

Table 1: Results

Problem Size	Method	$ \mathcal{X} $	$\min_{\mathbf{x} \in \mathcal{X}} \text{RMSD}(\mathbf{x}, \mathbf{x}_o)$	$i : \mathbf{x}_i \sim \mathbf{x}_o$	$\text{MDE}(\mathbf{x}_i)$	Time	Improv time
pdb1a57 698	ClassicAll	8	$3.1806 \times 10^{-11}$	5	$2.096 \times 10^{-11}$	$7.2168 \times 10^{-3}$	63.999
	QuaternionAll	8	$3.3550 \times 10^{-11}$	5	$2.092 \times 10^{-11}$	$4.4005 \times 10^{-3}$	
pdb1b4c 1108	ClassicAll	8	$2.6824 \times 10^{-12}$	5	$5.067 \times 10^{-13}$	$2.1307 \times 10^{-2}$	91.045
	QuaternionAll	8	$3.4662 \times 10^{-12}$	5	$5.493 \times 10^{-13}$	$1.1153 \times 10^{-2}$	
pdb1ba5 320	ClassicAll	8	$3.5621 \times 10^{-2}$	6	$9.363 \times 10^{-13}$	$2.2181 \times 10^{-3}$	57.428
	QuaternionAll	8	$3.5621 \times 10^{-2}$	6	$1.069 \times 10^{-12}$	$1.4090 \times 10^{-3}$	
pdb1d1n 594	ClassicAll	2	$2.9766 \times 10^{-11}$	1	$1.005 \times 10^{-11}$	$3.4262 \times 10^{-3}$	74.331
	QuaternionAll	2	$2.9311 \times 10^{-11}$	1	$9.672 \times 10^{-12}$	$1.9654 \times 10^{-3}$	
pdb1dp3 332	ClassicAll	8	$4.9981 \times 10^{-5}$	2	$7.704 \times 10^{-13}$	$2.2527 \times 10^{-3}$	56.765
	QuaternionAll	8	$4.9981 \times 10^{-5}$	2	$8.940 \times 10^{-13}$	$1.4370 \times 10^{-3}$	
pdb1du1 122	ClassicAll	8	$6.6600 \times 10^{-13}$	1	$8.225 \times 10^{-13}$	$7.7204 \times 10^{-4}$	54.055
	QuaternionAll	8	$1.6577 \times 10^{-12}$	1	$1.258 \times 10^{-12}$	$5.0114 \times 10^{-4}$	
pdb1eii 806	ClassicAll	8	$1.9451 \times 10^{-10}$	1	$1.393 \times 10^{-11}$	$5.7653 \times 10^{-3}$	53.735
	QuaternionAll	8	$1.8740 \times 10^{-10}$	1	$1.365 \times 10^{-11}$	$3.7502 \times 10^{-3}$	
pdb1fcl 338	ClassicAll	8	$1.5447 \times 10^{-11}$	2	$4.542 \times 10^{-12}$	$2.3463 \times 10^{-3}$	55.228
	QuaternionAll	8	$1.5223 \times 10^{-11}$	2	$4.515 \times 10^{-12}$	$1.5115 \times 10^{-3}$	
pdb1fd6 344	ClassicAll	8	$2.0242 \times 10^{-5}$	2	$3.182 \times 10^{-12}$	$2.4067 \times 10^{-3}$	55.707
	QuaternionAll	8	$2.0242 \times 10^{-5}$	2	$3.193 \times 10^{-12}$	$1.5457 \times 10^{-3}$	
pdb1hf9 496	ClassicAll	8	$9.0139 \times 10^{-10}$	6	$1.156 \times 10^{-11}$	$4.1394 \times 10^{-2}$	92.651
	QuaternionAll	8	$9.0282 \times 10^{-10}$	6	$1.180 \times 10^{-11}$	$2.1486 \times 10^{-2}$	
pdb1i2u 266	ClassicAll	8	$1.3842 \times 10^{-3}$	2	$5.562 \times 10^{-13}$	$1.8649 \times 10^{-3}$	54.043
	QuaternionAll	8	$1.3842 \times 10^{-3}$	2	$5.609 \times 10^{-13}$	$1.2106 \times 10^{-3}$	
pdb1i2v 266	ClassicAll	8	$8.9125 \times 10^{-13}$	5	$2.422 \times 10^{-13}$	$1.8297 \times 10^{-3}$	54.479
	QuaternionAll	8	$8.8206 \times 10^{-13}$	5	$2.525 \times 10^{-13}$	$1.1844 \times 10^{-3}$	
pdb1ijc 380	ClassicAll	8	$9.1858 \times 10^{-11}$	2	$1.408 \times 10^{-11}$	$2.9060 \times 10^{-3}$	57.083
	QuaternionAll	8	$9.4110 \times 10^{-11}$	2	$1.426 \times 10^{-11}$	$1.8500 \times 10^{-3}$	
pdb1jlz 140	ClassicAll	8	$1.2304 \times 10^{-4}$	1	$5.594 \times 10^{-13}$	$9.1346 \times 10^{-4}$	53.718
	QuaternionAll	8	$1.2304 \times 10^{-4}$	1	$5.965 \times 10^{-13}$	$5.9424 \times 10^{-4}$	
pdb1jw3 842	ClassicAll	8	$1.9618 \times 10^{-12}$	2	$5.936 \times 10^{-13}$	$5.9916 \times 10^{-3}$	54.421
	QuaternionAll	8	$1.8088 \times 10^{-12}$	2	$5.897 \times 10^{-13}$	$3.8800 \times 10^{-3}$	
pdb1k0v 440	ClassicAll	8	$8.3940 \times 10^{-5}$	2	$1.893 \times 10^{-13}$	$3.2384 \times 10^{-3}$	54.728
	QuaternionAll	8	$8.3940 \times 10^{-5}$	2	$1.894 \times 10^{-13}$	$2.0929 \times 10^{-3}$	
pdb1k2h 1120	ClassicAll	8	$1.9788 \times 10^{-4}$	2	$5.490 \times 10^{-13}$	$2.6758 \times 10^{-2}$	103.577
	QuaternionAll	8	$1.9788 \times 10^{-4}$	2	$5.198 \times 10^{-13}$	$1.3144 \times 10^{-2}$	
pdb1k36 278	ClassicAll	8	$1.6100 \times 10^{-10}$	1	$8.820 \times 10^{-12}$	$1.8692 \times 10^{-3}$	57.060
	QuaternionAll	8	$1.8077 \times 10^{-10}$	1	$1.081 \times 10^{-11}$	$1.1901 \times 10^{-3}$	
pdb1k37 278	ClassicAll	8	$2.1407 \times 10^{-12}$	2	$4.711 \times 10^{-13}$	$1.8674 \times 10^{-3}$	57.126
	QuaternionAll	8	$2.0318 \times 10^{-12}$	2	$4.988 \times 10^{-13}$	$1.1885 \times 10^{-3}$	
pdb1kuw 62	ClassicAll	8	$1.8706 \times 10^{-4}$	1	$9.229 \times 10^{-14}$	$3.9029 \times 10^{-4}$	50.741
	QuaternionAll	8	$1.8706 \times 10^{-4}$	1	$1.130 \times 10^{-13}$	$2.5891 \times 10^{-4}$	
pdb1kz0 98	ClassicAll	8	$6.7512 \times 10^{-13}$	1	$4.404 \times 10^{-14}$	$6.3022 \times 10^{-4}$	53.803
	QuaternionAll	8	$6.2568 \times 10^{-13}$	1	$5.880 \times 10^{-14}$	$4.0976 \times 10^{-4}$	
pdb1kz2 98	ClassicAll	8	$3.1076 \times 10^{-6}$	1	$2.119 \times 10^{-14}$	$6.4018 \times 10^{-4}$	52.740
	QuaternionAll	8	$3.1076 \times 10^{-6}$	1	$2.886 \times 10^{-14}$	$4.1913 \times 10^{-4}$	
pdb1kz5 74	ClassicAll	8	$4.8094 \times 10^{-13}$	1	$4.081 \times 10^{-14}$	$4.7184 \times 10^{-4}$	53.651
	QuaternionAll	8	$5.2716 \times 10^{-13}$	1	$4.738 \times 10^{-14}$	$3.0708 \times 10^{-4}$	
pdb1lvz 68	ClassicAll	8	$1.4708 \times 10^{-3}$	1	$6.336 \times 10^{-14}$	$4.2873 \times 10^{-4}$	52.337
	QuaternionAll	8	$1.4708 \times 10^{-3}$	1	$7.315 \times 10^{-14}$	$2.8144 \times 10^{-4}$	
pdb1m4e 122	ClassicAll	8	$5.4966 \times 10^{-12}$	1	$5.949 \times 10^{-13}$	$7.9497 \times 10^{-4}$	52.008
	QuaternionAll	8	$5.5048 \times 10^{-12}$	1	$5.972 \times 10^{-13}$	$5.2298 \times 10^{-4}$	
pdb1ma2 104	ClassicAll	8	$1.7458 \times 10^{-10}$	2	$8.695 \times 10^{-12}$	$6.6260 \times 10^{-4}$	54.281
	QuaternionAll	8	$1.7467 \times 10^{-10}$	2	$8.757 \times 10^{-12}$	$4.2948 \times 10^{-4}$	
pdb1ma4 104	ClassicAll	8	$5.4569 \times 10^{-4}$	2	$7.247 \times 10^{-14}$	$1.6390 \times 10^{-3}$	76.615
	QuaternionAll	8	$5.4569 \times 10^{-4}$	2	$7.977 \times 10^{-14}$	$9.2800 \times 10^{-4}$	
pdb1ma5	ClassicAll	8	$9.6358 \times 10^{-5}$	1	$8.169 \times 10^{-13}$	$6.7216 \times 10^{-4}$	

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104	QuaternionAll	8	$9.6358 \times 10^{-5}$	1	$9.044 \times 10^{-13}$	$4.3986 \times 10^{-4}$	52.813
pd1ma6	ClassicAll	8	$1.2440 \times 10^{-11}$	2	$6.283 \times 10^{-13}$	$6.7314 \times 10^{-4}$	
104	QuaternionAll	8	$1.4288 \times 10^{-11}$	2	$8.487 \times 10^{-13}$	$4.4000 \times 10^{-4}$	52.988
pd1mpe	ClassicAll	8	$5.1722 \times 10^{-10}$	2	$2.617 \times 10^{-11}$	$1.2925 \times 10^{-2}$	
1352	QuaternionAll	8	$5.1751 \times 10^{-10}$	2	$2.624 \times 10^{-11}$	$7.1170 \times 10^{-3}$	81.604
pd1nd9	ClassicAll	8	$1.0508 \times 10^{-12}$	2	$3.026 \times 10^{-13}$	$2.0602 \times 10^{-3}$	
296	QuaternionAll	8	$8.9082 \times 10^{-13}$	2	$3.845 \times 10^{-13}$	$1.3414 \times 10^{-3}$	53.589
pd1ne5	ClassicAll	128	$1.4845 \times 10^{-11}$	33	$1.214 \times 10^{-12}$	$3.1537 \times 10^{-2}$	
254	QuaternionAll	128	$1.5105 \times 10^{-11}$	33	$1.384 \times 10^{-12}$	$1.9559 \times 10^{-2}$	61.239
pd1nmj	ClassicAll	8	$2.3883 \times 10^{-13}$	7	$1.236 \times 10^{-14}$	$1.1175 \times 10^{-3}$	
170	QuaternionAll	8	$2.3832 \times 10^{-13}$	7	$1.422 \times 10^{-14}$	$7.2169 \times 10^{-4}$	54.843
pd1o53	ClassicAll	8	$1.0887 \times 10^{-11}$	2	$3.999 \times 10^{-13}$	$5.8817 \times 10^{-4}$	
92	QuaternionAll	8	$1.1252 \times 10^{-11}$	2	$4.527 \times 10^{-13}$	$3.8500 \times 10^{-4}$	52.771
pd1oqp	ClassicAll	8	$2.9348 \times 10^{-3}$	2	$7.045 \times 10^{-14}$	$2.6452 \times 10^{-2}$	
580	QuaternionAll	8	$2.9348 \times 10^{-3}$	2	$8.314 \times 10^{-14}$	$1.2882 \times 10^{-2}$	105.339
pd1plw	ClassicAll	8	$3.0310 \times 10^{-13}$	2	$2.830 \times 10^{-14}$	$1.8013 \times 10^{-4}$	
32	QuaternionAll	8	$3.2973 \times 10^{-13}$	2	$3.112 \times 10^{-14}$	$1.2037 \times 10^{-4}$	49.647
pd1plx	ClassicAll	8	$2.8525 \times 10^{-4}$	1	$1.574 \times 10^{-13}$	$1.8123 \times 10^{-4}$	
32	QuaternionAll	8	$2.8525 \times 10^{-4}$	1	$2.060 \times 10^{-13}$	$1.2033 \times 10^{-4}$	50.613
pd1pv0	ClassicAll	16	$1.3024 \times 10^{-11}$	1	$2.409 \times 10^{-13}$	$3.6764 \times 10^{-3}$	
278	QuaternionAll	16	$1.3017 \times 10^{-11}$	1	$2.723 \times 10^{-13}$	$2.3561 \times 10^{-3}$	56.037
pd1pzz	ClassicAll	8	$3.9940 \times 10^{-10}$	1	$5.644 \times 10^{-12}$	$1.3472 \times 10^{-1}$	
724	QuaternionAll	8	$3.9046 \times 10^{-10}$	1	$5.871 \times 10^{-12}$	$6.3919 \times 10^{-2}$	110.770
pd1qlk	ClassicAll	8	$3.1378 \times 10^{-5}$	5	$2.634 \times 10^{-13}$	$3.4224 \times 10^{-2}$	
1108	QuaternionAll	8	$3.1378 \times 10^{-5}$	5	$2.870 \times 10^{-13}$	$1.8366 \times 10^{-2}$	86.341
pd1r57	ClassicAll	8	$4.3330 \times 10^{-3}$	2	$1.847 \times 10^{-13}$	$4.3587 \times 10^{-3}$	
614	QuaternionAll	8	$4.3330 \times 10^{-3}$	2	$2.054 \times 10^{-13}$	$2.8209 \times 10^{-3}$	54.518
pd1ry3	ClassicAll	8	$9.1924 \times 10^{-12}$	2	$4.938 \times 10^{-13}$	$2.6880 \times 10^{-3}$	
386	QuaternionAll	8	$9.4285 \times 10^{-12}$	2	$5.913 \times 10^{-13}$	$1.6985 \times 10^{-3}$	58.256
pd1s4h	ClassicAll	8	$1.4643 \times 10^{-4}$	2	$4.696 \times 10^{-13}$	$5.0040 \times 10^{-4}$	
80	QuaternionAll	8	$1.4643 \times 10^{-4}$	2	$6.351 \times 10^{-13}$	$3.2503 \times 10^{-4}$	53.952
pd1s4j	ClassicAll	8	$5.8507 \times 10^{-12}$	2	$1.520 \times 10^{-13}$	$5.1183 \times 10^{-4}$	
80	QuaternionAll	8	$5.8479 \times 10^{-12}$	2	$2.083 \times 10^{-13}$	$3.3630 \times 10^{-4}$	52.193
pd1s6j	ClassicAll	8	$6.0202 \times 10^{-5}$	1	$6.073 \times 10^{-13}$	$3.7005 \times 10^{-3}$	
524	QuaternionAll	8	$6.0202 \times 10^{-5}$	1	$7.660 \times 10^{-13}$	$2.3304 \times 10^{-3}$	58.796
pd1sa8	ClassicAll	8	$1.7170 \times 10^{-3}$	1	$9.340 \times 10^{-13}$	$4.5346 \times 10^{-3}$	
638	QuaternionAll	8	$1.7170 \times 10^{-3}$	1	$1.034 \times 10^{-12}$	$3.0039 \times 10^{-3}$	50.957
pd1t2y	ClassicAll	8	$2.5460 \times 10^{-4}$	1	$1.887 \times 10^{-13}$	$1.0142 \times 10^{-3}$	
152	QuaternionAll	8	$2.5460 \times 10^{-4}$	1	$2.396 \times 10^{-13}$	$6.6476 \times 10^{-4}$	52.562
pd1t5q	ClassicAll	2	$1.0265 \times 10^{-12}$	1	$3.877 \times 10^{-14}$	$9.4120 \times 10^{-4}$	
180	QuaternionAll	2	$1.0480 \times 10^{-12}$	1	$5.093 \times 10^{-14}$	$5.2552 \times 10^{-4}$	79.096
pd1tot	ClassicAll	8	$3.4218 \times 10^{-3}$	5	$6.151 \times 10^{-14}$	$2.2365 \times 10^{-3}$	
314	QuaternionAll	8	$3.4218 \times 10^{-3}$	5	$6.855 \times 10^{-14}$	$1.4438 \times 10^{-3}$	54.902
pd1v6r	ClassicAll	8	$1.3650 \times 10^{-4}$	2	$6.835 \times 10^{-13}$	$8.2447 \times 10^{-4}$	
128	QuaternionAll	8	$1.3650 \times 10^{-4}$	2	$6.971 \times 10^{-13}$	$5.3590 \times 10^{-4}$	53.848
pd1v92	ClassicAll	8	$3.1327 \times 10^{-5}$	1	$1.463 \times 10^{-13}$	$1.9226 \times 10^{-3}$	
278	QuaternionAll	8	$3.1327 \times 10^{-5}$	1	$1.630 \times 10^{-13}$	$1.2375 \times 10^{-3}$	55.364
pd1vd7	ClassicAll	8	$7.8801 \times 10^{-12}$	1	$6.342 \times 10^{-13}$	$9.0575 \times 10^{-4}$	
140	QuaternionAll	8	$7.9022 \times 10^{-12}$	1	$7.439 \times 10^{-13}$	$5.9296 \times 10^{-4}$	52.750
pd1vd9	ClassicAll	8	$1.5514 \times 10^{-11}$	1	$1.290 \times 10^{-12}$	$9.0526 \times 10^{-4}$	
140	QuaternionAll	8	$1.5541 \times 10^{-11}$	1	$1.554 \times 10^{-12}$	$5.8499 \times 10^{-4}$	54.747
pd1vdb	ClassicAll	8	$8.5740 \times 10^{-12}$	2	$9.108 \times 10^{-13}$	$9.0390 \times 10^{-4}$	
140	QuaternionAll	8	$8.5291 \times 10^{-12}$	2	$1.082 \times 10^{-12}$	$5.8446 \times 10^{-4}$	54.655
pd1vpc	ClassicAll	8	$4.3482 \times 10^{-4}$	6	$8.510 \times 10^{-15}$	$1.8807 \times 10^{-3}$	
272	QuaternionAll	8	$4.3482 \times 10^{-4}$	6	$1.002 \times 10^{-14}$	$1.1963 \times 10^{-3}$	57.209

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pdb1wnk 140	ClassicAll	8	$2.2292 \times 10^{-10}$	1	$4.112 \times 10^{-12}$	$9.0852 \times 10^{-4}$	
	QuaternionAll	8	$2.2177 \times 10^{-10}$	1	$4.632 \times 10^{-12}$	$5.8888 \times 10^{-4}$	54.279
pdb1wo4 152	ClassicAll	8	$4.6193 \times 10^{-5}$	2	$9.957 \times 10^{-13}$	$9.9077 \times 10^{-4}$	
	QuaternionAll	8	$4.6193 \times 10^{-5}$	2	$9.634 \times 10^{-13}$	$6.3894 \times 10^{-4}$	55.065
pdb1wo5 152	ClassicAll	8	$2.7147 \times 10^{-10}$	1	$2.372 \times 10^{-12}$	$9.9623 \times 10^{-4}$	
	QuaternionAll	8	$2.7625 \times 10^{-10}$	1	$2.514 \times 10^{-12}$	$6.4531 \times 10^{-4}$	54.380
pdb1x60 476	ClassicAll	8	$6.7449 \times 10^{-12}$	1	$1.076 \times 10^{-12}$	$3.3136 \times 10^{-3}$	
	QuaternionAll	8	$6.9447 \times 10^{-12}$	1	$1.179 \times 10^{-12}$	$2.1603 \times 10^{-3}$	53.386
pdb1x9v 544	ClassicAll	8	$1.1547 \times 10^{-4}$	6	$8.968 \times 10^{-13}$	$4.1615 \times 10^{-2}$	
	QuaternionAll	8	$1.1547 \times 10^{-4}$	6	$9.611 \times 10^{-13}$	$2.1452 \times 10^{-2}$	93.994
pdb1y5c 68	ClassicAll	8	$8.7435 \times 10^{-13}$	1	$7.693 \times 10^{-14}$	$4.2161 \times 10^{-4}$	
	QuaternionAll	8	$8.2242 \times 10^{-13}$	1	$9.383 \times 10^{-14}$	$2.7276 \times 10^{-4}$	54.570
pdb1yx7 500	ClassicAll	8	$1.3647 \times 10^{-10}$	5	$3.509 \times 10^{-12}$	$3.5138 \times 10^{-3}$	
	QuaternionAll	8	$1.4245 \times 10^{-10}$	5	$4.348 \times 10^{-12}$	$2.2682 \times 10^{-3}$	54.917
pdb1yx8 500	ClassicAll	8	$2.5841 \times 10^{-10}$	6	$7.284 \times 10^{-12}$	$3.9642 \times 10^{-3}$	
	QuaternionAll	8	$2.6921 \times 10^{-10}$	6	$8.217 \times 10^{-12}$	$2.5052 \times 10^{-3}$	58.237
pdb1yxr 464	ClassicAll	8	$9.3459 \times 10^{-4}$	1	$6.979 \times 10^{-13}$	$3.2919 \times 10^{-3}$	
	QuaternionAll	8	$9.3459 \times 10^{-4}$	1	$7.989 \times 10^{-13}$	$2.1481 \times 10^{-3}$	53.244
pdb2a2y 1072	ClassicAll	8	$8.1076 \times 10^{-5}$	2	$1.150 \times 10^{-12}$	$2.0710 \times 10^{-1}$	
	QuaternionAll	8	$8.1076 \times 10^{-5}$	2	$1.151 \times 10^{-12}$	$9.7691 \times 10^{-2}$	111.993
pdb2a4j 580	ClassicAll	8	$1.0516 \times 10^{-4}$	2	$2.085 \times 10^{-14}$	$4.8461 \times 10^{-3}$	
	QuaternionAll	8	$1.0516 \times 10^{-4}$	2	$2.727 \times 10^{-14}$	$3.0597 \times 10^{-3}$	58.387
pdb2adl 868	ClassicAll	8	$3.1161 \times 10^{-11}$	1	$1.752 \times 10^{-11}$	$1.6403 \times 10^{-2}$	
	QuaternionAll	8	$3.3255 \times 10^{-11}$	1	$1.787 \times 10^{-11}$	$8.4920 \times 10^{-3}$	93.158
pdb2adn 868	ClassicAll	8	$2.3364 \times 10^{-10}$	1	$6.693 \times 10^{-12}$	$1.2112 \times 10^{-2}$	
	QuaternionAll	8	$2.3188 \times 10^{-10}$	1	$6.465 \times 10^{-12}$	$6.3753 \times 10^{-3}$	89.982
pdb2ajj 170	ClassicAll	8	$2.9810 \times 10^{-4}$	1	$5.641 \times 10^{-14}$	$1.1115 \times 10^{-3}$	
	QuaternionAll	8	$2.9810 \times 10^{-4}$	1	$6.584 \times 10^{-14}$	$7.1627 \times 10^{-4}$	55.172
pdb2ajm 170	ClassicAll	8	$2.4063 \times 10^{-12}$	2	$1.183 \times 10^{-13}$	$1.1195 \times 10^{-3}$	
	QuaternionAll	8	$2.7001 \times 10^{-12}$	2	$1.555 \times 10^{-13}$	$7.2295 \times 10^{-4}$	54.857
pdb2ajn 170	ClassicAll	8	$4.3268 \times 10^{-4}$	1	$1.076 \times 10^{-13}$	$1.1117 \times 10^{-3}$	
	QuaternionAll	8	$4.3268 \times 10^{-4}$	1	$1.217 \times 10^{-13}$	$7.1301 \times 10^{-4}$	55.920
pdb2ajo 170	ClassicAll	8	$2.4063 \times 10^{-12}$	2	$1.183 \times 10^{-13}$	$1.1267 \times 10^{-3}$	
	QuaternionAll	8	$2.7001 \times 10^{-12}$	2	$1.555 \times 10^{-13}$	$7.3113 \times 10^{-4}$	54.105
pdb2akk 446	ClassicAll	8	$3.0416 \times 10^{-3}$	2	$1.289 \times 10^{-13}$	$3.1293 \times 10^{-3}$	
	QuaternionAll	8	$3.0416 \times 10^{-3}$	2	$1.279 \times 10^{-13}$	$2.0386 \times 10^{-3}$	53.502
pdb2bzb 748	ClassicAll	8	$4.6498 \times 10^{-13}$	5	$9.361 \times 10^{-14}$	$4.3490 \times 10^{-2}$	
	QuaternionAll	8	$6.0113 \times 10^{-13}$	5	$1.224 \times 10^{-13}$	$2.2541 \times 10^{-2}$	92.941
pdb2c0s 386	ClassicAll	8	$1.0793 \times 10^{-2}$	6	$3.028 \times 10^{-13}$	$2.7425 \times 10^{-3}$	
	QuaternionAll	8	$1.0793 \times 10^{-2}$	6	$3.380 \times 10^{-13}$	$1.7394 \times 10^{-3}$	57.670
pdb2dci 120	ClassicAll	2	$2.0907 \times 10^{-13}$	1	$2.366 \times 10^{-14}$	$6.3428 \times 10^{-4}$	
	QuaternionAll	2	$3.3732 \times 10^{-13}$	1	$2.950 \times 10^{-14}$	$3.6157 \times 10^{-4}$	75.424
pdb2eem 206	ClassicAll	8	$9.5324 \times 10^{-12}$	1	$5.190 \times 10^{-13}$	$1.3738 \times 10^{-3}$	
	QuaternionAll	8	$9.5866 \times 10^{-12}$	1	$5.461 \times 10^{-13}$	$8.8063 \times 10^{-4}$	56.002
pdb2fva 494	ClassicAll	8	$1.2680 \times 10^{-11}$	2	$1.047 \times 10^{-12}$	$3.4355 \times 10^{-3}$	
	QuaternionAll	8	$1.2689 \times 10^{-11}$	2	$1.195 \times 10^{-12}$	$2.1902 \times 10^{-3}$	56.856
pdb2fvf 494	ClassicAll	8	$3.5796 \times 10^{-12}$	1	$3.106 \times 10^{-13}$	$3.4452 \times 10^{-3}$	
	QuaternionAll	8	$3.3286 \times 10^{-12}$	1	$3.445 \times 10^{-13}$	$2.2127 \times 10^{-3}$	55.699
pdb2fxz 80	ClassicAll	8	$4.2293 \times 10^{-12}$	1	$1.489 \times 10^{-12}$	$5.1456 \times 10^{-4}$	
	QuaternionAll	8	$5.3169 \times 10^{-12}$	1	$1.749 \times 10^{-12}$	$3.3937 \times 10^{-4}$	51.622
pdb2g9j 848	ClassicAll	8	$5.8011 \times 10^{-4}$	2	$3.282 \times 10^{-12}$	$2.6196 \times 10^{-1}$	
	QuaternionAll	8	$5.8011 \times 10^{-4}$	2	$3.535 \times 10^{-12}$	$1.2965 \times 10^{-1}$	102.051
pdb2g9l 224	ClassicAll	8	$1.0333 \times 10^{-4}$	2	$6.365 \times 10^{-14}$	$1.5112 \times 10^{-3}$	
	QuaternionAll	8	$1.0333 \times 10^{-4}$	2	$8.666 \times 10^{-14}$	$9.7433 \times 10^{-4}$	55.102

Table 2: Results - continued

Problem Size	Method	$ \mathcal{X} $	$\min_{\mathbf{x} \in \mathcal{X}} \text{RMSD}(\mathbf{x}, \mathbf{x}_o)$	$i : \mathbf{x}_i \sim \mathbf{x}_o$	$\text{MDE}(\mathbf{x}_i)$	Time	Improv time
pdb2h5m 614	ClassicAll	8	$1.2267 \times 10^{-3}$	1	$9.692 \times 10^{-13}$	$4.3038 \times 10^{-3}$	55.110
	QuaternionAll	8	$1.2267 \times 10^{-3}$	1	$1.032 \times 10^{-12}$	$2.7747 \times 10^{-3}$	
pdb2hep 252	ClassicAll	2	$2.1758 \times 10^{-11}$	1	$1.191 \times 10^{-12}$	$1.3721 \times 10^{-3}$	82.177
	QuaternionAll	2	$2.2038 \times 10^{-11}$	1	$1.268 \times 10^{-12}$	$7.5315 \times 10^{-4}$	
pdb2j0z 752	ClassicAll	8	$1.3100 \times 10^{-10}$	6	$4.392 \times 10^{-12}$	$1.6122 \times 10^{-1}$	108.703
	QuaternionAll	8	$1.3116 \times 10^{-10}$	6	$4.954 \times 10^{-12}$	$7.7250 \times 10^{-2}$	
pdb2j10 752	ClassicAll	1024	$2.9952 \times 10^{-5}$	574	$9.196 \times 10^{-12}$	$6.8913 \times 10^{-1}$	23.678
	QuaternionAll	1024	$2.9952 \times 10^{-5}$	574	$9.529 \times 10^{-12}$	$5.5720 \times 10^{-1}$	
pdb2j11 752	ClassicAll	1024	$2.7803 \times 10^{-11}$	549	$5.256 \times 10^{-12}$	$6.8328 \times 10^{-1}$	22.844
	QuaternionAll	1024	$2.7661 \times 10^{-11}$	549	$5.631 \times 10^{-12}$	$5.5622 \times 10^{-1}$	
pdb2jmy 92	ClassicAll	8	$7.0432 \times 10^{-5}$	1	$9.834 \times 10^{-13}$	$5.9855 \times 10^{-4}$	50.662
	QuaternionAll	8	$7.0432 \times 10^{-5}$	1	$9.967 \times 10^{-13}$	$3.9728 \times 10^{-4}$	
pdb2jn5 74	ClassicAll	8	$6.6339 \times 10^{-12}$	1	$1.104 \times 10^{-11}$	$4.6229 \times 10^{-4}$	53.793
	QuaternionAll	8	$2.0459 \times 10^{-11}$	1	$2.456 \times 10^{-11}$	$3.0059 \times 10^{-4}$	
pdb2jnk 842	ClassicAll	8	$3.4995 \times 10^{-11}$	1	$2.246 \times 10^{-12}$	$6.1159 \times 10^{-3}$	54.384
	QuaternionAll	8	$3.4653 \times 10^{-11}$	1	$2.319 \times 10^{-12}$	$3.9615 \times 10^{-3}$	
pdb2jpn 476	ClassicAll	8	$6.4192 \times 10^{-12}$	2	$6.730 \times 10^{-14}$	$4.5397 \times 10^{-3}$	65.366
	QuaternionAll	8	$6.5904 \times 10^{-12}$	2	$6.984 \times 10^{-14}$	$2.7453 \times 10^{-3}$	
pdb2jua 614	ClassicAll	8	$1.8734 \times 10^{-4}$	2	$1.740 \times 10^{-11}$	$4.4263 \times 10^{-3}$	57.461
	QuaternionAll	8	$1.8734 \times 10^{-4}$	2	$1.882 \times 10^{-11}$	$2.8110 \times 10^{-3}$	
pdb2jvd 288	ClassicAll	2	$9.4244 \times 10^{-13}$	1	$3.339 \times 10^{-14}$	$1.5850 \times 10^{-3}$	82.264
	QuaternionAll	2	$9.4967 \times 10^{-13}$	1	$3.898 \times 10^{-14}$	$8.6960 \times 10^{-4}$	
pdb2jwe 984	ClassicAll	2	$9.2597 \times 10^{-11}$	1	$2.695 \times 10^{-11}$	$5.7134 \times 10^{-3}$	76.233
	QuaternionAll	2	$9.2052 \times 10^{-11}$	1	$2.734 \times 10^{-11}$	$3.2419 \times 10^{-3}$	
pdb2jws 338	ClassicAll	8	$4.5612 \times 10^{-4}$	2	$1.251 \times 10^{-13}$	$2.4140 \times 10^{-3}$	56.376
	QuaternionAll	8	$4.5612 \times 10^{-4}$	2	$1.543 \times 10^{-13}$	$1.5437 \times 10^{-3}$	
pdb2jwu 338	ClassicAll	8	$3.0876 \times 10^{-4}$	1	$4.421 \times 10^{-12}$	$2.3899 \times 10^{-3}$	54.854
	QuaternionAll	8	$3.0876 \times 10^{-4}$	1	$4.373 \times 10^{-12}$	$1.5433 \times 10^{-3}$	
pdb2jxf 182	ClassicAll	8	$2.4000 \times 10^{-4}$	1	$1.399 \times 10^{-13}$	$1.2131 \times 10^{-3}$	55.782
	QuaternionAll	8	$2.4000 \times 10^{-4}$	1	$1.734 \times 10^{-13}$	$7.7873 \times 10^{-4}$	
pdb2jz5 548	ClassicAll	8	$1.7460 \times 10^{-3}$	1	$2.860 \times 10^{-13}$	$3.7907 \times 10^{-3}$	56.177
	QuaternionAll	8	$1.7460 \times 10^{-3}$	1	$2.854 \times 10^{-13}$	$2.4272 \times 10^{-3}$	
pdb2k2a 422	ClassicAll	8	$4.7195 \times 10^{-3}$	5	$3.810 \times 10^{-14}$	$2.9808 \times 10^{-3}$	56.839
	QuaternionAll	8	$4.7195 \times 10^{-3}$	5	$5.148 \times 10^{-14}$	$1.9006 \times 10^{-3}$	
pdb2k2f 1268	ClassicAll	8	$1.2926 \times 10^{-11}$	1	$2.639 \times 10^{-13}$	$2.9746 \times 10^1$	115.049
	QuaternionAll	8	$1.2956 \times 10^{-11}$	1	$2.818 \times 10^{-13}$	$1.3832 \times 10^1$	
pdb2k36 896	ClassicAll	8	$1.6972 \times 10^{-12}$	1	$1.922 \times 10^{-13}$	$6.4707 \times 10^{-3}$	55.621
	QuaternionAll	8	$1.6007 \times 10^{-12}$	1	$2.045 \times 10^{-13}$	$4.1580 \times 10^{-3}$	
pdb2k37 356	ClassicAll	8	$3.7147 \times 10^{-12}$	1	$1.921 \times 10^{-13}$	$2.5637 \times 10^{-3}$	56.576
	QuaternionAll	8	$3.6185 \times 10^{-12}$	1	$2.525 \times 10^{-13}$	$1.6373 \times 10^{-3}$	
pdb2k3i 656	ClassicAll	8	$4.6225 \times 10^{-3}$	2	$3.810 \times 10^{-13}$	$5.9071 \times 10^{-3}$	64.615
	QuaternionAll	8	$4.6225 \times 10^{-3}$	2	$4.009 \times 10^{-13}$	$3.5884 \times 10^{-3}$	
pdb2k6s 494	ClassicAll	8	$8.2998 \times 10^{-12}$	2	$2.100 \times 10^{-13}$	$7.3740 \times 10^{-3}$	75.280
	QuaternionAll	8	$8.4519 \times 10^{-12}$	2	$2.651 \times 10^{-13}$	$4.2070 \times 10^{-3}$	
pdb2k7o 1096	ClassicAll	8	$1.8663 \times 10^{-4}$	1	$1.279 \times 10^{-13}$	$5.1186 \times 10^{-2}$	91.784
	QuaternionAll	8	$1.8663 \times 10^{-4}$	1	$1.416 \times 10^{-13}$	$2.6689 \times 10^{-2}$	
pdb2kbm 1268	ClassicAll	8	$1.5487 \times 10^{-12}$	2	$2.165 \times 10^{-13}$	$2.5000 \times 10^1$	112.296
	QuaternionAll	8	$1.6865 \times 10^{-12}$	2	$2.226 \times 10^{-13}$	$1.1776 \times 10^1$	
pdb2kdh 434	ClassicAll	8	$7.2209 \times 10^{-5}$	2	$1.947 \times 10^{-11}$	$3.0999 \times 10^{-3}$	55.644
	QuaternionAll	8	$7.2209 \times 10^{-5}$	2	$2.228 \times 10^{-11}$	$1.9917 \times 10^{-3}$	
pdb2kdl 338	ClassicAll	8	$4.4591 \times 10^{-12}$	2	$2.301 \times 10^{-13}$	$2.3135 \times 10^{-3}$	56.185
	QuaternionAll	8	$4.4513 \times 10^{-12}$	2	$2.919 \times 10^{-13}$	$1.4812 \times 10^{-3}$	
pdb2kdm 338	ClassicAll	8	$2.1896 \times 10^{-11}$	1	$3.191 \times 10^{-12}$	$2.3738 \times 10^{-3}$	56.347
	QuaternionAll	8	$2.1643 \times 10^{-11}$	1	$3.284 \times 10^{-12}$	$1.5183 \times 10^{-3}$	

Table 2: Results - continued

Problem Size	Method	$ \mathcal{X} $	$\min_{\mathbf{x} \in \mathcal{X}} \text{RMSD}(\mathbf{x}, \mathbf{x}_o)$	$i : \mathbf{x}_i \sim \mathbf{x}_o$	$\text{MDE}(\mathbf{x}_i)$	Time	Improv time
pdb2kdp 428	ClassicAll	8	$3.0283 \times 10^{-12}$	1	$2.621 \times 10^{-13}$	$3.0102 \times 10^{-3}$	56.709
	QuaternionAll	8	$3.0741 \times 10^{-12}$	1	$2.865 \times 10^{-13}$	$1.9209 \times 10^{-3}$	
pdb2kdr 170	ClassicAll	8	$6.3024 \times 10^{-5}$	2	$6.618 \times 10^{-14}$	$1.1171 \times 10^{-3}$	56.243
	QuaternionAll	8	$6.3024 \times 10^{-5}$	2	$8.490 \times 10^{-14}$	$7.1496 \times 10^{-4}$	
pdb2kes 290	ClassicAll	8	$1.8528 \times 10^{-4}$	7	$4.467 \times 10^{-14}$	$1.9606 \times 10^{-3}$	57.266
	QuaternionAll	8	$1.8528 \times 10^{-4}$	7	$5.425 \times 10^{-14}$	$1.2466 \times 10^{-3}$	
pdb2kib 352	ClassicAll	8	$2.9706 \times 10^{-5}$	1	$2.533 \times 10^{-12}$	$3.5759 \times 10^{-2}$	100.203
	QuaternionAll	8	$2.9706 \times 10^{-5}$	1	$2.539 \times 10^{-12}$	$1.7861 \times 10^{-2}$	
pdb2kjin 158	ClassicAll	8	$1.9764 \times 10^{-12}$	2	$9.827 \times 10^{-14}$	$1.0281 \times 10^{-3}$	54.686
	QuaternionAll	8	$1.9265 \times 10^{-12}$	2	$1.174 \times 10^{-13}$	$6.6463 \times 10^{-4}$	
pdb2kjo 158	ClassicAll	8	$1.2876 \times 10^{-11}$	1	$2.284 \times 10^{-13}$	$1.0360 \times 10^{-3}$	55.247
	QuaternionAll	8	$1.2921 \times 10^{-11}$	1	$2.421 \times 10^{-13}$	$6.6731 \times 10^{-4}$	
pdb2kjr 572	ClassicAll	8	$5.1341 \times 10^{-11}$	2	$3.247 \times 10^{-12}$	$3.9453 \times 10^{-3}$	55.966
	QuaternionAll	8	$5.1082 \times 10^{-11}$	2	$3.252 \times 10^{-12}$	$2.5296 \times 10^{-3}$	
pdb2kko 1300	ClassicAll	8	$6.9643 \times 10^{-4}$	2	$1.191 \times 10^{-13}$	$5.7810 \times 10^{-2}$	93.315
	QuaternionAll	8	$6.9643 \times 10^{-4}$	2	$1.284 \times 10^{-13}$	$2.9904 \times 10^{-2}$	
pdb2kl5 662	ClassicAll	8	$2.4505 \times 10^{-12}$	1	$1.820 \times 10^{-13}$	$4.6640 \times 10^{-3}$	55.690
	QuaternionAll	8	$2.5206 \times 10^{-12}$	1	$2.020 \times 10^{-13}$	$2.9957 \times 10^{-3}$	
pdb2klz 276	ClassicAll	2	$3.9786 \times 10^{-13}$	1	$3.439 \times 10^{-14}$	$1.5068 \times 10^{-3}$	82.307
	QuaternionAll	2	$3.7834 \times 10^{-13}$	1	$4.443 \times 10^{-14}$	$8.2650 \times 10^{-4}$	
pdb2ko1 1060	ClassicAll	8	$9.3273 \times 10^{-4}$	2	$1.150 \times 10^{-12}$	$8.1329 \times 10^{-2}$	111.278
	QuaternionAll	8	$9.3273 \times 10^{-4}$	2	$1.151 \times 10^{-12}$	$3.8494 \times 10^{-2}$	
pdb2koz 200	ClassicAll	8	$4.7204 \times 10^{-5}$	2	$1.067 \times 10^{-12}$	$1.3638 \times 10^{-3}$	54.047
	QuaternionAll	8	$4.7204 \times 10^{-5}$	2	$1.151 \times 10^{-12}$	$8.8530 \times 10^{-4}$	
pdb2kp0 200	ClassicAll	8	$7.8392 \times 10^{-11}$	2	$4.894 \times 10^{-12}$	$1.3497 \times 10^{-3}$	54.739
	QuaternionAll	8	$8.2404 \times 10^{-11}$	2	$5.595 \times 10^{-12}$	$8.7224 \times 10^{-4}$	
pdb2ksg 290	ClassicAll	8	$9.2027 \times 10^{-13}$	1	$3.215 \times 10^{-14}$	$1.9883 \times 10^{-3}$	55.337
	QuaternionAll	8	$9.2208 \times 10^{-13}$	1	$3.967 \times 10^{-14}$	$1.2800 \times 10^{-3}$	
pdb2kt8 458	ClassicAll	8	$4.1573 \times 10^{-4}$	1	$3.314 \times 10^{-12}$	$3.1420 \times 10^{-3}$	54.738
	QuaternionAll	8	$4.1573 \times 10^{-4}$	1	$3.535 \times 10^{-12}$	$2.0305 \times 10^{-3}$	
pdb2kuh 404	ClassicAll	8	$1.1667 \times 10^{-3}$	6	$2.015 \times 10^{-14}$	$2.8482 \times 10^{-3}$	54.954
	QuaternionAll	8	$1.1667 \times 10^{-3}$	6	$2.491 \times 10^{-14}$	$1.8381 \times 10^{-3}$	
pdb2kwh 338	ClassicAll	8	$2.0587 \times 10^{-3}$	2	$1.408 \times 10^{-13}$	$2.3177 \times 10^{-3}$	56.804
	QuaternionAll	8	$2.0587 \times 10^{-3}$	2	$1.825 \times 10^{-13}$	$1.4781 \times 10^{-3}$	
pdb2kxa 144	ClassicAll	2	$3.9712 \times 10^{-12}$	1	$1.325 \times 10^{-12}$	$7.8119 \times 10^{-4}$	73.810
	QuaternionAll	2	$3.7392 \times 10^{-12}$	1	$1.351 \times 10^{-12}$	$4.4945 \times 10^{-4}$	
pdb2kyb 362	ClassicAll	8	$3.1200 \times 10^{-6}$	2	$1.321 \times 10^{-11}$	$3.4027 \times 10^{-3}$	63.943
	QuaternionAll	8	$3.1200 \times 10^{-6}$	2	$1.373 \times 10^{-11}$	$2.0755 \times 10^{-3}$	
pdb2l3m 428	ClassicAll	8	$1.5178 \times 10^{-3}$	1	$1.028 \times 10^{-12}$	$2.9766 \times 10^{-3}$	54.897
	QuaternionAll	8	$1.5178 \times 10^{-3}$	1	$9.340 \times 10^{-13}$	$1.9217 \times 10^{-3}$	
pdb2l3n 626	ClassicAll	8	$3.9987 \times 10^{-4}$	5	$3.024 \times 10^{-14}$	$1.8277 \times 10^{-2}$	98.537
	QuaternionAll	8	$3.9987 \times 10^{-4}$	5	$3.632 \times 10^{-14}$	$9.2061 \times 10^{-3}$	
pdb2l45 116	ClassicAll	8	$5.9466 \times 10^{-13}$	1	$2.236 \times 10^{-14}$	$7.6098 \times 10^{-4}$	52.412
	QuaternionAll	8	$6.7808 \times 10^{-13}$	1	$3.033 \times 10^{-14}$	$4.9929 \times 10^{-4}$	
pdb2l5r 138	ClassicAll	2	$3.0491 \times 10^{-13}$	2	$3.535 \times 10^{-14}$	$7.1230 \times 10^{-4}$	78.007
	QuaternionAll	2	$3.0031 \times 10^{-13}$	2	$4.436 \times 10^{-14}$	$4.0015 \times 10^{-4}$	
pdb2l6q 374	ClassicAll	4	$1.6115 \times 10^{-9}$	1	$4.435 \times 10^{-11}$	$1.9704 \times 10^{-3}$	67.872
	QuaternionAll	4	$1.6752 \times 10^{-9}$	1	$5.413 \times 10^{-11}$	$1.1738 \times 10^{-3}$	
pdb2l6r 374	ClassicAll	8	$1.0970 \times 10^{-10}$	2	$2.060 \times 10^{-12}$	$2.6361 \times 10^{-3}$	57.422
	QuaternionAll	8	$9.8250 \times 10^{-11}$	2	$2.174 \times 10^{-12}$	$1.6745 \times 10^{-3}$	
pdb2l98 434	ClassicAll	8	$5.6413 \times 10^{-12}$	2	$3.273 \times 10^{-13}$	$3.0147 \times 10^{-3}$	56.372
	QuaternionAll	8	$6.2089 \times 10^{-12}$	2	$3.637 \times 10^{-13}$	$1.9279 \times 10^{-3}$	
pdb2lci 806	ClassicAll	8	$1.2015 \times 10^{-12}$	1	$2.579 \times 10^{-13}$	$5.6616 \times 10^{-3}$	55.707
	QuaternionAll	8	$1.1830 \times 10^{-12}$	1	$2.404 \times 10^{-13}$	$3.6360 \times 10^{-3}$	

Table 2: Results - continued

Problem Size	Method	$ \mathcal{X} $	$\min_{\mathbf{x} \in \mathcal{X}} \text{RMSD}(\mathbf{x}, \mathbf{x}_o)$	$i : \mathbf{x}_i \sim \mathbf{x}_o$	$\text{MDE}(\mathbf{x}_i)$	Time	Improv time
pdb2lde 152	ClassicAll	8	$6.0406 \times 10^{-3}$	2	$3.154 \times 10^{-14}$	$9.8617 \times 10^{-4}$	
	QuaternionAll	8	$6.0406 \times 10^{-3}$	2	$3.766 \times 10^{-14}$	$6.3873 \times 10^{-4}$	54.396
pdb2le2 676	ClassicAll	8	$1.5317 \times 10^{-12}$	2	$2.064 \times 10^{-13}$	$2.2512 \times 10^{-1}$	
	QuaternionAll	8	$1.4989 \times 10^{-12}$	2	$2.042 \times 10^{-13}$	$1.0961 \times 10^{-1}$	105.376
pdb2le7 122	ClassicAll	8	$8.8940 \times 10^{-14}$	2	$2.111 \times 10^{-14}$	$7.8547 \times 10^{-4}$	
	QuaternionAll	8	$1.1008 \times 10^{-13}$	2	$2.749 \times 10^{-14}$	$5.1159 \times 10^{-4}$	53.534
pdb2ler 68	ClassicAll	8	$5.1096 \times 10^{-14}$	2	$1.314 \times 10^{-14}$	$4.2376 \times 10^{-4}$	
	QuaternionAll	8	$6.2001 \times 10^{-14}$	2	$1.532 \times 10^{-14}$	$2.7519 \times 10^{-4}$	53.992
pdb2lgi 338	ClassicAll	8	$9.7255 \times 10^{-12}$	2	$1.068 \times 10^{-12}$	$2.3776 \times 10^{-3}$	
	QuaternionAll	8	$9.6518 \times 10^{-12}$	2	$1.052 \times 10^{-12}$	$1.5301 \times 10^{-3}$	55.393
pdb2lhc 338	ClassicAll	8	$3.8367 \times 10^{-10}$	1	$2.902 \times 10^{-12}$	$2.4365 \times 10^{-3}$	
	QuaternionAll	8	$3.8166 \times 10^{-10}$	1	$2.997 \times 10^{-12}$	$1.5379 \times 10^{-3}$	58.426
pdb2lhd 338	ClassicAll	8	$1.3048 \times 10^{-11}$	2	$1.930 \times 10^{-12}$	$2.3559 \times 10^{-3}$	
	QuaternionAll	8	$1.4592 \times 10^{-11}$	2	$2.033 \times 10^{-12}$	$1.5150 \times 10^{-3}$	55.502
pdb2lhe 338	ClassicAll	8	$9.7862 \times 10^{-10}$	2	$4.963 \times 10^{-11}$	$2.5781 \times 10^{-3}$	
	QuaternionAll	8	$9.7867 \times 10^{-10}$	2	$4.967 \times 10^{-11}$	$1.6370 \times 10^{-3}$	57.493
pdb2lhg 338	ClassicAll	8	$5.0995 \times 10^{-13}$	6	$6.485 \times 10^{-14}$	$2.3862 \times 10^{-3}$	
	QuaternionAll	8	$5.4683 \times 10^{-13}$	6	$7.343 \times 10^{-14}$	$1.5279 \times 10^{-3}$	56.176
pdb2lix 162	ClassicAll	2	$4.9988 \times 10^{-13}$	1	$4.842 \times 10^{-14}$	$8.5831 \times 10^{-4}$	
	QuaternionAll	2	$5.1517 \times 10^{-13}$	1	$5.614 \times 10^{-14}$	$4.8839 \times 10^{-4}$	75.743
pdb2lld 242	ClassicAll	8	$3.3972 \times 10^{-3}$	5	$1.938 \times 10^{-13}$	$1.6492 \times 10^{-3}$	
	QuaternionAll	8	$3.3972 \times 10^{-3}$	5	$2.216 \times 10^{-13}$	$1.0697 \times 10^{-3}$	54.176
pdb2lm9 578	ClassicAll	8	$2.2967 \times 10^{-3}$	2	$6.254 \times 10^{-14}$	$4.0365 \times 10^{-3}$	
	QuaternionAll	8	$2.2967 \times 10^{-3}$	2	$7.713 \times 10^{-14}$	$2.5617 \times 10^{-3}$	57.571
pdb2lmf 140	ClassicAll	8	$1.0942 \times 10^{-4}$	1	$1.282 \times 10^{-13}$	$9.1035 \times 10^{-4}$	
	QuaternionAll	8	$1.0942 \times 10^{-4}$	1	$1.462 \times 10^{-13}$	$5.8702 \times 10^{-4}$	55.081
pdb2ln3 500	ClassicAll	8	$2.5821 \times 10^{-13}$	1	$1.292 \times 10^{-13}$	$3.4688 \times 10^{-3}$	
	QuaternionAll	8	$2.9987 \times 10^{-13}$	1	$1.359 \times 10^{-13}$	$2.2326 \times 10^{-3}$	55.367
pdb2lo2 230	ClassicAll	8	$1.4423 \times 10^{-2}$	2	$2.068 \times 10^{-14}$	$1.5525 \times 10^{-3}$	
	QuaternionAll	8	$1.4423 \times 10^{-2}$	2	$2.571 \times 10^{-14}$	$1.0000 \times 10^{-3}$	55.244
pdb2lqp 428	ClassicAll	8	$5.7815 \times 10^{-4}$	2	$2.950 \times 10^{-13}$	$2.9691 \times 10^{-3}$	
	QuaternionAll	8	$5.7815 \times 10^{-4}$	2	$3.085 \times 10^{-13}$	$1.9058 \times 10^{-3}$	55.794
pdb2lr0 806	ClassicAll	8	$1.2202 \times 10^{-11}$	1	$3.549 \times 10^{-12}$	$5.6876 \times 10^{-3}$	
	QuaternionAll	8	$1.1747 \times 10^{-11}$	1	$3.440 \times 10^{-12}$	$3.6523 \times 10^{-3}$	55.724
pdb2lrh 806	ClassicAll	8	$2.9721 \times 10^{-12}$	1	$5.631 \times 10^{-13}$	$5.6939 \times 10^{-3}$	
	QuaternionAll	8	$2.9099 \times 10^{-12}$	1	$6.564 \times 10^{-13}$	$3.6372 \times 10^{-3}$	56.546
pdb2ls9 152	ClassicAll	8	$2.7045 \times 10^{-12}$	1	$1.122 \times 10^{-13}$	$1.0102 \times 10^{-3}$	
	QuaternionAll	8	$3.0425 \times 10^{-12}$	1	$1.471 \times 10^{-13}$	$6.5577 \times 10^{-4}$	54.050
pdb2lsa 140	ClassicAll	8	$2.5535 \times 10^{-3}$	2	$5.235 \times 10^{-14}$	$9.2737 \times 10^{-4}$	
	QuaternionAll	8	$2.5535 \times 10^{-3}$	2	$6.998 \times 10^{-14}$	$6.0696 \times 10^{-4}$	52.790
pdb2lss 422	ClassicAll	8	$1.2372 \times 10^{-3}$	1	$1.230 \times 10^{-13}$	$3.0024 \times 10^{-3}$	
	QuaternionAll	8	$1.2372 \times 10^{-3}$	1	$1.455 \times 10^{-13}$	$1.9476 \times 10^{-3}$	54.157
pdb2lt3 680	ClassicAll	8	$9.6961 \times 10^{-13}$	6	$7.245 \times 10^{-14}$	$4.7925 \times 10^{-3}$	
	QuaternionAll	8	$1.0253 \times 10^{-12}$	6	$7.760 \times 10^{-14}$	$3.0730 \times 10^{-3}$	55.954
pdb2lu6 86	ClassicAll	8	$7.7550 \times 10^{-3}$	1	$5.356 \times 10^{-15}$	$5.3249 \times 10^{-4}$	
	QuaternionAll	8	$7.7550 \times 10^{-3}$	1	$6.922 \times 10^{-15}$	$3.4442 \times 10^{-4}$	54.604
pdb2lwa 432	ClassicAll	2048	$4.9078 \times 10^{-12}$	449	$3.616 \times 10^{-13}$	1.2911	
	QuaternionAll	2048	$4.0818 \times 10^{-12}$	449	$4.436 \times 10^{-13}$	$9.2788 \times 10^{-1}$	39.145
pdb2lx0 194	ClassicAll	8	$7.4851 \times 10^{-12}$	1	$3.569 \times 10^{-13}$	$1.3161 \times 10^{-3}$	
	QuaternionAll	8	$7.5304 \times 10^{-12}$	1	$4.035 \times 10^{-13}$	$8.5217 \times 10^{-4}$	54.440
pdb2lxb 892	ClassicAll	8	$9.0172 \times 10^{-13}$	1	$1.542 \times 10^{-13}$	$1.6539 \times 10^{-2}$	
	QuaternionAll	8	$8.6577 \times 10^{-13}$	1	$1.585 \times 10^{-13}$	$8.5426 \times 10^{-3}$	93.606
pdb2lxy 404	ClassicAll	8	$1.1155 \times 10^{-10}$	2	$9.313 \times 10^{-13}$	$2.8074 \times 10^{-3}$	
	QuaternionAll	8	$1.1215 \times 10^{-10}$	2	$1.025 \times 10^{-12}$	$1.7838 \times 10^{-3}$	57.383

Table 2: Results - continued

Problem Size	Method	$ \mathcal{X} $	$\min_{\mathbf{x} \in \mathcal{X}} \text{RMSD}(\mathbf{x}, \mathbf{x}_o)$	$i : \mathbf{x}_i \sim \mathbf{x}_o$	$\text{MDE}(\mathbf{x}_i)$	Time	Improv time
pdb2lxx 194	ClassicAll	8	$1.1003 \times 10^{-4}$	2	$2.371 \times 10^{-12}$	$1.3136 \times 10^{-3}$	54.545
	QuaternionAll	8	$1.1003 \times 10^{-4}$	2	$2.792 \times 10^{-12}$	$8.4998 \times 10^{-4}$	
pdb2lzf 820	ClassicAll	8	$5.9653 \times 10^{-4}$	2	$3.217 \times 10^{-14}$	$2.6541 \times 10^{-1}$	108.709
	QuaternionAll	8	$5.9653 \times 10^{-4}$	2	$3.959 \times 10^{-14}$	$1.2717 \times 10^{-1}$	
pdb2m1a 158	ClassicAll	8	$9.1771 \times 10^{-14}$	1	$6.346 \times 10^{-15}$	$1.0358 \times 10^{-3}$	55.437
	QuaternionAll	8	$9.0451 \times 10^{-14}$	1	$7.612 \times 10^{-15}$	$6.6637 \times 10^{-4}$	
pdb2m1j 182	ClassicAll	8	$1.5890 \times 10^{-13}$	2	$1.865 \times 10^{-14}$	$1.2810 \times 10^{-3}$	56.375
	QuaternionAll	8	$1.6894 \times 10^{-13}$	2	$2.212 \times 10^{-14}$	$8.1920 \times 10^{-4}$	
pdb2m2y 110	ClassicAll	8	$1.8177 \times 10^{-3}$	1	$2.699 \times 10^{-13}$	$7.1505 \times 10^{-4}$	53.774
	QuaternionAll	8	$1.8177 \times 10^{-3}$	1	$2.808 \times 10^{-13}$	$4.6500 \times 10^{-4}$	
pdb2m3f 134	ClassicAll	8	$9.5240 \times 10^{-14}$	1	$3.629 \times 10^{-14}$	$8.6816 \times 10^{-4}$	54.117
	QuaternionAll	8	$5.7597 \times 10^{-14}$	1	$4.641 \times 10^{-14}$	$5.6331 \times 10^{-4}$	
pdb2m4j 2178	ClassicAll	8	$5.2912 \times 10^{-4}$	1	$1.463 \times 10^{-11}$	$7.0056 \times 10^{-2}$	94.747
	QuaternionAll	8	$5.2912 \times 10^{-4}$	1	$1.455 \times 10^{-11}$	$3.5973 \times 10^{-2}$	
pdb2m8m 170	ClassicAll	8	$6.9769 \times 10^{-3}$	5	$2.424 \times 10^{-14}$	$1.1181 \times 10^{-3}$	56.229
	QuaternionAll	8	$6.9769 \times 10^{-3}$	5	$3.058 \times 10^{-14}$	$7.1566 \times 10^{-4}$	
pdb2m8o 170	ClassicAll	8	$4.7097 \times 10^{-3}$	5	$1.798 \times 10^{-14}$	$1.1217 \times 10^{-3}$	55.446
	QuaternionAll	8	$4.7097 \times 10^{-3}$	5	$2.301 \times 10^{-14}$	$7.2157 \times 10^{-4}$	
pdb2m97 416	ClassicAll	8	$2.4560 \times 10^{-12}$	6	$4.654 \times 10^{-14}$	$2.9099 \times 10^{-3}$	56.502
	QuaternionAll	8	$2.4592 \times 10^{-12}$	6	$5.847 \times 10^{-14}$	$1.8594 \times 10^{-3}$	
pdb2m9g 1108	ClassicAll	8	$4.9692 \times 10^{-12}$	1	$2.939 \times 10^{-13}$	$1.0016 \times 10^{-2}$	89.107
	QuaternionAll	8	$4.9567 \times 10^{-12}$	1	$3.170 \times 10^{-13}$	$5.2963 \times 10^{-3}$	
pdb2m9r 242	ClassicAll	8	$3.7505 \times 10^{-12}$	1	$3.537 \times 10^{-14}$	$1.6064 \times 10^{-3}$	62.840
	QuaternionAll	8	$3.6480 \times 10^{-12}$	1	$4.406 \times 10^{-14}$	$9.8646 \times 10^{-4}$	
pdb2mdv 460	ClassicAll	8	$4.7210 \times 10^{-4}$	2	$3.178 \times 10^{-12}$	$3.3404 \times 10^{-3}$	54.706
	QuaternionAll	8	$4.7210 \times 10^{-4}$	2	$3.178 \times 10^{-12}$	$2.1592 \times 10^{-3}$	
pdb2me1 164	ClassicAll	8	$1.4934 \times 10^{-4}$	2	$1.886 \times 10^{-13}$	$1.0737 \times 10^{-3}$	56.114
	QuaternionAll	8	$1.4934 \times 10^{-4}$	2	$2.202 \times 10^{-13}$	$6.8778 \times 10^{-4}$	
pdb2me2 164	ClassicAll	8	$1.3863 \times 10^{-4}$	1	$3.667 \times 10^{-13}$	$1.1361 \times 10^{-3}$	58.383
	QuaternionAll	8	$1.3863 \times 10^{-4}$	1	$5.098 \times 10^{-13}$	$7.1731 \times 10^{-4}$	
pdb2me3 164	ClassicAll	8	$3.4823 \times 10^{-5}$	2	$1.425 \times 10^{-13}$	$1.0830 \times 10^{-3}$	56.590
	QuaternionAll	8	$3.4823 \times 10^{-5}$	2	$1.590 \times 10^{-13}$	$6.9159 \times 10^{-4}$	
pdb2me4 164	ClassicAll	8	$2.9945 \times 10^{-5}$	2	$5.547 \times 10^{-13}$	$1.1386 \times 10^{-3}$	57.477
	QuaternionAll	8	$2.9945 \times 10^{-5}$	2	$6.221 \times 10^{-13}$	$7.2300 \times 10^{-4}$	
pdb2mg1 164	ClassicAll	8	$4.4954 \times 10^{-13}$	6	$4.400 \times 10^{-14}$	$1.0749 \times 10^{-3}$	56.100
	QuaternionAll	8	$5.4976 \times 10^{-13}$	6	$5.374 \times 10^{-14}$	$6.8859 \times 10^{-4}$	
pdb2mg2 170	ClassicAll	8	$1.0745 \times 10^{-3}$	6	$1.831 \times 10^{-14}$	$1.1148 \times 10^{-3}$	55.223
	QuaternionAll	8	$1.0745 \times 10^{-3}$	6	$2.481 \times 10^{-14}$	$7.1821 \times 10^{-4}$	
pdb2mg3 170	ClassicAll	8	$6.2977 \times 10^{-13}$	6	$3.542 \times 10^{-14}$	$1.1292 \times 10^{-3}$	56.277
	QuaternionAll	8	$6.7812 \times 10^{-13}$	6	$4.459 \times 10^{-14}$	$7.2254 \times 10^{-4}$	
pdb2mh8 338	ClassicAll	8	$4.2246 \times 10^{-12}$	6	$1.547 \times 10^{-13}$	$2.3125 \times 10^{-3}$	55.656
	QuaternionAll	8	$4.0208 \times 10^{-12}$	6	$1.883 \times 10^{-13}$	$1.4856 \times 10^{-3}$	
pdb2mhw 164	ClassicAll	8	$3.6932 \times 10^{-3}$	2	$6.229 \times 10^{-14}$	$1.1199 \times 10^{-3}$	53.778
	QuaternionAll	8	$3.6932 \times 10^{-3}$	2	$7.130 \times 10^{-14}$	$7.2828 \times 10^{-4}$	
pdb2mi1 84	ClassicAll	4	$2.1485 \times 10^{-11}$	4	$1.828 \times 10^{-12}$	$7.9150 \times 10^{-4}$	75.987
	QuaternionAll	4	$2.2963 \times 10^{-11}$	4	$2.053 \times 10^{-12}$	$4.4975 \times 10^{-4}$	
pdb2mi7 404	ClassicAll	8	$8.0637 \times 10^{-12}$	2	$6.022 \times 10^{-13}$	$2.7539 \times 10^{-3}$	57.280
	QuaternionAll	8	$8.8714 \times 10^{-12}$	2	$6.815 \times 10^{-13}$	$1.7510 \times 10^{-3}$	
pdb2mij 224	ClassicAll	8	$1.2077 \times 10^{-12}$	1	$1.244 \times 10^{-13}$	$1.5043 \times 10^{-3}$	55.973
	QuaternionAll	8	$1.2294 \times 10^{-12}$	1	$1.522 \times 10^{-13}$	$9.6447 \times 10^{-4}$	
pdb2mix 128	ClassicAll	8	$3.7545 \times 10^{-13}$	1	$4.816 \times 10^{-14}$	$8.4472 \times 10^{-4}$	52.794
	QuaternionAll	8	$3.4098 \times 10^{-13}$	1	$4.684 \times 10^{-14}$	$5.5285 \times 10^{-4}$	
pdb2mj1 110	ClassicAll	8	$2.0809 \times 10^{-3}$	1	$1.309 \times 10^{-13}$	$7.1806 \times 10^{-4}$	54.318
	QuaternionAll	8	$2.0809 \times 10^{-3}$	1	$1.646 \times 10^{-13}$	$4.6531 \times 10^{-4}$	

Table 2: Results - continued

Problem Size	Method	$ \mathcal{X} $	$\min_{\mathbf{x} \in \mathcal{X}} \text{RMSD}(\mathbf{x}, \mathbf{x}_o)$	$i : \mathbf{x}_i \sim \mathbf{x}_o$	$\text{MDE}(\mathbf{x}_i)$	Time	Improv time
pdb2mj2 218	ClassicAll	8	$3.9018 \times 10^{-3}$	2	$9.775 \times 10^{-14}$	$1.4385 \times 10^{-3}$	
	QuaternionAll	8	$3.9018 \times 10^{-3}$	2	$1.192 \times 10^{-13}$	$9.1651 \times 10^{-4}$	56.956
pdb2mjg 556	ClassicAll	8	$1.4497 \times 10^{-3}$	2	$5.503 \times 10^{-14}$	$2.1163 \times 10^{-2}$	
	QuaternionAll	8	$1.4497 \times 10^{-3}$	2	$6.579 \times 10^{-14}$	$1.0643 \times 10^{-2}$	98.846
pdb2mji 788	ClassicAll	8	$1.3090 \times 10^{-11}$	1	$3.207 \times 10^{-12}$	$5.6582 \times 10^{-3}$	
	QuaternionAll	8	$1.2949 \times 10^{-11}$	1	$3.247 \times 10^{-12}$	$3.6855 \times 10^{-3}$	53.528
pdb2mle 434	ClassicAll	8	$1.6719 \times 10^{-3}$	2	$1.491 \times 10^{-13}$	$3.0881 \times 10^{-3}$	
	QuaternionAll	8	$1.6719 \times 10^{-3}$	2	$1.535 \times 10^{-13}$	$1.9706 \times 10^{-3}$	56.705
pdb2mlf 434	ClassicAll	8	$8.3036 \times 10^{-13}$	2	$9.918 \times 10^{-14}$	$3.0447 \times 10^{-3}$	
	QuaternionAll	8	$8.8493 \times 10^{-13}$	2	$1.127 \times 10^{-13}$	$1.9552 \times 10^{-3}$	55.724
pdb2mo5 854	ClassicAll	8	$1.9007 \times 10^{-11}$	1	$1.394 \times 10^{-12}$	$6.1861 \times 10^{-3}$	
	QuaternionAll	8	$1.8458 \times 10^{-11}$	1	$1.403 \times 10^{-12}$	$3.9989 \times 10^{-3}$	54.695
pdb2mpu 554	ClassicAll	8	$2.5305 \times 10^{-12}$	1	$9.785 \times 10^{-14}$	$3.9406 \times 10^{-3}$	
	QuaternionAll	8	$2.5592 \times 10^{-12}$	1	$1.016 \times 10^{-13}$	$2.5394 \times 10^{-3}$	55.178
pdb2mra 704	ClassicAll	8	$4.3616 \times 10^{-12}$	1	$2.632 \times 10^{-13}$	$5.9738 \times 10^{-3}$	
	QuaternionAll	8	$4.3117 \times 10^{-12}$	1	$2.768 \times 10^{-13}$	$3.7144 \times 10^{-3}$	60.829
pdb2msu 122	ClassicAll	8	$3.6237 \times 10^{-12}$	1	$7.813 \times 10^{-14}$	$7.9014 \times 10^{-4}$	
	QuaternionAll	8	$3.6441 \times 10^{-12}$	1	$8.765 \times 10^{-14}$	$5.1566 \times 10^{-4}$	53.229
pdb2mty 120	ClassicAll	2	$5.1232 \times 10^{-12}$	2	$1.848 \times 10^{-14}$	$6.7409 \times 10^{-4}$	
	QuaternionAll	2	$5.2129 \times 10^{-12}$	2	$2.363 \times 10^{-14}$	$3.7637 \times 10^{-4}$	79.103
pdb2muh 98	ClassicAll	8	$8.0615 \times 10^{-5}$	2	$2.008 \times 10^{-13}$	$6.2151 \times 10^{-4}$	
	QuaternionAll	8	$8.0615 \times 10^{-5}$	2	$2.279 \times 10^{-13}$	$3.9926 \times 10^{-4}$	55.666
pdb2mvj 156	ClassicAll	2	$6.1752 \times 10^{-12}$	1	$1.534 \times 10^{-13}$	$8.1384 \times 10^{-4}$	
	QuaternionAll	2	$6.1858 \times 10^{-12}$	1	$1.647 \times 10^{-13}$	$4.5906 \times 10^{-4}$	77.282
pdb2mvt 284	ClassicAll	8	$1.5441 \times 10^{-4}$	2	$6.053 \times 10^{-12}$	$1.9649 \times 10^{-3}$	
	QuaternionAll	8	$1.5441 \times 10^{-4}$	2	$6.225 \times 10^{-12}$	$1.2743 \times 10^{-3}$	54.200
pdb2mvx 2360	ClassicAll	8	$5.8655 \times 10^{-5}$	6	$1.968 \times 10^{-10}$	$3.1667 \times 10^{-2}$	
	QuaternionAll	8	$5.8655 \times 10^{-5}$	6	$1.971 \times 10^{-10}$	$1.7955 \times 10^{-2}$	76.369
pdb2mz6 220	ClassicAll	8	$2.3371 \times 10^{-10}$	1	$2.141 \times 10^{-11}$	$4.7695 \times 10^{-2}$	
	QuaternionAll	8	$2.3374 \times 10^{-10}$	1	$2.153 \times 10^{-11}$	$2.4584 \times 10^{-2}$	94.004
pdb2n00 572	ClassicAll	8	$1.2439 \times 10^{-4}$	2	$2.703 \times 10^{-13}$	$4.0558 \times 10^{-3}$	
	QuaternionAll	8	$1.2439 \times 10^{-4}$	2	$3.466 \times 10^{-13}$	$2.6001 \times 10^{-3}$	55.986
pdb2n0b 60	ClassicAll	2	$1.0219 \times 10^{-11}$	2	$7.123 \times 10^{-13}$	$2.9131 \times 10^{-4}$	
	QuaternionAll	2	$1.0781 \times 10^{-11}$	2	$9.477 \times 10^{-13}$	$1.6266 \times 10^{-4}$	79.095
pdb2n0c 60	ClassicAll	2	$1.0471 \times 10^{-12}$	1	$1.293 \times 10^{-13}$	$2.8892 \times 10^{-4}$	
	QuaternionAll	2	$9.1394 \times 10^{-13}$	1	$1.682 \times 10^{-13}$	$1.6213 \times 10^{-4}$	78.206
pdb2n0d 60	ClassicAll	2	$5.2061 \times 10^{-11}$	2	$3.639 \times 10^{-12}$	$2.9353 \times 10^{-4}$	
	QuaternionAll	2	$5.7645 \times 10^{-11}$	2	$4.540 \times 10^{-12}$	$1.6380 \times 10^{-4}$	79.201
pdb2n0e 60	ClassicAll	2	$1.1503 \times 10^{-11}$	2	$3.314 \times 10^{-12}$	$2.9862 \times 10^{-4}$	
	QuaternionAll	2	$1.8786 \times 10^{-11}$	2	$4.286 \times 10^{-12}$	$1.7032 \times 10^{-4}$	75.335
pdb2n0f 60	ClassicAll	2	$2.2697 \times 10^{-12}$	1	$3.185 \times 10^{-13}$	$2.9557 \times 10^{-4}$	
	QuaternionAll	2	$2.7490 \times 10^{-12}$	1	$4.023 \times 10^{-13}$	$1.6613 \times 10^{-4}$	77.919
pdb2n0g 60	ClassicAll	2	$1.4896 \times 10^{-11}$	1	$8.315 \times 10^{-13}$	$2.9465 \times 10^{-4}$	
	QuaternionAll	2	$1.4974 \times 10^{-11}$	1	$9.618 \times 10^{-13}$	$1.6859 \times 10^{-4}$	74.774
pdb2n0h 60	ClassicAll	2	$4.1935 \times 10^{-12}$	2	$7.716 \times 10^{-13}$	$2.9523 \times 10^{-4}$	
	QuaternionAll	2	$4.1379 \times 10^{-12}$	2	$8.755 \times 10^{-13}$	$1.6501 \times 10^{-4}$	78.920
pdb2n35 314	ClassicAll	8	$1.4478 \times 10^{-4}$	6	$3.658 \times 10^{-14}$	$2.1553 \times 10^{-3}$	
	QuaternionAll	8	$1.4478 \times 10^{-4}$	6	$4.617 \times 10^{-14}$	$1.3703 \times 10^{-3}$	57.290
pdb2n3a 574	ClassicAll	8	$2.1457 \times 10^{-3}$	5	$8.770 \times 10^{-14}$	$7.4548 \times 10^{-2}$	
	QuaternionAll	8	$2.1457 \times 10^{-3}$	5	$1.049 \times 10^{-13}$	$3.7047 \times 10^{-2}$	101.227
pdb2n41 638	ClassicAll	8	$5.9366 \times 10^{-3}$	2	$1.812 \times 10^{-13}$	$4.5500 \times 10^{-3}$	
	QuaternionAll	8	$5.9366 \times 10^{-3}$	2	$1.836 \times 10^{-13}$	$2.8766 \times 10^{-3}$	58.176
pdb2n4e 638	ClassicAll	8	$5.1960 \times 10^{-3}$	2	$1.494 \times 10^{-13}$	$4.4792 \times 10^{-3}$	
	QuaternionAll	8	$5.1960 \times 10^{-3}$	2	$1.687 \times 10^{-13}$	$2.9218 \times 10^{-3}$	53.305



Table 2: Results - continued

Problem Size	Method	$ \mathcal{X} $	$\min_{\mathbf{x} \in \mathcal{X}} \text{RMSD}(\mathbf{x}, \mathbf{x}_o)$	$i : \mathbf{x}_i \sim \mathbf{x}_o$	$\text{MDE}(\mathbf{x}_i)$	Time	Improv time
pdb2n5q 164	ClassicAll	8	$1.1051 \times 10^{-11}$	1	$1.732 \times 10^{-12}$	$1.1036 \times 10^{-3}$	
	QuaternionAll	8	$9.3428 \times 10^{-12}$	1	$1.745 \times 10^{-12}$	$7.1961 \times 10^{-4}$	53.367
pdb2n67 566	ClassicAll	8	$2.0736 \times 10^{-12}$	1	$4.443 \times 10^{-13}$	$4.0023 \times 10^{-3}$	
	QuaternionAll	8	$2.0936 \times 10^{-12}$	1	$4.465 \times 10^{-13}$	$2.5811 \times 10^{-3}$	55.062
pdb2n6n 192	ClassicAll	2	$1.6681 \times 10^{-12}$	2	$6.557 \times 10^{-13}$	$1.1880 \times 10^{-3}$	
	QuaternionAll	2	$1.2630 \times 10^{-12}$	2	$7.492 \times 10^{-13}$	$6.6004 \times 10^{-4}$	79.991
pdb2n7i 224	ClassicAll	8	$1.3998 \times 10^{-4}$	1	$9.212 \times 10^{-13}$	$1.5001 \times 10^{-3}$	
	QuaternionAll	8	$1.3998 \times 10^{-4}$	1	$1.126 \times 10^{-12}$	$9.5671 \times 10^{-4}$	56.801
pdb2n7j 336	ClassicAll	2	$2.5110 \times 10^{-12}$	1	$5.969 \times 10^{-13}$	$1.8835 \times 10^{-3}$	
	QuaternionAll	2	$2.6436 \times 10^{-12}$	1	$6.094 \times 10^{-13}$	$1.0410 \times 10^{-3}$	80.945
pdb2n9b 832	ClassicAll	8	$4.0200 \times 10^{-10}$	1	$1.196 \times 10^{-12}$	$1.1441 \times 10^{-1}$	
	QuaternionAll	8	$4.0126 \times 10^{-10}$	1	$1.238 \times 10^{-12}$	$5.3057 \times 10^{-2}$	115.633
pdb2na9 266	ClassicAll	8	$2.3390 \times 10^{-12}$	1	$5.440 \times 10^{-14}$	$1.8226 \times 10^{-3}$	
	QuaternionAll	8	$2.3721 \times 10^{-12}$	1	$6.690 \times 10^{-14}$	$1.1543 \times 10^{-3}$	57.894
pdb2ndc 110	ClassicAll	8	$3.1313 \times 10^{-3}$	2	$3.365 \times 10^{-14}$	$7.1114 \times 10^{-4}$	
	QuaternionAll	8	$3.1313 \times 10^{-3}$	2	$4.481 \times 10^{-14}$	$4.6542 \times 10^{-4}$	52.796
pdb2nde 110	ClassicAll	8	$8.5286 \times 10^{-5}$	2	$7.022 \times 10^{-14}$	$7.0378 \times 10^{-4}$	
	QuaternionAll	8	$8.5286 \times 10^{-5}$	2	$8.855 \times 10^{-14}$	$4.5662 \times 10^{-4}$	54.126
pdb2ndk 290	ClassicAll	8	$9.0150 \times 10^{-5}$	1	$5.022 \times 10^{-13}$	$1.9955 \times 10^{-3}$	
	QuaternionAll	8	$9.0150 \times 10^{-5}$	1	$6.279 \times 10^{-13}$	$1.2676 \times 10^{-3}$	57.420
pdb2nvj 152	ClassicAll	8	$6.7520 \times 10^{-3}$	7	$2.082 \times 10^{-14}$	$1.0271 \times 10^{-3}$	
	QuaternionAll	8	$6.7520 \times 10^{-3}$	7	$2.293 \times 10^{-14}$	$6.7479 \times 10^{-4}$	52.215
pdb2p6j 314	ClassicAll	8	$3.2640 \times 10^{-13}$	1	$4.795 \times 10^{-14}$	$2.1604 \times 10^{-3}$	
	QuaternionAll	8	$3.5480 \times 10^{-13}$	1	$6.389 \times 10^{-14}$	$1.3869 \times 10^{-3}$	55.769
pdb2p81 266	ClassicAll	8	$6.8538 \times 10^{-11}$	2	$7.881 \times 10^{-13}$	$1.8154 \times 10^{-3}$	
	QuaternionAll	8	$6.8914 \times 10^{-11}$	2	$8.226 \times 10^{-13}$	$1.1458 \times 10^{-3}$	58.435
pdb2pqe 896	ClassicAll	8	$4.1258 \times 10^{-5}$	2	$1.127 \times 10^{-11}$	$6.4705 \times 10^{-3}$	
	QuaternionAll	8	$4.1258 \times 10^{-5}$	2	$1.248 \times 10^{-11}$	$4.1703 \times 10^{-3}$	55.156
pdb2rlg 108	ClassicAll	2	$4.8140 \times 10^{-13}$	1	$5.501 \times 10^{-14}$	$5.5687 \times 10^{-4}$	
	QuaternionAll	2	$5.3066 \times 10^{-13}$	1	$6.973 \times 10^{-14}$	$3.1140 \times 10^{-4}$	78.828
pdb2rlh 108	ClassicAll	2	$1.0750 \times 10^{-12}$	1	$4.772 \times 10^{-14}$	$5.6031 \times 10^{-4}$	
	QuaternionAll	2	$1.0423 \times 10^{-12}$	1	$5.801 \times 10^{-14}$	$3.1601 \times 10^{-4}$	77.306
pdb2rmy 206	ClassicAll	8	$1.2240 \times 10^{-4}$	1	$1.872 \times 10^{-13}$	$1.3607 \times 10^{-3}$	
	QuaternionAll	8	$1.2240 \times 10^{-4}$	1	$2.498 \times 10^{-13}$	$8.7649 \times 10^{-4}$	55.244
pdb2rnd 206	ClassicAll	128	$3.4031 \times 10^{-12}$	33	$2.626 \times 10^{-13}$	$2.2644 \times 10^{-2}$	
	QuaternionAll	128	$3.8842 \times 10^{-12}$	33	$3.569 \times 10^{-13}$	$1.2864 \times 10^{-2}$	76.027
pdb2roo 260	ClassicAll	8	$3.3639 \times 10^{-4}$	6	$2.933 \times 10^{-12}$	$3.1899 \times 10^{-3}$	
	QuaternionAll	8	$3.3639 \times 10^{-4}$	6	$3.525 \times 10^{-12}$	$1.8971 \times 10^{-3}$	68.144
pdb2rq1 572	ClassicAll	8	$9.9510 \times 10^{-11}$	1	$2.345 \times 10^{-12}$	$3.9594 \times 10^{-3}$	
	QuaternionAll	8	$1.0013 \times 10^{-10}$	1	$2.496 \times 10^{-12}$	$2.5420 \times 10^{-3}$	55.758
pdb2rut 218	ClassicAll	8	$2.0579 \times 10^{-13}$	2	$4.389 \times 10^{-14}$	$1.4384 \times 10^{-3}$	
	QuaternionAll	8	$4.0527 \times 10^{-13}$	2	$5.013 \times 10^{-14}$	$9.2275 \times 10^{-4}$	55.878
pdb2ruv 224	ClassicAll	8	$5.4278 \times 10^{-13}$	2	$5.775 \times 10^{-14}$	$1.5078 \times 10^{-3}$	
	QuaternionAll	8	$6.5510 \times 10^{-13}$	2	$7.404 \times 10^{-14}$	$9.5680 \times 10^{-4}$	57.593
pdb2rux 218	ClassicAll	8	$3.6084 \times 10^{-3}$	1	$2.671 \times 10^{-14}$	$1.4544 \times 10^{-3}$	
	QuaternionAll	8	$3.6084 \times 10^{-3}$	1	$3.016 \times 10^{-14}$	$9.3587 \times 10^{-4}$	55.411
pdb2ruy 224	ClassicAll	8	$4.1535 \times 10^{-13}$	1	$1.968 \times 10^{-14}$	$1.4661 \times 10^{-3}$	
	QuaternionAll	8	$3.5981 \times 10^{-13}$	1	$2.387 \times 10^{-14}$	$9.3448 \times 10^{-4}$	56.889
pdb2rv3 218	ClassicAll	8	$3.0630 \times 10^{-4}$	1	$3.656 \times 10^{-14}$	$1.4407 \times 10^{-3}$	
	QuaternionAll	8	$3.0630 \times 10^{-4}$	1	$4.118 \times 10^{-14}$	$9.2552 \times 10^{-4}$	55.664
pdb2rv5 212	ClassicAll	8	$8.6519 \times 10^{-4}$	1	$1.145 \times 10^{-14}$	$1.4125 \times 10^{-3}$	
	QuaternionAll	8	$8.6519 \times 10^{-4}$	1	$1.338 \times 10^{-14}$	$9.0624 \times 10^{-4}$	55.864
pdb2y4q 476	ClassicAll	8	$4.6451 \times 10^{-11}$	2	$1.410 \times 10^{-12}$	$3.3001 \times 10^{-3}$	
	QuaternionAll	8	$4.6324 \times 10^{-11}$	2	$1.451 \times 10^{-12}$	$2.1201 \times 10^{-3}$	55.657