.185×10^{-24}	1.3041×10^{-12}	3.0644×10^{-2}	$0.769\,29$
pdb2mg2	Classic	1.707×10^{-25}		3.2009×10^{-2}	
	Quaternion	3.530×10^{-25}	1.4276×10^{-13}	3.1769×10^{-2}	$0.755\,33$
pdb2mg3	Classic	6.270×10^{-24}		3.5170×10^{-2}	
	Quaternion	3.333×10^{-24}	8.2131×10^{-13}	3.4969×10^{-2}	$0.574\,90$
pdb2mh8	Classic	2.558×10^{-23}		1.4083×10^{-1}	
	Quaternion	5.209×10^{-23}	1.4713×10^{-12}	1.3972×10^{-1}	$0.796\,40$
pdb2mhw	Classic	8.217×10^{-24}		3.6546×10^{-2}	

Table 2: Results - continued

Problem	Method	LDE	RMSD	Time	Improv time
	Quaternion	1.076×10^{-23}	4.0488×10^{-13}	3.6219×10^{-2}	0.904 38
pdb2mi1	Classic	1.251×10^{-10}		1.3810×10^{-1}	
	Quaternion	1.251×10^{-10}	3.2567×10^{-12}	1.3661×10^{-1}	1.093 75
pdb2mi7	Classic	7.286×10^{-11}		1.9134×10^{-1}	
	Quaternion	7.286×10^{-11}	1.0262×10^{-11}	1.9018×10^{-1}	0.611 20
pdb2mij	Classic	2.770×10^{-23}		6.3742×10^{-2}	
	Quaternion	2.702×10^{-23}	3.5837×10^{-12}	6.3251×10^{-2}	0.775 51
pdb2mix	Classic	2.388×10^{-24}		2.2331×10^{-2}	
	Quaternion	4.043×10^{-24}	2.2543×10^{-13}	2.2094×10^{-2}	1.071 22
pdb2mj1	Classic	8.148×10^{-24}		2.0482×10^{-2}	
	Quaternion	2.934×10^{-23}	1.5286×10^{-12}	2.0268×10^{-2}	1.056 37
pdb2mj2	Classic	3.199×10^{-23}		6.4609×10^{-2}	
	Quaternion	1.252×10^{-23}	2.8888×10^{-12}	6.4032×10^{-2}	0.901 21
pdb2mji	Classic	1.888×10^{-11}		8.1435×10^{-1}	
	Quaternion	1.888×10^{-11}	2.9688×10^{-11}	8.0890×10^{-1}	0.673 53
pdb2mle	Classic	2.703×10^{-22}		2.4228×10^{-1}	
	Quaternion	2.802×10^{-22}	1.1519×10^{-12}	2.4057×10^{-1}	0.713 77
pdb2mlf	Classic	5.630×10^{-23}		2.4821×10^{-1}	
	Quaternion	5.903×10^{-23}	1.9392×10^{-12}	2.4708×10^{-1}	0.457 80
pdb2mpu	Classic	8.827×10^{-23}		3.7798×10^{-1}	
	Quaternion	4.845×10^{-23}	9.0462×10^{-13}	3.7626×10^{-1}	0.455 97
pdb2msu	Classic	1.417×10^{-23}		2.4935×10^{-2}	
	Quaternion	1.122×10^{-23}	8.7849×10^{-13}	2.4704×10^{-2}	0.937 80
pdb2mty	Classic	1.003×10^{-24}		2.1482×10^{-2}	
	Quaternion	3.669×10^{-24}	2.2229×10^{-12}	2.1335×10^{-2}	0.692 94
pdb2muh	Classic	9.401×10^{-11}		2.7358×10^{-2}	
	Quaternion	9.401×10^{-11}	9.0669×10^{-12}	2.7176×10^{-2}	0.668 83
pdb2mvj	Classic	3.303×10^{-22}		3.6213×10^{-2}	
	Quaternion	6.049×10^{-23}	1.4707×10^{-11}	3.5941×10^{-2}	0.758 36
pdb2mvt	Classic	6.824×10^{-11}		1.6847×10^{-1}	
	Quaternion	6.824×10^{-11}	2.7781×10^{-10}	1.6763×10^{-1}	0.502 25
pdb2n00	Classic	4.943×10^{-11}		5.8688×10^{-1}	
	Quaternion	4.943×10^{-11}	3.0781×10^{-12}	5.8337×10^{-1}	0.602 83
pdb2n0b	Classic	9.255×10^{-10}		6.1460×10^{-3}	
	Quaternion	9.255×10^{-10}	8.1641×10^{-13}	6.0688×10^{-3}	1.272 37
pdb2n0c	Classic	8.868×10^{-10}		5.0337×10^{-3}	
	Quaternion	8.868×10^{-10}	3.1194×10^{-13}	4.9691×10^{-3}	1.299 21
pdb2n0d	Classic	1.185×10^{-9}		5.5065×10^{-3}	
	Quaternion	1.185×10^{-9}	1.1993×10^{-11}	5.4424×10^{-3}	1.177 79
pdb2n0e	Classic	1.631×10^{-20}		5.7785×10^{-3}	
	Quaternion	2.503×10^{-20}	3.9902×10^{-12}	5.7114×10^{-3}	1.173 33
pdb2n0f	Classic	2.798×10^{-12}		6.2746×10^{-3}	
	Quaternion	2.798×10^{-12}	1.3315×10^{-12}	6.2053×10^{-3}	1.116 54
pdb2n0g	Classic	4.724×10^{-11}		6.4728×10^{-3}	
	Quaternion	4.724×10^{-11}	1.1667×10^{-11}	6.4026×10^{-3}	1.096 60

Table 2: Results - continued

Problem	Method	LDE	RMSD	Time	Improv time
pdb2n0h	Classic	4.855×10^{-11}		5.8792×10^{-3}	
	Quaternion	4.855×10^{-11}	1.1609×10^{-11}	5.8166×10^{-3}	1.075 89
pdb2n35	Classic	3.985×10^{-24}		1.1930×10^{-1}	
	Quaternion	1.389×10^{-24}	1.2116×10^{-12}	1.1892×10^{-1}	0.319 49
pdb2n41	Classic	4.628×10^{-23}		6.5166×10^{-1}	
	Quaternion	1.314×10^{-22}	3.5667×10^{-13}	6.4724×10^{-1}	0.683 80
pdb2n4e	Classic	2.212×10^{-22}		5.1972×10^{-1}	
	Quaternion	7.882×10^{-23}	8.8287×10^{-13}	5.1657×10^{-1}	0.607 99
pdb2n5q	Classic	1.337×10^{-10}		8.7929×10^{-2}	
	Quaternion	1.337×10^{-10}	5.7950×10^{-12}	8.7304×10^{-2}	0.716 29
pdb2n67	Classic	1.030×10^{-21}		3.9051×10^{-1}	
	Quaternion	1.111×10^{-21}	4.6338×10^{-13}	3.8929×10^{-1}	0.313 35
pdb2n6n	Classic	6.310×10^{-12}		1.4140×10^{-1}	
	Quaternion	6.309×10^{-12}	8.3196×10^{-12}	1.4077×10^{-1}	0.450 37
pdb2n7i	Classic	1.245×10^{-11}		6.1675×10^{-2}	
	Quaternion	1.245×10^{-11}	1.4499×10^{-11}	6.1367×10^{-2}	0.502 72
pdb2n7j	Classic	3.115×10^{-22}		2.2875×10^{-1}	
	Quaternion	9.101×10^{-22}	9.7846×10^{-13}	2.2750×10^{-1}	0.548 06
pdb2na9	Classic	2.734×10^{-23}		8.8161×10^{-2}	
	Quaternion	8.610×10^{-24}	1.0478×10^{-12}	8.7559×10^{-2}	0.687 40
pdb2ndc	Classic	5.633×10^{-25}		2.0757×10^{-2}	
	Quaternion	7.826×10^{-25}	5.7876×10^{-13}	2.0556×10^{-2}	0.976 54
pdb2nde	Classic	7.159×10^{-24}		1.6123×10^{-2}	
	Quaternion	8.570×10^{-24}	8.1870×10^{-13}	1.5962×10^{-2}	1.012 52
pdb2ndk	Classic	3.106×10^{-10}		1.0467×10^{-1}	
	Quaternion	3.106×10^{-10}	1.5147×10^{-11}	1.0385×10^{-1}	0.796 44
pdb2nvj	Classic	4.326×10^{-24}		2.8261×10^{-2}	
	Quaternion	5.563×10^{-25}	5.8671×10^{-14}	2.8010×10^{-2}	0.894 52
pdb2p6j	Classic	4.017×10^{-24}		1.3058×10^{-1}	
	Quaternion	8.387×10^{-24}	1.7099×10^{-13}	1.3025×10^{-1}	0.249 27
pdb2p81	Classic	2.121×10^{-10}		8.4485×10^{-2}	
	Quaternion	2.121×10^{-10}	8.9719×10^{-12}	8.4084×10^{-2}	0.476 60
pdb2rlg	Classic	8.367×10^{-25}		1.8970×10^{-2}	
	Quaternion	1.460×10^{-24}	6.7346×10^{-13}	1.8810×10^{-2}	0.848 83
pdb2rlh	Classic	1.086×10^{-23}		2.0733×10^{-2}	
	Quaternion	3.476×10^{-24}	1.0733×10^{-12}	2.0553×10^{-2}	0.875 58
pdb2rmy	Classic	4.829×10^{-11}		6.1916×10^{-2}	
	Quaternion	4.829×10^{-11}	1.7484×10^{-12}	6.1598×10^{-2}	0.516 05
pdb2rnd	Classic	6.754×10^{-23}		5.9113×10^{-2}	
	Quaternion	7.833×10^{-23}	5.1117×10^{-12}	5.8774×10^{-2}	0.576 22
pdb2roo	Classic	3.674×10^{-20}		6.0056×10^{-1}	
	Quaternion	4.516×10^{-20}	5.3127×10^{-12}	5.9484×10^{-1}	0.961 83
pdb2rut	Classic	1.305×10^{-24}		6.5395×10^{-2}	
	Quaternion	3.227×10^{-24}	1.0520×10^{-12}	6.4825×10^{-2}	0.878 82
pdb2ruv	Classic	6.723×10^{-23}		7.0057×10^{-2}	

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Table 2: Results - continued

Problem	Method	LDE	RMSD	Time	Improv time
	Quaternion	1.728×10^{-23}	1.2232×10^{-12}	6.9627×10^{-2}	0.617 43
pdb2rux	Classic	7.500×10^{-25}		7.0486×10^{-2}	
	Quaternion	1.207×10^{-24}	9.3591×10^{-14}	6.9966×10^{-2}	0.743 66
pdb2ruy	Classic	6.585×10^{-25}		7.1120×10^{-2}	
	Quaternion	4.031×10^{-25}	1.1711×10^{-12}	7.0733×10^{-2}	0.547 56
pdb2rv3	Classic	3.543×10^{-24}		7.1410×10^{-2}	
	Quaternion	3.084×10^{-24}	8.5139×10^{-13}	7.0936×10^{-2}	0.667 59
pdb2rv5	Classic	2.414×10^{-25}		6.1965×10^{-2}	
	Quaternion	1.035×10^{-25}	1.3358×10^{-13}	6.1747×10^{-2}	0.352 71
pdb2y4q	Classic	2.687×10^{-11}		9.5763×10^{-1}	
	Quaternion	2.687×10^{-11}	2.2850×10^{-11}	9.5674×10^{-1}	0.092 94

Table 3: Operation Results

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
pdb1ba5	Classic	83480	41875	5212		735
		141083	71478	3382		637
		8276	4595	0		
		4966	2757	0		
	Quaternion	72313	38858	5212	15.44	
		106219	48441	3382	32.82	
		3310	1838	0	150.03	
		8275	4595	0	−39.99	
pdb1d1n	Classic	130125	67954	8136		1180
		221108	115731	5214		831
		13276	7370	0		
		7966	4422	0		
	Quaternion	112771	62720	8136	15.39	
		165959	78222	5214	33.23	
		5310	2948	0	150.02	
		13275	7370	0	−39.99	
pdb1dp3	Classic	169984	85389	10096		1511
		287240	145497	6566		1271
		16846	9285	0		
		10108	5571	0		
	Quaternion	147039	78906	10096	15.60	
		215989	98399	6566	32.99	
		6738	3714	0	150.01	
		16845	9285	0	−39.99	
pdb1du1	Classic	26241	13651	1444		244
		44657	23232	930		159
		2701	1475	0		
		1621	885	0		
	Quaternion	22753	12578	1444	15.33	
		33502	15689	930	33.30	
		1080	590	0	150.09	
		2700	1475	0	−39.96	
pdb1fcl	Classic	414889	213238	25630		3464
		700070	363957	16680		3255
		40716	23390	0		
		24430	14034	0		
	Quaternion	358787	197840	25630	15.64	
		526695	246634	16680	32.92	
		16286	9356	0	150.01	
		40715	23390	0	−40.00	
pdb1fd6	Classic	183487	95609	10799		1562
		310472	163119	7015		1339
		18281	10465	0		
		10969	6279	0		
	Quaternion	158833	88618	10799	15.52	
		233386	110483	7015	33.03	
		7312	4186	0	150.01	
		18280	10465	0	−39.99	
pdb1i2u	Classic	62369	32665	3796		564
		106004	55638	2436		396
		6371	3545	0		
		3823	2127	0		
	Quaternion	54060	30158	3796	15.37	
		79562	37611	2436	33.23	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		2548	1418	0	150.04	
		6370	3545	0	−39.98	
pdb1i2v	Classic	69525	35201	4416		616
		117686	60093	2854		511
		6951	3865	0		
		4171	2319	0		
	Quaternion	60273	32674	4416	15.35	
		88580	40731	2854	32.86	
		2780	1546	0	150.04	
		6950	3865	0	−39.99	
pdb1jlz	Classic	31396	16338	1778		287
		53369	27819	1146		198
		3211	1770	0		
		1927	1062	0		
	Quaternion	27214	15072	1778	15.37	
		40054	18798	1146	33.24	
		1284	708	0	150.08	
		3210	1770	0	−39.97	
pdb1k0v	Classic	96812	50399	5864		891
		164612	85800	3760		604
		9916	5455	0		
		5950	3273	0		
	Quaternion	83918	46474	5864	15.36	
		123529	57965	3760	33.26	
		3966	2182	0	150.03	
		9915	5455	0	−39.99	
pdb1k37	Classic	241008	125971	13455		1999
		407294	215061	8803		1825
		23836	13835	0		
		14302	8301	0		
	Quaternion	208553	116942	13455	15.56	
		306299	145777	8803	32.97	
		9534	5534	0	150.01	
		23835	13835	0	−40.00	
pdb1kuw	Classic	12648	6648	747		115
		21524	11319	479		77
		1301	720	0		
		781	432	0		
	Quaternion	10967	6132	747	15.33	
		16146	7648	479	33.31	
		520	288	0	150.19	
		1300	720	0	−39.92	
pdb1kz0	Classic	19469	10254	1114		180
		33173	17457	714		114
		2016	1110	0		
		1210	666	0		
	Quaternion	16892	9456	1114	15.26	
		24881	11794	714	33.33	
		806	444	0	150.12	
		2015	1110	0	−39.95	
pdb1kz2	Classic	20847	11064	1258		190
		35516	18843	804		123
		2156	1200	0		
		1294	720	0		

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	18087	10212	1258	15.26	
		26639	12736	804	33.32	
		862	480	0	150.12	
		2155	1200	0	−39.95	
pdb1kz5	Classic	15288	8120	850		139
		26045	13827	546		90
		1581	880	0		
		949	528	0		
	Quaternion	13262	7492	850	15.28	
		19532	9344	546	33.35	
		632	352	0	150.16	
		1580	880	0	−39.94	
pdb1lvz	Classic	13003	6844	743		122
		22184	11649	475		73
		1356	740	0		
		814	444	0		
	Quaternion	11289	6308	743	15.18	
		16635	7868	475	33.36	
		542	296	0	150.18	
		1355	740	0	−39.93	
pdb1m4e	Classic	23886	12658	1348		217
		40664	21549	866		143
		2461	1370	0		
		1477	822	0		
	Quaternion	20709	11672	1348	15.34	
		30494	14558	866	33.35	
		984	548	0	150.10	
		2460	1370	0	−39.96	
pdb1ma2	Classic	214798	107766	13505		1817
		361754	183843	8805		1755
		20881	11790	0		
		12529	7074	0		
	Quaternion	185593	99864	13505	15.74	
		272290	124506	8805	32.86	
		8352	4716	0	150.01	
		20880	11790	0	−40.00	
pdb1ma4	Classic	63291	32634	3356		538
		106961	55671	2204		476
		6266	3570	0		
		3760	2142	0		
	Quaternion	54758	30240	3356	15.58	
		80427	37702	2204	32.99	
		2506	1428	0	150.04	
		6265	3570	0	−39.98	
pdb1ma5	Classic	20920	10953	1199		191
		35582	18645	771		129
		2146	1185	0		
		1288	711	0		
	Quaternion	18133	10098	1199	15.37	
		26693	12595	771	33.30	
		858	474	0	150.12	
		2145	1185	0	−39.95	
pdb1ma6	Classic	19349	10106	1180		180
		32942	17193	754		115

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		1996	1090	0		
		1198	654	0		
	Quaternion	16775	9304	1180	15.34	
		24703	11606	754	33.35	
		798	436	0	150.13	
		1995	1090	0	−39.95	
pdb1nd9	Classic	210912	110485	13437		1759
		356639	188595	8691		1572
		20926	12125	0		
		12556	7275	0		
	Quaternion	182542	102530	13437	15.54	
		268151	127815	8691	33.00	
		8370	4850	0	150.01	
		20925	12125	0	−40.00	
pdb1ne5	Classic	107267	55770	6676		930
		181673	95106	4310		761
		10746	6090	0		
		6448	3654	0		
	Quaternion	92881	51636	6676	15.49	
		136525	64382	4310	33.07	
		4298	2436	0	150.02	
		10745	6090	0	−39.99	
pdb1nmj	Classic	37189	18624	2392		332
		62906	31779	1546		277
		3706	2040	0		
		2224	1224	0		
	Quaternion	32225	17268	2392	15.40	
		47349	21528	1546	32.86	
		1482	816	0	150.07	
		3705	2040	0	−39.97	
pdb1o53	Classic	20580	10757	1209		187
		34988	18315	777		129
		2106	1165	0		
		1264	699	0		
	Quaternion	17837	9922	1209	15.38	
		26253	12375	777	33.27	
		842	466	0	150.12	
		2105	1165	0	−39.95	
pdb1plw	Classic	6193	3238	318		56
		10535	5511	206		38
		636	350	0		
		382	210	0		
	Quaternion	5368	2984	318	15.37	
		7901	3722	206	33.34	
		254	140	0	150.39	
		635	350	0	−39.84	
pdb1plx	Classic	5722	2968	294		53
		9743	5049	190		34
		591	320	0		
		355	192	0		
	Quaternion	4962	2732	294	15.32	
		7306	3408	190	33.36	
		236	128	0	150.42	
		590	320	0	−39.83	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
pdb1pv0	Classic	71354	37610	4104		645
		121382	64086	2640		444
		7321	4090	0		
		4393	2454	0		
	Quaternion	61888	34756	4104	15.30	
		91108	43342	2640	33.23	
		2928	1636	0	150.03	
		7320	4090	0	−39.99	
pdb1r57	Classic	182496	96250	10868		1603
		309812	164076	7004		1208
		18511	10490	0		
		11107	6294	0		
	Quaternion	158136	89036	10868	15.40	
		232630	111022	7004	33.18	
		7404	4196	0	150.01	
		18510	10490	0	−39.99	
pdb1ry3	Classic	96805	50488	5516		884
		164579	85998	3554		611
		9906	5480	0		
		5944	3288	0		
	Quaternion	83935	46616	5516	15.33	
		123545	58136	3554	33.21	
		3962	2192	0	150.03	
		9905	5480	0	−39.99	
pdb1s4h	Classic	14601	7604	792		136
		24857	12936	510		87
		1506	820	0		
		904	492	0		
	Quaternion	12659	7000	792	15.34	
		18641	8732	510	33.35	
		602	328	0	150.17	
		1505	820	0	−39.93	
pdb1s4j	Classic	16767	8721	959		154
		28520	14850	617		104
		1721	945	0		
		1033	567	0		
	Quaternion	14540	8046	959	15.32	
		21404	10035	617	33.25	
		688	378	0	150.15	
		1720	945	0	−39.94	
pdb1sa8	Classic	139784	72971	8646		1263
		237443	124278	5548		901
		14236	7915	0		
		8542	4749	0		
	Quaternion	121121	67354	8646	15.41	
		178227	84001	5548	33.23	
		5694	3166	0	150.02	
		14235	7915	0	−39.99	
pdb1t2y	Classic	33960	17884	1956		307
		57758	30459	1258		211
		3481	1940	0		
		2089	1164	0		
	Quaternion	29441	16508	1956	15.35	
		43338	20588	1258	33.27	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		1392	776	0	150.07	
		3480	1940	0	−39.97	
pdb1t5q	Classic	34263	18165	2034		322
		58484	30921	1296		189
		3581	1965	0		
		2149	1179	0		
	Quaternion	29751	16746	2034	15.17	
		43850	20887	1296	33.37	
		1432	786	0	150.07	
		3580	1965	0	−39.97	
pdb1tot	Classic	66500	33507	4369		603
		112703	57189	2811		474
		6696	3675	0		
		4018	2205	0		
	Quaternion	57692	31086	4369	15.27	
		84825	38753	2811	32.87	
		2678	1470	0	150.04	
		6695	3675	0	−39.99	
pdb1v6r	Classic	27545	14535	1490		252
		46901	24750	960		165
		2841	1575	0		
		1705	945	0		
	Quaternion	23891	13410	1490	15.29	
		35182	16725	960	33.31	
		1136	630	0	150.09	
		2840	1575	0	−39.96	
pdb1v92	Classic	61359	32419	3727		562
		104486	55209	2383		367
		6331	3515	0		
		3799	2109	0		
	Quaternion	53225	29918	3727	15.28	
		78384	37313	2383	33.30	
		2532	1406	0	150.04	
		6330	3515	0	−39.98	
pdb1vd7	Classic	29723	15134	1760		282
		50531	25740	1130		185
		3046	1630	0		
		1828	978	0		
	Quaternion	25761	13924	1760	15.38	
		37921	17370	1130	33.25	
		1218	652	0	150.08	
		3045	1630	0	−39.97	
pdb1vd9	Classic	39904	20669	2345		359
		67724	35211	1513		265
		4046	2245	0		
		2428	1347	0		
	Quaternion	34573	19090	2345	15.42	
		50857	23807	1513	33.17	
		1618	898	0	150.06	
		4045	2245	0	−39.98	
pdb1vdb	Classic	27918	14472	1678		265
		47561	24618	1072		163
		2891	1560	0		
		1735	936	0		

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	24217	13320	1678	15.28	
		35672	16616	1072	33.33	
		1156	624	0	150.09	
		2890	1560	0	−39.97	
pdb1vpc	Classic	57845	28782	3900		516
		97754	49104	2516		440
		5736	3150	0		
		3442	1890	0		
	Quaternion	50098	26676	3900	15.46	
		73589	33258	2516	32.84	
		2294	1260	0	150.04	
		5735	3150	0	−39.98	
pdb1wnk	Classic	29441	15393	1752		276
		50168	26202	1120		172
		3051	1665	0		
		1831	999	0		
	Quaternion	25548	14190	1752	15.24	
		37634	17699	1120	33.30	
		1220	666	0	150.08	
		3050	1665	0	−39.97	
pdb1wo4	Classic	213327	109958	12556		1774
		360005	187704	8202		1671
		20946	12070	0		
		12568	7242	0		
	Quaternion	184499	102052	12556	15.63	
		270849	127218	8202	32.92	
		8378	4828	0	150.01	
		20945	12070	0	−40.00	
pdb1wo5	Classic	70051	35931	4111		614
		118544	61248	2669		506
		6991	3915	0		
		4195	2349	0		
	Quaternion	60630	33234	4111	15.54	
		89098	41441	2669	33.05	
		2796	1566	0	150.04	
		6990	3915	0	−39.99	
pdb1y5c	Classic	12843	6709	673		118
		21854	11418	435		78
		1321	725	0		
		793	435	0		
	Quaternion	11134	6182	673	15.35	
		16392	7711	435	33.32	
		528	290	0	150.19	
		1320	725	0	−39.92	
pdb1yxr	Classic	213046	110728	13594		1841
		360665	188793	8766		1524
		21291	12080	0		
		12775	7248	0		
	Quaternion	184400	102476	13594	15.53	
		271010	127776	8766	33.08	
		8516	4832	0	150.01	
		21290	12080	0	−40.00	
pdb2a4j	Classic	146397	74907	8068		1360
		248663	127545	5220		948

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Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	14921	8115	0		
		8953	4869	0		
		126900	69102	8068	15.36	
		186740	86185	5220	33.16	
		5968	3246	0	150.02	
		14920	8115	0	−39.99	
pdb2ajj	Classic	34965	18411	1994		328
		59639	31350	1276		199
		3641	1995	0		
		2185	1197	0		
	Quaternion	30361	16986	1994	15.16	
		44738	21185	1276	33.31	
		1456	798	0	150.07	
		3640	1995	0	−39.97	
pdb2ajm	Classic	37240	19552	2143		347
		63467	33297	1373		218
		3861	2120	0		
		2317	1272	0		
	Quaternion	32326	18044	2143	15.20	
		47620	22504	1373	33.28	
		1544	848	0	150.06	
		3860	2120	0	−39.97	
pdb2ajn	Classic	36973	19491	2074		344
		63038	33198	1330		214
		3841	2115	0		
		2305	1269	0		
	Quaternion	32102	17994	2074	15.17	
		47296	22441	1330	33.28	
		1536	846	0	150.07	
		3840	2115	0	−39.97	
pdb2ajo	Classic	37240	19552	2143		347
		63467	33297	1373		218
		3861	2120	0		
		2317	1272	0		
	Quaternion	32326	18044	2143	15.20	
		47620	22504	1373	33.28	
		1544	848	0	150.06	
		3860	2120	0	−39.97	
pdb2akk	Classic	274636	143720	16449		2303
		464483	245289	10683		2034
		27281	15760	0		
		16369	9456	0		
	Quaternion	237702	133324	16449	15.54	
		349208	166208	10683	33.01	
		10912	6304	0	150.01	
		27280	15760	0	−40.00	
pdb2c0s	Classic	86654	42868	5989		777
		146429	73161	3859		664
		8591	4700	0		
		5155	2820	0		
	Quaternion	75076	39764	5989	15.42	
		110278	49572	3859	32.78	
		3436	1880	0	150.03	
		8590	4700	0	−39.99	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
pdb2dci	Classic	22355	11750	1332		210
		38123	19998	850		127
		2326	1270	0		
		1396	762	0		
	Quaternion	19403	10828	1332	15.21	
		28589	13506	850	33.35	
		930	508	0	150.11	
		2325	1270	0	−39.96	
pdb2eem	Classic	96164	50387	5369		819
		162830	85965	3497		689
		9616	5515	0		
		5770	3309	0		
	Quaternion	83265	46702	5369	15.49	
		122375	58225	3497	33.06	
		3846	2206	0	150.03	
		9615	5515	0	−39.99	
pdb2fxz	Classic	17059	8843	1050		158
		29015	15048	672		105
		1751	955	0		
		1051	573	0		
	Quaternion	14787	8146	1050	15.36	
		21768	10161	672	33.29	
		700	382	0	150.14	
		1750	955	0	−39.94	
pdb2g9l	Classic	47386	25170	2808		437
		80792	42867	1794		273
		4921	2730	0		
		2953	1638	0		
	Quaternion	41131	23232	2808	15.21	
		60598	28974	1794	33.32	
		1968	1092	0	150.05	
		4920	2730	0	−39.98	
pdb2h5m	Classic	148675	78371	8722		1334
		252722	133518	5610		942
		15191	8515	0		
		9115	5109	0		
	Quaternion	128874	72394	8722	15.36	
		189674	90281	5610	33.24	
		6076	3406	0	150.02	
		15190	8515	0	−39.99	
pdb2hep	Classic	142643	74581	8803		1206
		241337	127248	5699		1043
		14201	8165	0		
		8521	4899	0		
	Quaternion	123461	69134	8803	15.54	
		181402	86191	5699	33.04	
		5680	3266	0	150.02	
		14200	8165	0	−39.99	
pdb2jmy	Classic	19673	10463	1194		180
		33536	17820	762		114
		2041	1135	0		
		1225	681	0		
	Quaternion	17074	9658	1194	15.22	
		25152	12045	762	33.33	

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Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		816	454	0	150.12	
		2040	1135	0	−39.95	
pdb2jn5	Classic	18689	9764	1015		168
		31754	16632	657		120
		1906	1060	0		
		1144	636	0		
	Quaternion	16198	9016	1015	15.38	
		23835	11244	657	33.22	
		762	424	0	150.13	
		1905	1060	0	−39.95	
pdb2jpn	Classic	173586	89881	9778		1537
		294236	153186	6346		1198
		17476	9785	0		
		10486	5871	0		
	Quaternion	150332	83102	9778	15.47	
		221045	103627	6346	33.11	
		6990	3914	0	150.01	
		17475	9785	0	−39.99	
pdb2jua	Classic	169740	88466	10191		1543
		288461	150711	6549		1086
		17331	9610	0		
		10399	5766	0		
	Quaternion	147158	81712	10191	15.35	
		216574	101902	6549	33.19	
		6932	3844	0	150.01	
		17330	9610	0	−39.99	
pdb2jvd	Classic	66132	35217	3836		595
		112571	59994	2462		401
		6806	3825	0		
		4084	2295	0		
	Quaternion	57353	32526	3836	15.31	
		84449	40563	2462	33.30	
		2722	1530	0	150.04	
		6805	3825	0	−39.99	
pdb2jws	Classic	78173	41055	4527		720
		133097	69927	2905		472
		8061	4455	0		
		4837	2673	0		
	Quaternion	67824	37902	4527	15.26	
		99880	47269	2905	33.26	
		3224	1782	0	150.03	
		8060	4455	0	−39.99	
pdb2jwu	Classic	318363	165871	19412		2638
		537776	283173	12622		2437
		31411	18215	0		
		18847	10929	0		
	Quaternion	275435	153974	19412	15.59	
		404468	191941	12622	32.96	
		12564	7286	0	150.01	
		31410	18215	0	−40.00	
pdb2jxf	Classic	39326	20582	2334		369
		67031	35046	1492		229
		4081	2230	0		
		2449	1338	0		

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Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	34139	18988	2334	15.19	
		50294	23682	1492	33.28	
		1632	892	0	150.06	
		4080	2230	0	−39.98	
pdb2jz5	Classic	235721	124317	13559		2004
		399341	212091	8801		1664
		23631	13605	0		
		14179	8163	0		
	Quaternion	204124	115218	13559	15.48	
		300054	143647	8801	33.09	
		9452	5442	0	150.01	
		23630	13605	0	−40.00	
pdb2k2a	Classic	100223	50391	6501		882
		169430	86031	4205		761
		9951	5535	0		
		5971	3321	0		
	Quaternion	86839	46782	6501	15.41	
		127568	58317	4205	32.82	
		3980	2214	0	150.03	
		9950	5535	0	−39.99	
pdb2k36	Classic	188603	100312	11053		1722
		321296	170841	7077		1113
		19496	10880	0		
		11698	6528	0		
	Quaternion	163617	92588	11053	15.27	
		240991	115472	7077	33.32	
		7798	4352	0	150.01	
		19495	10880	0	−39.99	
pdb2k37	Classic	85097	45190	5343		768
		144845	76989	3413		518
		8756	4910	0		
		5254	2946	0		
	Quaternion	73808	41744	5343	15.30	
		108677	52058	3413	33.28	
		3502	1964	0	150.03	
		8755	4910	0	−39.99	
pdb2k3i	Classic	208025	109857	11720		1812
		353009	187308	7590		1395
		21051	11985	0		
		12631	7191	0		
	Quaternion	180233	101670	11720	15.42	
		265096	126771	7590	33.16	
		8420	4794	0	150.01	
		21050	11985	0	−40.00	
pdb2kdh	Classic	199272	100562	12172		1771
		336872	171336	7892		1472
		19791	10930	0		
		11875	6558	0		
	Quaternion	172384	92908	12172	15.60	
		253254	115862	7892	33.02	
		7916	4372	0	150.01	
		19790	10930	0	−39.99	
pdb2kdl	Classic	209921	109758	12469		1776
		355220	187308	8095		1534

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	20916	12030	0		
		12550	7218	0		
		181740	101796	12469	15.51	
		267045	126906	8095	33.02	
		8366	4812	0	150.01	
		20915	12030	0	−40.00	
pdb2kdm	Classic	127278	66246	7858		1105
		215597	112959	5074		898
		12761	7230	0		
	Quaternion	7657	4338	0		
		110206	61320	7858	15.49	
		162000	76458	5074	33.08	
		5104	2892	0	150.02	
		12760	7230	0	−39.99	
pdb2kdp	Classic	94222	49530	5364		857
		160256	84348	3452		584
		9661	5370	0		
	Quaternion	5797	3222	0		
		81684	45708	5364	15.35	
		120248	57006	3452	33.27	
		3864	2148	0	150.03	
		9660	5370	0	−39.99	
pdb2kdr	Classic	38185	20055	2263		356
		65084	34155	1447		223
		3961	2175	0		
	Quaternion	2377	1305	0		
		33149	18510	2263	15.19	
		48834	23085	1447	33.28	
		1584	870	0	150.06	
		3960	2175	0	−39.97	
pdb2kes	Classic	71544	38531	4216		631
		121778	65670	2704		436
		7356	4195	0		
	Quaternion	4414	2517	0		
		62046	35626	4216	15.31	
		91353	44425	2704	33.30	
		2942	1678	0	150.03	
		7355	4195	0	−39.99	
pdb2kjn	Classic	33963	18019	1896		310
		57857	30690	1218		201
		3511	1955	0		
	Quaternion	2107	1173	0		
		29467	16634	1896	15.26	
		43400	20745	1218	33.31	
		1404	782	0	150.07	
		3510	1955	0	−39.97	
pdb2kjo	Classic	30672	16264	1722		283
		52280	27687	1104		177
		3181	1760	0		
	Quaternion	1909	1056	0		
		26611	14996	1722	15.26	
		39202	18704	1104	33.36	
		1272	704	0	150.08	
		3180	1760	0	−39.97	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
pdb2kl5	Classic	159613	84124	9031		1436
		271367	143319	5821		1006
		16326	9140	0		
		9796	5484	0		
	Quaternion	138372	77708	9031	15.35	
		203667	96908	5821	33.24	
		6530	3656	0	150.02	
		16325	9140	0	−39.99	
pdb2klz	Classic	65400	35071	3735		583
		111350	59763	2399		395
		6736	3815	0		
		4042	2289	0		
	Quaternion	56727	32414	3735	15.29	
		83531	40421	2399	33.30	
		2694	1526	0	150.04	
		6735	3815	0	−39.99	
pdb2koz	Classic	58090	29967	3509		521
		98513	51051	2263		394
		5866	3255	0		
		3520	1953	0		
	Quaternion	50312	27678	3509	15.46	
		73991	34517	2263	33.14	
		2346	1302	0	150.04	
		5865	3255	0	−39.98	
pdb2kp0	Classic	149202	76900	8972		1261
		252029	131208	5838		1137
		14731	8420	0		
		8839	5052	0		
	Quaternion	129067	71288	8972	15.60	
		189540	88876	5838	32.97	
		5892	3368	0	150.02	
		14730	8420	0	−39.99	
pdb2ksg	Classic	58327	30934	3302		542
		99470	52668	2114		332
		6066	3350	0		
		3640	2010	0		
	Quaternion	50626	28532	3302	15.21	
		74595	35586	2114	33.35	
		2426	1340	0	150.04	
		6065	3350	0	−39.98	
pdb2kt8	Classic	437553	228164	25962		3616
		739043	389532	16920		3357
		43146	25060	0		
		25888	15036	0		
	Quaternion	378533	211816	25962	15.59	
		555845	264044	16920	32.96	
		17258	10024	0	150.01	
		43145	25060	0	−40.00	
pdb2kuh	Classic	91679	46047	6213		810
		155009	78606	4005		693
		9111	5055	0		
		5467	3033	0		
	Quaternion	79439	42738	6213	15.41	
		116704	53277	4005	32.82	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		3644	2022	0	150.03	
		9110	5055	0	−39.99	
pdb2kwh	Classic	80098	42614	4706		725
		136397	72600	3016		481
		8261	4630	0		
		4957	2778	0		
	Quaternion	69487	39364	4706	15.27	
		102330	49090	3016	33.29	
		3304	1852	0	150.03	
		8260	4630	0	−39.99	
pdb2kxa	Classic	26245	13847	1765		248
		44789	23562	1117		145
		2741	1495	0		
		1645	897	0		
	Quaternion	22783	12754	1765	15.20	
		33578	15909	1117	33.39	
		1096	598	0	150.09	
		2740	1495	0	−39.96	
pdb2l3m	Classic	88306	46819	5237		809
		150422	79728	3351		522
		9126	5075	0		
		5476	3045	0		
	Quaternion	76604	43202	5237	15.28	
		112827	53881	3351	33.32	
		3650	2030	0	150.03	
		9125	5075	0	−39.99	
pdb2l45	Classic	35486	18757	1996		309
		60233	31977	1292		236
		3596	2045	0		
		2158	1227	0		
	Quaternion	30746	17354	1996	15.42	
		45225	21639	1292	33.19	
		1438	818	0	150.07	
		3595	2045	0	−39.97	
pdb2l5r	Classic	34227	17202	2254		298
		57824	29370	1458		264
		3386	1890	0		
		2032	1134	0		
	Quaternion	29646	15972	2254	15.45	
		43539	19910	1458	32.81	
		1354	756	0	150.07	
		3385	1890	0	−39.97	
pdb2l6q	Classic	210155	109140	12741		1794
		355517	186186	8261		1541
		20916	11940	0		
		12550	7164	0		
	Quaternion	181897	101136	12741	15.54	
		267259	126092	8261	33.02	
		8366	4776	0	150.01	
		20915	11940	0	−40.00	
pdb2l6r	Classic	86164	44966	5006		791
		146528	76560	3218		536
		8831	4870	0		
		5299	2922	0		

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	74696	41476	5006	15.35	
		109958	51730	3218	33.26	
		3532	1948	0	150.03	
		8830	4870	0	−39.99	
pdb2l98	Classic	297656	155067	17565		2511
		503357	264627	11423		2210
		29556	16995	0		
		17734	10197	0		
	Quaternion	257620	143814	17565	15.54	
		378461	179289	11423	33.00	
		11822	6798	0	150.01	
		29555	16995	0	−40.00	
pdb2lci	Classic	219340	116342	12795		1943
		372809	198297	8237		1400
		22391	12670	0		
		13435	7602	0		
	Quaternion	190148	107584	12795	15.35	
		279838	134154	8237	33.22	
		8956	5068	0	150.01	
		22390	12670	0	−40.00	
pdb2lde	Classic	31206	16362	1731		289
		53138	27852	1113		186
		3221	1770	0		
		1933	1062	0		
	Quaternion	27066	15084	1731	15.30	
		39860	18814	1113	33.31	
		1288	708	0	150.08	
		3220	1770	0	−39.97	
pdb2le7	Classic	24708	13198	1386		223
		42083	22473	890		146
		2551	1430	0		
		1531	858	0		
	Quaternion	21426	12176	1386	15.32	
		31554	15186	890	33.37	
		1020	572	0	150.10	
		2550	1430	0	−39.96	
pdb2ler	Classic	13109	6979	695		120
		22349	11880	447		75
		1361	755	0		
		817	453	0		
	Quaternion	11373	6434	695	15.26	
		16754	8025	447	33.40	
		544	302	0	150.18	
		1360	755	0	−39.93	
pdb2lgi	Classic	166792	87193	10138		1415
		282257	148764	6568		1213
		16626	9545	0		
		9976	5727	0		
	Quaternion	144381	80822	10138	15.52	
		212157	100763	6568	33.04	
		6650	3818	0	150.02	
		16625	9545	0	−39.99	
pdb2lhc	Classic	143466	75278	7961		1237
		243152	128403	5177		1001

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		14421	8230	0		
		8653	4938	0		
	Quaternion	124267	69736	7961	15.45	
		182698	86946	5177	33.09	
		5768	3292	0	150.02	
		14420	8230	0	−39.99	
pdb2lhe	Classic	264195	136824	16111		2218
		446333	233508	10471		2011
		26096	15000	0		
		15658	9000	0		
	Quaternion	228571	126912	16111	15.59	
		335675	158216	10471	32.97	
		10438	6000	0	150.01	
		26095	15000	0	−40.00	
pdb2lhg	Classic	72998	36022	5204		657
		123362	61479	3346		559
		7241	3950	0		
		4345	2370	0		
	Quaternion	63253	33416	5204	15.41	
		92914	41658	3346	32.77	
		2896	1580	0	150.03	
		7240	3950	0	−39.99	
pdb2lix	Classic	34093	17982	1966		308
		57989	30624	1264		211
		3496	1950	0		
		2098	1170	0		
	Quaternion	29555	16596	1966	15.35	
		43507	20698	1264	33.29	
		1398	780	0	150.07	
		3495	1950	0	−39.97	
pdb2lld	Classic	51732	25986	3406		463
		87557	44352	2196		381
		5171	2850	0		
		3103	1710	0		
	Quaternion	44847	24108	3406	15.35	
		65908	30054	2196	32.85	
		2068	1140	0	150.05	
		5170	2850	0	−39.98	
pdb2lm9	Classic	125265	66974	7614		1144
		213551	114081	4858		724
		12996	7270	0		
		7798	4362	0		
	Quaternion	108714	61840	7614	15.22	
		160161	77122	4858	33.34	
		5198	2908	0	150.02	
		12995	7270	0	−39.99	
pdb2lmf	Classic	27046	14252	1608		257
		46175	24255	1024		148
		2831	1540	0		
		1699	924	0		
	Quaternion	23488	13132	1608	15.15	
		34622	16380	1024	33.37	
		1132	616	0	150.09	
		2830	1540	0	−39.96	

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Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
pdb2ln3	Classic	110586	58756	6404		997
		188207	100089	4112		674
		11371	6380	0		
		6823	3828	0		
	Quaternion	95898	54260	6404	15.32	
		141198	67668	4112	33.29	
		4548	2552	0	150.02	
		11370	6380	0	−39.99	
pdb2lo2	Classic	46982	24961	2697		429
		80033	42504	1729		277
		4856	2705	0		
		2914	1623	0		
	Quaternion	40753	23030	2697	15.28	
		60023	28723	1729	33.34	
		1942	1082	0	150.05	
		4855	2705	0	−39.98	
pdb2lqp	Classic	89690	47862	5226		813
		152765	81510	3348		531
		9261	5190	0		
		5557	3114	0		
	Quaternion	77789	44172	5226	15.30	
		114566	55090	3348	33.34	
		3704	2076	0	150.03	
		9260	5190	0	−39.99	
pdb2ls9	Classic	27531	14583	1557		262
		47033	24816	993		147
		2891	1575	0		
		1735	945	0		
	Quaternion	23913	13434	1557	15.13	
		35256	16757	993	33.40	
		1156	630	0	150.09	
		2890	1575	0	−39.97	
pdb2lsa	Classic	27572	14596	1714		255
		47000	24849	1092		159
		2861	1580	0		
		1717	948	0		
	Quaternion	23925	13460	1714	15.24	
		35246	16788	1092	33.35	
		1144	632	0	150.09	
		2860	1580	0	−39.97	
pdb2lss	Classic	84615	44193	5283		778
		143921	75240	3379		523
		8681	4785	0		
		5209	2871	0		
	Quaternion	73357	40758	5283	15.35	
		107994	50835	3379	33.27	
		3472	1914	0	150.03	
		8680	4785	0	−39.99	
pdb2lt3	Classic	146127	72116	9841		1318
		246947	123057	6351		1116
		14496	7900	0		
		8698	4740	0		
	Quaternion	126602	66868	9841	15.42	
		185973	83364	6351	32.79	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		5798	3160	0	150.02	
		14495	7900	0	−39.99	
pdb2lu6	Classic	18106	9727	918		161
		30830	16566	594		108
		1866	1055	0		
		1120	633	0		
	Quaternion	15698	8978	918	15.34	
		23115	11197	594	33.38	
		746	422	0	150.13	
		1865	1055	0	−39.95	
pdb2lwa	Classic	86036	45885	5212		795
		146726	78111	3322		487
		8946	4965	0		
		5368	2979	0		
	Quaternion	74655	42306	5212	15.24	
		110001	52767	3322	33.39	
		3578	1986	0	150.03	
		8945	4965	0	−39.99	
pdb2lx0	Classic	42165	22152	2564		388
		71783	37719	1640		254
		4346	2400	0		
		2608	1440	0		
	Quaternion	36572	20436	2564	15.29	
		53855	25488	1640	33.29	
		1738	960	0	150.06	
		4345	2400	0	−39.98	
pdb2lxz	Classic	508422	260506	29900		4201
		857051	444741	19576		4090
		49621	28610	0		
		29773	17166	0		
	Quaternion	439526	241832	29900	15.68	
		644996	301462	19576	32.88	
		19848	11444	0	150.01	
		49620	28610	0	−40.00	
pdb2m1a	Classic	40691	21934	2284		354
		69209	37389	1472		254
		4166	2390	0		
		2500	1434	0		
	Quaternion	35276	20288	2284	15.35	
		51923	25298	1472	33.29	
		1666	956	0	150.06	
		4165	2390	0	−39.98	
pdb2m1j	Classic	40290	20826	2278		373
		68483	35442	1468		253
		4121	2250	0		
		2473	1350	0		
	Quaternion	34915	19188	2278	15.39	
		51390	23934	1468	33.26	
		1648	900	0	150.06	
		4120	2250	0	−39.98	
pdb2m2y	Classic	22290	11726	1248		205
		37958	19965	802		133
		2301	1270	0		
		1381	762	0		

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	19335	10816	1248	15.28	
		28474	13490	802	33.31	
		920	508	0	150.11	
		2300	1270	0	-39.96	
pdb2m3f	Classic	25794	13725	1552		241
		44030	23364	988		142
		2696	1485	0		
		1618	891	0		
	Quaternion	22396	12654	1552	15.17	
		33009	15783	988	33.39	
		1078	594	0	150.09	
		2695	1485	0	-39.96	
pdb2m8m	Classic	33124	16305	2338		299
		55976	27819	1504		253
		3286	1785	0		
		1972	1071	0		
	Quaternion	28697	15114	2338	15.43	
		42153	18843	1504	32.79	
		1314	714	0	150.08	
		3285	1785	0	-39.97	
pdb2m8o	Classic	32108	15765	2295		291
		54260	26895	1475		245
		3186	1725	0		
		1912	1035	0		
	Quaternion	27817	14610	2295	15.43	
		40861	18215	1475	32.79	
		1274	690	0	150.08	
		3185	1725	0	-39.97	
pdb2m97	Classic	86374	42598	5896		785
		146066	72699	3798		651
		8601	4670	0		
		5161	2802	0		
	Quaternion	74873	39512	5896	15.36	
		110010	49258	3798	32.78	
		3440	1868	0	150.03	
		8600	4670	0	-39.99	
pdb2m9r	Classic	54997	28678	2615		500
		93464	48840	1709		350
		5616	3110	0		
		3370	1866	0		
	Quaternion	47668	26468	2615	15.38	
		70153	33010	1709	33.23	
		2246	1244	0	150.04	
		5615	3110	0	-39.98	
pdb2me1	Classic	35007	18509	1991		322
		59639	31515	1277		206
		3621	2005	0		
		2173	1203	0		
	Quaternion	30370	17074	1991	15.27	
		44732	21295	1277	33.33	
		1448	802	0	150.07	
		3620	2005	0	-39.97	
pdb2me2	Classic	34241	17821	1899		324
		58352	30327	1219		199

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		3551	1925	0		
		2131	1155	0		
	Quaternion	29713	16418	1899	15.24	
		43772	20479	1219	33.31	
		1420	770	0	150.07	
		3550	1925	0	−39.97	
pdb2me3	Classic	29895	15748	1666		286
		51059	26796	1064		161
		3136	1700	0		
		1882	1020	0		
	Quaternion	25965	14504	1666	15.14	
		38279	18092	1064	33.39	
		1254	680	0	150.08	
		3135	1700	0	−39.97	
pdb2me4	Classic	37165	19441	2004		344
		63269	33099	1292		224
		3831	2105	0		
		2299	1263	0		
	Quaternion	32236	17930	2004	15.29	
		47470	22363	1292	33.28	
		1532	842	0	150.07	
		3830	2105	0	−39.97	
pdb2mg1	Classic	32521	15900	2304		296
		54953	27126	1482		249
		3226	1740	0		
		1936	1044	0		
	Quaternion	28177	14736	2304	15.42	
		41389	18372	1482	32.77	
		1290	696	0	150.08	
		3225	1740	0	−39.97	
pdb2mg2	Classic	33138	16268	2332		301
		56009	27753	1500		252
		3291	1780	0		
		1975	1068	0		
	Quaternion	28712	15076	2332	15.42	
		42178	18796	1500	32.79	
		1316	712	0	150.08	
		3290	1780	0	−39.97	
pdb2mg3	Classic	34481	16980	2307		312
		58286	28974	1489		262
		3426	1860	0		
		2056	1116	0		
	Quaternion	29880	15744	2307	15.40	
		43895	19628	1489	32.79	
		1370	744	0	150.07	
		3425	1860	0	−39.97	
pdb2mh8	Classic	76925	38354	5231		684
		130028	65472	3373		586
		7636	4210	0		
		4582	2526	0		
	Quaternion	66656	35596	5231	15.41	
		97917	44374	3373	32.79	
		3054	1684	0	150.03	
		7635	4210	0	−39.99	

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Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
pdb2mhw	Classic	32755	17405	2038		302
		55844	29634	1298		188
		3401	1885	0		
		2041	1131	0		
	Quaternion	28424	16054	2038	15.24	
		41876	20023	1298	33.36	
		1360	754	0	150.07	
		3400	1885	0	−39.97	
pdb2mi1	Classic	224647	110671	14915		1922
		377891	188760	9703		1885
		21711	12095	0		
		13027	7257	0		
	Quaternion	194031	102506	14915	15.78	
		284568	127805	9703	32.79	
		8684	4838	0	150.01	
		21710	12095	0	−40.00	
pdb2mi7	Classic	80929	42978	4814		752
		138014	73161	3072		459
		8416	4650	0		
		5050	2790	0		
	Quaternion	70231	39624	4814	15.23	
		103483	49422	3072	33.37	
		3366	1860	0	150.03	
		8415	4650	0	−39.99	
pdb2mij	Classic	44984	24090	2577		411
		76700	41019	1649		257
		4671	2610	0		
		2803	1566	0		
	Quaternion	39031	22224	2577	15.25	
		57504	27718	1649	33.38	
		1868	1044	0	150.05	
		4670	2610	0	−39.98	
pdb2mix	Classic	24954	13124	1455		229
		42479	22341	933		150
		2571	1420	0		
		1543	852	0		
	Quaternion	21638	12100	1455	15.32	
		31862	15092	933	33.32	
		1028	568	0	150.10	
		2570	1420	0	−39.96	
pdb2mj1	Classic	24211	12904	1365		218
		41225	21978	877		145
		2496	1400	0		
		1498	840	0		
	Quaternion	20997	11912	1365	15.31	
		30919	14856	877	33.33	
		998	560	0	150.10	
		2495	1400	0	−39.96	
pdb2mj2	Classic	47064	25072	2644		427
		80165	42702	1698		279
		4861	2720	0		
		2917	1632	0		
	Quaternion	40825	23144	2644	15.28	
		60126	28864	1698	33.33	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		1944	1088	0	150.05	
		4860	2720	0	−39.98	
pdb2mji	Classic	186713	96889	11820		1692
		317006	165000	7580		1220
		18971	10505	0		
		11383	6303	0		
	Quaternion	161756	89414	11820	15.43	
		237986	111515	7580	33.20	
		7588	4202	0	150.01	
		18970	10505	0	−39.99	
pdb2mle	Classic	94386	50009	5349		865
		160784	85173	3433		559
		9756	5425	0		
		5854	3255	0		
	Quaternion	81891	46162	5349	15.26	
		120615	57571	3433	33.30	
		3902	2170	0	150.03	
		9755	5425	0	−39.99	
pdb2mlf	Classic	96716	51396	5498		879
		164711	87549	3530		578
		9981	5580	0		
		5989	3348	0		
	Quaternion	83902	47460	5498	15.27	
		123564	59188	3530	33.30	
		3992	2232	0	150.03	
		9980	5580	0	−39.99	
pdb2mpu	Classic	118672	62545	6910		1079
		201902	106524	4438		730
		12186	6785	0		
		7312	4071	0		
	Quaternion	102900	57734	6910	15.33	
		151495	72003	4438	33.27	
		4874	2714	0	150.02	
		12185	6785	0	−39.99	
pdb2msu	Classic	28149	14707	1632		256
		47858	25047	1050		177
		2881	1595	0		
		1729	957	0		
	Quaternion	24403	13574	1632	15.35	
		35918	16929	1050	33.24	
		1152	638	0	150.09	
		2880	1595	0	−39.97	
pdb2mty	Classic	29614	14341	1838		269
		49970	24453	1196		233
		2916	1565	0		
		1750	939	0		
	Quaternion	25633	13274	1838	15.53	
		37635	16551	1196	32.78	
		1166	626	0	150.09	
		2915	1565	0	−39.97	
pdb2muh	Classic	33511	17383	1934		290
		56735	29634	1256		239
		3351	1895	0		
		2011	1137	0		

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	29005	16082	1934	15.54	
		42628	20053	1256	33.09	
		1340	758	0	150.07	
		3350	1895	0	−39.97	
pdb2mvj	Classic	32681	17381	1894		300
		55712	29601	1212		189
		3391	1885	0		
		2035	1131	0		
	Quaternion	28363	16042	1894	15.22	
		41784	20007	1212	33.33	
		1356	754	0	150.07	
		3390	1885	0	−39.97	
pdb2mvt	Classic	93074	48036	5728		837
		157880	81840	3688		628
		9411	5220	0		
		5647	3132	0		
	Quaternion	80628	44376	5728	15.44	
		118586	55340	3688	33.14	
		3764	2088	0	150.03	
		9410	5220	0	−39.99	
pdb2n00	Classic	216594	113735	12993		1897
		367496	193941	8381		1463
		21906	12415	0		
		13144	7449	0		
	Quaternion	187687	105286	12993	15.40	
		276049	131277	8381	33.13	
		8762	4966	0	150.01	
		21905	12415	0	−40.00	
pdb2n0b	Classic	12711	6232	727		118
		21524	10626	473		92
		1276	680	0		
		766	408	0		
	Quaternion	11022	5768	727	15.32	
		16201	7192	473	32.86	
		510	272	0	150.20	
		1275	680	0	−39.92	
pdb2n0c	Classic	10718	5322	551		105
		18224	9042	357		66
		1101	570	0		
		661	342	0		
	Quaternion	9290	4884	551	15.37	
		13676	6094	357	33.26	
		440	228	0	150.23	
		1100	570	0	−39.91	
pdb2n0d	Classic	11272	5496	659		107
		19115	9372	427		79
		1141	600	0		
		685	360	0		
	Quaternion	9785	5088	659	15.20	
		14390	6344	427	32.84	
		456	240	0	150.22	
		1140	600	0	−39.91	
pdb2n0e	Classic	12310	6036	801		113
		20831	10296	517		91

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		1231	660	0		
		739	396	0		
	Quaternion	10673	5592	801	15.34	
		15684	6972	517	32.82	
		492	264	0	150.20	
		1230	660	0	−39.92	
pdb2n0f	Classic	12568	6365	744		119
		21359	10824	478		79
		1286	685	0		
		772	411	0		
	Quaternion	10891	5854	744	15.40	
		16029	7303	478	33.25	
		514	274	0	150.19	
		1285	685	0	−39.92	
pdb2n0g	Classic	12675	6537	728		118
		21557	11121	468		78
		1301	705	0		
		781	423	0		
	Quaternion	10986	6018	728	15.37	
		16172	7507	468	33.30	
		520	282	0	150.19	
		1300	705	0	−39.92	
pdb2n0h	Classic	12444	5999	805		115
		21029	10230	521		95
		1236	655	0		
		742	393	0		
	Quaternion	10783	5554	805	15.40	
		15839	6925	521	32.77	
		494	262	0	150.20	
		1235	655	0	−39.92	
pdb2n35	Classic	68250	33740	4642		613
		115343	57585	2994		522
		6771	3700	0		
		4063	2220	0		
	Quaternion	59138	31300	4642	15.41	
		86870	39020	2994	32.78	
		2708	1480	0	150.04	
		6770	3700	0	−39.99	
pdb2n41	Classic	195544	103551	11115		1703
		331922	176550	7189		1300
		19816	11295	0		
		11890	6777	0		
	Quaternion	169430	95826	11115	15.41	
		249229	119485	7189	33.18	
		7926	4518	0	150.01	
		19815	11295	0	−39.99	
pdb2n4e	Classic	141076	74702	7992		1271
		239984	127248	5144		872
		14471	8110	0		
		8683	4866	0		
	Quaternion	122312	68980	7992	15.34	
		180062	86026	5144	33.28	
		5788	3244	0	150.02	
		14470	8110	0	−39.99	

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
pdb2n5q	Classic	84933	44018	5197		724
		143624	75075	3369		627
		8436	4810	0		
		5062	2886	0		
	Quaternion	73487	40768	5197	15.58	
		107959	50830	3369	33.04	
		3374	1924	0	150.03	
		8435	4810	0	−39.99	
pdb2n67	Classic	120036	63268	7045		1087
		204146	107745	4525		745
		12301	6860	0		
		7381	4116	0		
	Quaternion	104051	58388	7045	15.36	
		153170	72820	4525	33.28	
		4920	2744	0	150.02	
		12300	6860	0	−39.99	
pdb2n6n	Classic	100436	51312	5944		855
		169661	87615	3876		774
		9921	5640	0		
		5953	3384	0		
	Quaternion	86954	47652	5944	15.50	
		127696	59400	3876	32.86	
		3968	2256	0	150.03	
		9920	5640	0	−39.99	
pdb2n7i	Classic	49022	24292	3291		441
		82871	41448	2123		371
		4871	2660	0		
		2923	1596	0		
	Quaternion	42473	22520	3291	15.42	
		62396	28076	2123	32.81	
		1948	1064	0	150.05	
		4870	2660	0	−39.98	
pdb2n7j	Classic	122973	64530	7168		1060
		208403	110055	4644		858
		12356	7050	0		
		7414	4230	0		
	Quaternion	106500	59760	7168	15.47	
		156573	74510	4644	33.10	
		4942	2820	0	150.02	
		12355	7050	0	−39.99	
pdb2na9	Classic	53708	28702	3148		495
		91616	48873	2010		303
		5591	3110	0		
		3355	1866	0		
	Quaternion	46617	26480	3148	15.21	
		68692	33026	2010	33.37	
		2236	1244	0	150.04	
		5590	3110	0	−39.98	
pdb2ndc	Classic	23594	12536	1327		213
		40169	21351	853		142
		2431	1360	0		
		1459	816	0		
	Quaternion	20462	11572	1327	15.31	
		30130	14432	853	33.32	

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		972	544	0	150.10	
		2430	1360	0	−39.96	
pdb2nde	Classic	20464	10781	1157		191
		34889	18348	741		117
		2126	1165	0		
		1276	699	0		
	Quaternion	17757	9934	1157	15.24	
		26161	12391	741	33.36	
		850	466	0	150.12	
		2125	1165	0	−39.95	
pdb2ndk	Classic	60298	31583	3711		569
		102803	53757	2365		346
		6266	3415	0		
		3760	2049	0		
	Quaternion	52336	29110	3711	15.21	
		77111	36309	2365	33.32	
		2506	1366	0	150.04	
		6265	3415	0	−39.98	
pdb2nvj	Classic	26611	14043	1623		254
		45449	23892	1031		143
		2791	1515	0		
		1675	909	0		
	Quaternion	23109	12930	1623	15.15	
		34068	16129	1031	33.41	
		1116	606	0	150.09	
		2790	1515	0	−39.96	
pdb2p6j	Classic	67180	35805	3896		611
		114452	60984	2496		396
		6946	3885	0		
		4168	2331	0		
	Quaternion	58282	33054	3896	15.27	
		85843	41223	2496	33.33	
		2778	1554	0	150.04	
		6945	3885	0	−39.99	
pdb2p81	Classic	53401	27903	3130		500
		90956	47487	2004		315
		5521	3015	0		
		3313	1809	0		
	Quaternion	46321	25710	3130	15.28	
		68226	32069	2004	33.32	
		2208	1206	0	150.05	
		5520	3015	0	−39.98	
pdb2rlg	Classic	23053	12168	1341		212
		39278	20724	859		136
		2386	1320	0		
		1432	792	0		
	Quaternion	20006	11232	1341	15.23	
		29467	14008	859	33.29	
		954	528	0	150.10	
		2385	1320	0	−39.96	
pdb2rlh	Classic	25024	13248	1516		227
		42611	22572	970		151
		2581	1440	0		
		1549	864	0		

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
	Quaternion	21713	12240	1516	15.25	
		31974	15264	970	33.27	
		1032	576	0	150.10	
		2580	1440	0	−39.96	
pdb2rmy	Classic	44945	23968	2585		408
		76568	40821	1657		265
		4646	2600	0		
		2788	1560	0		
	Quaternion	38989	22124	2585	15.28	
		57425	27592	1657	33.34	
		1858	1040	0	150.05	
		4645	2600	0	−39.98	
pdb2rnd	Classic	42833	22753	2460		396
		73037	38742	1574		245
		4451	2465	0		
		2671	1479	0		
	Quaternion	37175	20990	2460	15.22	
		54772	26179	1574	33.35	
		1780	986	0	150.06	
		4450	2465	0	−39.98	
pdb2roo	Classic	519661	224120	31129		4964
		868568	380523	20621		4859
		48746	23920	0		
		29248	14352	0		
	Quaternion	447347	205348	31129	16.17	
		654945	256256	20621	32.62	
		19498	9568	0	150.01	
		48745	23920	0	−40.00	
pdb2rut	Classic	45728	24164	2495		411
		77756	41151	1611		285
		4681	2620	0		
		2809	1572	0		
	Quaternion	39631	22300	2495	15.38	
		58334	27812	1611	33.29	
		1872	1048	0	150.05	
		4680	2620	0	−39.98	
pdb2ruv	Classic	47284	24900	2599		431
		80462	42405	1675		289
		4861	2700	0		
		2917	1620	0		
	Quaternion	41003	22980	2599	15.32	
		60370	28660	1675	33.28	
		1944	1080	0	150.05	
		4860	2700	0	−39.98	
pdb2rux	Classic	48007	25379	2615		434
		81683	43230	1687		295
		4931	2755	0		
		2959	1653	0		
	Quaternion	41629	23434	2615	15.32	
		61288	29225	1687	33.28	
		1972	1102	0	150.05	
		4930	2755	0	−39.98	
pdb2ruy	Classic	48465	25575	2578		436
		82409	43560	1668		303

Table 4: Results - continued

Problem	Method	Operation Nodes	Operation Virtual Path	Operation ddf	No. Operations Improvments	Branchs Prunes
		4961	2775	0		
		2977	1665	0		
	Quaternion	42009	23610	2578	15.37	
		61834	29445	1668	33.27	
		1984	1110	0	150.05	
		4960	2775	0	−39.98	
pdb2rv3	Classic	49503	26189	2702		442
		84158	44616	1746		312
		5061	2845	0		
		3037	1707	0		
	Quaternion	42908	24190	2702	15.37	
		63152	30167	1746	33.26	
		2024	1138	0	150.05	
		5060	2845	0	−39.98	
pdb2rv5	Classic	45259	23968	2505		410
		77030	40821	1613		275
		4656	2600	0		
		2794	1560	0		
	Quaternion	39247	22124	2505	15.32	
		57787	27592	1613	33.30	
		1862	1040	0	150.05	
		4655	2600	0	−39.98	
pdb2y4q	Classic	343918	179004	21257		2897
		581468	305481	13781		2567
		34111	19620	0		
		20467	11772	0		
	Quaternion	297633	166020	21257	15.55	
		437212	206972	13781	32.99	
		13644	7848	0	150.01	
		34110	19620	0	−40.00	