

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
pdb1ba5 320	ClassicAll	16384	$3.5079 \times 10^{-2}$	10070	$7.453 \times 10^{-7}$	5.5325	
	QuaternionAll	16384	$3.5079 \times 10^{-2}$	10070	$7.453 \times 10^{-7}$	4.7959	15.359
pdb1d1n 594	ClassicAll	5376	$2.9766 \times 10^{-11}$	1707	$1.005 \times 10^{-11}$	$1.0156 \times 10^1$	
	QuaternionAll	5376	$2.9311 \times 10^{-11}$	1707	$9.672 \times 10^{-12}$	5.6835	78.694
pdb1du1 122	ClassicAll	212992	$6.6600 \times 10^{-13}$	45549	$8.225 \times 10^{-13}$	$2.5062 \times 10^1$	
	QuaternionAll	212992	$1.6576 \times 10^{-12}$	45549	$1.258 \times 10^{-12}$	$2.5012 \times 10^1$	0.201
pdb1i2u 266	ClassicAll	48	$1.1301 \times 10^{-3}$	22	$5.676 \times 10^{-7}$	$1.0456 \times 10^{-1}$	
	QuaternionAll	48	$1.1301 \times 10^{-3}$	22	$5.676 \times 10^{-7}$	$5.2997 \times 10^{-2}$	97.300
pdb1i2v 266	ClassicAll	8	$8.9125 \times 10^{-13}$	5	$2.422 \times 10^{-13}$	$1.5406 \times 10^{-2}$	
	QuaternionAll	8	$8.8206 \times 10^{-13}$	5	$2.525 \times 10^{-13}$	$7.3820 \times 10^{-3}$	108.701
pdb1jlz 140	ClassicAll	256	$1.2003 \times 10^{-4}$	73	$3.238 \times 10^{-7}$	$3.0876 \times 10^{-2}$	
	QuaternionAll	256	$1.2003 \times 10^{-4}$	73	$3.238 \times 10^{-7}$	$2.0054 \times 10^{-2}$	53.970
pdb1k0v 440	ClassicAll	8	$8.3940 \times 10^{-5}$	2	$1.893 \times 10^{-13}$	$4.1180 \times 10^{-3}$	
	QuaternionAll	8	$8.3940 \times 10^{-5}$	2	$1.894 \times 10^{-13}$	$2.5508 \times 10^{-3}$	61.436
pdb1k2h 1120	ClassicAll	64	$1.9334 \times 10^{-4}$	6	$4.671 \times 10^{-7}$	1.9235	
	QuaternionAll	64	$1.9334 \times 10^{-4}$	6	$4.671 \times 10^{-7}$	$8.8912 \times 10^{-1}$	116.338
pdb1k37 278	ClassicAll	224	$2.1407 \times 10^{-12}$	30	$4.711 \times 10^{-13}$	$2.9754 \times 10^1$	
	QuaternionAll	224	$2.0318 \times 10^{-12}$	30	$4.988 \times 10^{-13}$	$1.4785 \times 10^1$	101.243
pdb1kuw 62	ClassicAll	16	$1.8706 \times 10^{-4}$	1	$9.229 \times 10^{-14}$	$1.1271 \times 10^{-3}$	
	QuaternionAll	16	$1.8706 \times 10^{-4}$	1	$1.130 \times 10^{-13}$	$6.9661 \times 10^{-4}$	61.798
pdb1kz0 98	ClassicAll	16	$6.7512 \times 10^{-13}$	1	$4.404 \times 10^{-14}$	$9.1368 \times 10^{-4}$	
	QuaternionAll	16	$6.2568 \times 10^{-13}$	1	$5.880 \times 10^{-14}$	$6.4383 \times 10^{-4}$	41.913
pdb1kz2 98	ClassicAll	16	$3.1076 \times 10^{-6}$	5	$2.119 \times 10^{-14}$	$1.0205 \times 10^{-3}$	
	QuaternionAll	16	$3.1076 \times 10^{-6}$	5	$2.886 \times 10^{-14}$	$7.0401 \times 10^{-4}$	44.959
pdb1kz5 74	ClassicAll	16	$4.8094 \times 10^{-13}$	1	$4.081 \times 10^{-14}$	$1.0049 \times 10^{-3}$	
	QuaternionAll	16	$5.2716 \times 10^{-13}$	1	$4.738 \times 10^{-14}$	$6.4642 \times 10^{-4}$	55.449
pdb1lvz 68	ClassicAll	16	$1.1842 \times 10^{-3}$	1	$6.483 \times 10^{-8}$	$6.1571 \times 10^{-4}$	
	QuaternionAll	16	$1.1842 \times 10^{-3}$	1	$6.483 \times 10^{-8}$	$4.4316 \times 10^{-4}$	38.938
pdb1m4e 122	ClassicAll	384	$5.4966 \times 10^{-12}$	25	$5.949 \times 10^{-13}$	$3.5242 \times 10^{-2}$	
	QuaternionAll	384	$5.5048 \times 10^{-12}$	25	$5.972 \times 10^{-13}$	$2.3349 \times 10^{-2}$	50.933
pdb1ma4 104	ClassicAll	192	$5.0392 \times 10^{-4}$	54	$7.441 \times 10^{-7}$	$3.1803 \times 10^{-2}$	
	QuaternionAll	192	$5.0392 \times 10^{-4}$	54	$7.441 \times 10^{-7}$	$1.8756 \times 10^{-2}$	69.565
pdb1ma5 104	ClassicAll	4608	$6.1895 \times 10^{-5}$	1665	$7.863 \times 10^{-7}$	$3.0799 \times 10^{-1}$	
	QuaternionAll	4608	$6.1895 \times 10^{-5}$	1665	$7.863 \times 10^{-7}$	$2.9139 \times 10^{-1}$	5.694
pdb1ma6 104	ClassicAll	24576	$1.2440 \times 10^{-11}$	5094	$6.283 \times 10^{-13}$	2.0697	
	QuaternionAll	24576	$1.4288 \times 10^{-11}$	5094	$8.487 \times 10^{-13}$	2.3901	-13.406
pdb1nd9 296	ClassicAll	512	$1.0508 \times 10^{-12}$	2	$3.026 \times 10^{-13}$	$8.4278 \times 10^{-1}$	
	QuaternionAll	512	$8.9082 \times 10^{-13}$	2	$3.845 \times 10^{-13}$	$4.6467 \times 10^{-1}$	81.372
pdb1nmj 170	ClassicAll	8	$2.3883 \times 10^{-13}$	7	$1.236 \times 10^{-14}$	$1.2173 \times 10^{-3}$	
	QuaternionAll	8	$2.3832 \times 10^{-13}$	7	$1.422 \times 10^{-14}$	$7.6976 \times 10^{-4}$	58.144
pdb1o53 92	ClassicAll	294912	$1.0887 \times 10^{-11}$	69346	$3.999 \times 10^{-13}$	$7.7107 \times 10^1$	
	QuaternionAll	294912	$1.1252 \times 10^{-11}$	69346	$4.527 \times 10^{-13}$	$2.7689 \times 10^1$	178.470
pdb1oqp 580	ClassicAll	8	$2.9348 \times 10^{-3}$	2	$7.045 \times 10^{-14}$	$2.7797 \times 10^{-2}$	
	QuaternionAll	8	$2.9348 \times 10^{-3}$	2	$8.314 \times 10^{-14}$	$1.3325 \times 10^{-2}$	108.609
pdb1plw 32	ClassicAll	64	$3.0310 \times 10^{-13}$	26	$2.830 \times 10^{-14}$	$9.2563 \times 10^{-4}$	
	QuaternionAll	64	$3.2973 \times 10^{-13}$	26	$3.112 \times 10^{-14}$	$6.9320 \times 10^{-4}$	33.530
pdb1plx 32	ClassicAll	256	$1.8321 \times 10^{-4}$	105	$2.751 \times 10^{-6}$	$2.2670 \times 10^{-3}$	
	QuaternionAll	256	$1.8321 \times 10^{-4}$	105	$2.751 \times 10^{-6}$	$2.0063 \times 10^{-3}$	12.992
pdb1r57 614	ClassicAll	64	$4.1216 \times 10^{-3}$	6	$2.080 \times 10^{-9}$	$5.1769 \times 10^{-2}$	
	QuaternionAll	64	$4.1216 \times 10^{-3}$	6	$2.080 \times 10^{-9}$	$3.0150 \times 10^{-2}$	71.703
pdb1s4h 80	ClassicAll	393216	$3.7288 \times 10^{-6}$	114246	$1.026 \times 10^{-6}$	$1.4783 \times 10^2$	
	QuaternionAll	393216	$3.7288 \times 10^{-6}$	114246	$1.026 \times 10^{-6}$	$1.2240 \times 10^2$	20.775
pdb1s4j 80	ClassicAll	512	$5.8507 \times 10^{-12}$	106	$1.520 \times 10^{-13}$	$1.4515 \times 10^{-2}$	
	QuaternionAll	512	$5.8479 \times 10^{-12}$	106	$2.083 \times 10^{-13}$	$1.3990 \times 10^{-2}$	3.753
pdb1sa8	ClassicAll	8	$1.7170 \times 10^{-3}$	1	$9.340 \times 10^{-13}$	$2.4228 \times 10^{-2}$	

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
638	QuaternionAll	8	$1.7170 \times 10^{-3}$	1	$1.034 \times 10^{-12}$	$1.2110 \times 10^{-2}$	100.076
pdb1t2y 152	ClassicAll	384	$2.2800 \times 10^{-4}$	169	$5.096 \times 10^{-7}$	$2.8234 \times 10^{-2}$	28.667
	QuaternionAll	384	$2.2800 \times 10^{-4}$	169	$5.096 \times 10^{-7}$	$2.1943 \times 10^{-2}$	
pdb1t5q 180	ClassicAll	2	$1.0265 \times 10^{-12}$	1	$3.877 \times 10^{-14}$	$9.9171 \times 10^{-4}$	82.966
	QuaternionAll	2	$1.0480 \times 10^{-12}$	1	$5.093 \times 10^{-14}$	$5.4202 \times 10^{-4}$	
pdb1tot 314	ClassicAll	8	$3.4218 \times 10^{-3}$	5	$6.151 \times 10^{-14}$	$2.3885 \times 10^{-3}$	56.400
	QuaternionAll	8	$3.4218 \times 10^{-3}$	5	$6.855 \times 10^{-14}$	$1.5272 \times 10^{-3}$	
pdb1v6r 128	ClassicAll	448	$7.3125 \times 10^{-5}$	122	$1.648 \times 10^{-6}$	$7.7798 \times 10^{-2}$	62.652
	QuaternionAll	448	$7.3125 \times 10^{-5}$	122	$1.648 \times 10^{-6}$	$4.7831 \times 10^{-2}$	
pdb1v92 278	ClassicAll	25600	$2.3012 \times 10^{-5}$	9449	$1.890 \times 10^{-6}$	6.3087	12.949
	QuaternionAll	25600	$2.3012 \times 10^{-5}$	9449	$1.890 \times 10^{-6}$	5.5854	
pdb1vpc 272	ClassicAll	16	$4.3482 \times 10^{-4}$	14	$8.510 \times 10^{-15}$	$3.8676 \times 10^{-3}$	58.683
	QuaternionAll	16	$4.3482 \times 10^{-4}$	14	$1.002 \times 10^{-14}$	$2.4373 \times 10^{-3}$	
pdb1wnk 140	ClassicAll	24576	$2.2292 \times 10^{-10}$	2433	$4.112 \times 10^{-12}$	2.5894	10.310
	QuaternionAll	24576	$2.2177 \times 10^{-10}$	2433	$4.632 \times 10^{-12}$	2.3474	
pdb1wo4 152	ClassicAll	62720	$1.0961 \times 10^{-5}$	20998	$2.477 \times 10^{-6}$	$1.3822 \times 10^1$	18.488
	QuaternionAll	62720	$1.0961 \times 10^{-5}$	20998	$2.477 \times 10^{-6}$	$1.1665 \times 10^1$	
pdb1y5c 68	ClassicAll	8192	$8.7435 \times 10^{-13}$	2929	$7.693 \times 10^{-14}$	$2.0069 \times 10^{-1}$	-28.353
	QuaternionAll	8192	$8.2242 \times 10^{-13}$	2929	$9.383 \times 10^{-14}$	$2.8012 \times 10^{-1}$	
pdb2a4j 580	ClassicAll	16	$1.0516 \times 10^{-4}$	2	$2.085 \times 10^{-14}$	$1.4460 \times 10^{-2}$	89.524
	QuaternionAll	16	$1.0516 \times 10^{-4}$	2	$2.727 \times 10^{-14}$	$7.6298 \times 10^{-3}$	
pdb2a4j 170	ClassicAll	640	$7.2549 \times 10^{-5}$	121	$1.229 \times 10^{-6}$	$4.6544 \times 10^{-2}$	8.453
	QuaternionAll	640	$7.2549 \times 10^{-5}$	121	$1.229 \times 10^{-6}$	$4.2916 \times 10^{-2}$	
pdb2ajm 170	ClassicAll	12288	$2.4063 \times 10^{-12}$	1074	$1.183 \times 10^{-13}$	1.4240	9.517
	QuaternionAll	12288	$2.7001 \times 10^{-12}$	1074	$1.555 \times 10^{-13}$	1.3003	
pdb2ajn 170	ClassicAll	53760	$3.7478 \times 10^{-4}$	15665	$2.380 \times 10^{-6}$	9.4979	19.252
	QuaternionAll	53760	$3.7478 \times 10^{-4}$	15665	$2.380 \times 10^{-6}$	7.9646	
pdb2ajo 170	ClassicAll	12288	$2.4063 \times 10^{-12}$	1074	$1.183 \times 10^{-13}$	1.4322	9.805
	QuaternionAll	12288	$2.7001 \times 10^{-12}$	1074	$1.555 \times 10^{-13}$	1.3043	
pdb2akk 446	ClassicAll	8	$3.0416 \times 10^{-3}$	2	$1.289 \times 10^{-13}$	$1.0365 \times 10^{-1}$	100.826
	QuaternionAll	8	$3.0416 \times 10^{-3}$	2	$1.279 \times 10^{-13}$	$5.1613 \times 10^{-2}$	
pdb2bzb 748	ClassicAll	32	$4.6498 \times 10^{-13}$	29	$9.361 \times 10^{-14}$	$3.2063 \times 10^{-1}$	104.728
	QuaternionAll	32	$6.0113 \times 10^{-13}$	29	$1.224 \times 10^{-13}$	$1.5661 \times 10^{-1}$	
pdb2c0s 386	ClassicAll	8	$1.0793 \times 10^{-2}$	6	$3.028 \times 10^{-13}$	$3.8909 \times 10^{-3}$	65.184
	QuaternionAll	8	$1.0793 \times 10^{-2}$	6	$3.380 \times 10^{-13}$	$2.3555 \times 10^{-3}$	
pdb2dci 120	ClassicAll	2	$2.0907 \times 10^{-13}$	1	$2.366 \times 10^{-14}$	$6.6909 \times 10^{-4}$	79.389
	QuaternionAll	2	$3.3732 \times 10^{-13}$	1	$2.950 \times 10^{-14}$	$3.7298 \times 10^{-4}$	
pdb2eem 206	ClassicAll	128	$9.5324 \times 10^{-12}$	29	$5.190 \times 10^{-13}$	$4.5197 \times 10^{-1}$	95.375
	QuaternionAll	128	$9.5866 \times 10^{-12}$	29	$5.461 \times 10^{-13}$	$2.3134 \times 10^{-1}$	
pdb2fxz 80	ClassicAll	41472	$4.2293 \times 10^{-12}$	13441	$1.489 \times 10^{-12}$	2.7845	0.900
	QuaternionAll	41472	$5.3169 \times 10^{-12}$	13441	$1.749 \times 10^{-12}$	2.7597	
pdb2g9j 848	ClassicAll	16	$5.8011 \times 10^{-4}$	2	$3.282 \times 10^{-12}$	$8.6313 \times 10^{-1}$	101.888
	QuaternionAll	16	$5.8011 \times 10^{-4}$	2	$3.535 \times 10^{-12}$	$4.2753 \times 10^{-1}$	
pdb2g9l 224	ClassicAll	8	$1.0333 \times 10^{-4}$	2	$6.365 \times 10^{-14}$	$1.6101 \times 10^{-3}$	57.122
	QuaternionAll	8	$1.0333 \times 10^{-4}$	2	$8.666 \times 10^{-14}$	$1.0247 \times 10^{-3}$	
pdb2h5m 614	ClassicAll	128	$1.2260 \times 10^{-3}$	21	$2.131 \times 10^{-7}$	$1.1055 \times 10^{-1}$	61.026
	QuaternionAll	128	$1.2260 \times 10^{-3}$	21	$2.131 \times 10^{-7}$	$6.8655 \times 10^{-2}$	
pdb2hep 252	ClassicAll	676	$2.1758 \times 10^{-11}$	224	$1.191 \times 10^{-12}$	3.2206	98.178
	QuaternionAll	676	$2.2038 \times 10^{-11}$	224	$1.268 \times 10^{-12}$	1.6251	
pdb2jmy 92	ClassicAll	24	$2.4695 \times 10^{-5}$	9	$3.958 \times 10^{-6}$	$1.5905 \times 10^{-3}$	46.738
	QuaternionAll	24	$2.4695 \times 10^{-5}$	9	$3.958 \times 10^{-6}$	$1.0839 \times 10^{-3}$	
pdb2jn5 74	ClassicAll	96	$6.6339 \times 10^{-12}$	45	$1.104 \times 10^{-11}$	$3.1163 \times 10^{-3}$	31.954
	QuaternionAll	96	$2.0459 \times 10^{-11}$	45	$2.456 \times 10^{-11}$	$2.3617 \times 10^{-3}$	
pdb2jpn 476	ClassicAll	8	$6.4192 \times 10^{-12}$	2	$6.730 \times 10^{-14}$	$4.7008 \times 10^{-3}$	66.341
	QuaternionAll	8	$6.5904 \times 10^{-12}$	2	$6.984 \times 10^{-14}$	$2.8260 \times 10^{-3}$	

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pdb2jvd 288	ClassicAll	16	$9.4244 \times 10^{-13}$	6	$3.339 \times 10^{-14}$	$5.0341 \times 10^{-3}$	
	QuaternionAll	16	$9.4969 \times 10^{-13}$	6	$3.898 \times 10^{-14}$	$3.0724 \times 10^{-3}$	63.848
pdb2jxf 182	ClassicAll	2048	$1.1644 \times 10^{-4}$	305	$1.841 \times 10^{-6}$	$1.2165 \times 10^{-1}$	
	QuaternionAll	2048	$1.1644 \times 10^{-4}$	305	$1.841 \times 10^{-6}$	$1.2608 \times 10^{-1}$	-3.510
pdb2jz5 548	ClassicAll	64	$1.7154 \times 10^{-3}$	5	$1.691 \times 10^{-7}$	7.6168	
	QuaternionAll	64	$1.7154 \times 10^{-3}$	5	$1.691 \times 10^{-7}$	3.6348	109.551
pdb2k2a 422	ClassicAll	8	$4.7195 \times 10^{-3}$	5	$3.810 \times 10^{-14}$	$4.2185 \times 10^{-3}$	
	QuaternionAll	8	$4.7195 \times 10^{-3}$	5	$5.148 \times 10^{-14}$	$2.5402 \times 10^{-3}$	66.069
pdb2k36 896	ClassicAll	32	$1.6972 \times 10^{-12}$	13	$1.922 \times 10^{-13}$	$3.5895 \times 10^{-2}$	
	QuaternionAll	32	$1.6007 \times 10^{-12}$	13	$2.045 \times 10^{-13}$	$2.2363 \times 10^{-2}$	60.512
pdb2k37 356	ClassicAll	192	$3.7147 \times 10^{-12}$	45	$1.921 \times 10^{-13}$	$3.2952 \times 10^{-2}$	
	QuaternionAll	192	$3.6176 \times 10^{-12}$	45	$2.525 \times 10^{-13}$	$2.5747 \times 10^{-2}$	27.985
pdb2k3i 656	ClassicAll	1024	$2.8710 \times 10^{-3}$	393	$6.869 \times 10^{-7}$	$1.4346 \times 10^1$	
	QuaternionAll	1024	$2.8710 \times 10^{-3}$	393	$6.869 \times 10^{-7}$	6.7963	111.093
pdb2k6s 494	ClassicAll	256	$8.2998 \times 10^{-12}$	114	$2.100 \times 10^{-13}$	1.1219	
	QuaternionAll	256	$8.4519 \times 10^{-12}$	114	$2.651 \times 10^{-13}$	$5.6482 \times 10^{-1}$	98.633
pdb2kdp 428	ClassicAll	128	$3.0283 \times 10^{-12}$	5	$2.621 \times 10^{-13}$	$4.8129 \times 10^{-2}$	
	QuaternionAll	128	$3.0741 \times 10^{-12}$	5	$2.865 \times 10^{-13}$	$3.0679 \times 10^{-2}$	56.876
pdb2kdr 170	ClassicAll	192	$6.3024 \times 10^{-5}$	86	$6.618 \times 10^{-14}$	$1.1125 \times 10^{-2}$	
	QuaternionAll	192	$6.3024 \times 10^{-5}$	86	$8.490 \times 10^{-14}$	$8.3046 \times 10^{-3}$	33.968
pdb2kes 290	ClassicAll	64	$1.7403 \times 10^{-4}$	43	$1.149 \times 10^{-6}$	$1.1603 \times 10^{-2}$	
	QuaternionAll	64	$1.7403 \times 10^{-4}$	43	$1.149 \times 10^{-6}$	$6.8773 \times 10^{-3}$	68.711
pdb2kjin 158	ClassicAll	4608	$1.9764 \times 10^{-12}$	1194	$9.827 \times 10^{-14}$	$5.4626 \times 10^{-1}$	
	QuaternionAll	4608	$1.9265 \times 10^{-12}$	1194	$1.174 \times 10^{-13}$	$4.8765 \times 10^{-1}$	12.019
pdb2kjo 158	ClassicAll	384	$1.2876 \times 10^{-11}$	165	$2.284 \times 10^{-13}$	$2.4887 \times 10^{-2}$	
	QuaternionAll	384	$1.2921 \times 10^{-11}$	165	$2.421 \times 10^{-13}$	$2.0677 \times 10^{-2}$	20.361
pdb2kko 1300	ClassicAll	32	$6.9298 \times 10^{-4}$	10	$1.852 \times 10^{-7}$	2.0477	
	QuaternionAll	32	$6.9298 \times 10^{-4}$	10	$1.852 \times 10^{-7}$	1.0247	99.835
pdb2kl5 662	ClassicAll	96	$2.4505 \times 10^{-12}$	5	$1.820 \times 10^{-13}$	$6.3858 \times 10^{-2}$	
	QuaternionAll	96	$2.5206 \times 10^{-12}$	5	$2.020 \times 10^{-13}$	$4.0071 \times 10^{-2}$	59.361
pdb2klz 276	ClassicAll	24	$3.9786 \times 10^{-13}$	9	$3.439 \times 10^{-14}$	$6.3768 \times 10^{-3}$	
	QuaternionAll	24	$3.7834 \times 10^{-13}$	9	$4.443 \times 10^{-14}$	$3.9236 \times 10^{-3}$	62.523
pdb2ko1 1060	ClassicAll	128	$7.9853 \times 10^{-4}$	46	$7.782 \times 10^{-8}$	4.6840	
	QuaternionAll	128	$7.9853 \times 10^{-4}$	46	$7.782 \times 10^{-8}$	2.2980	103.828
pdb2ksg 290	ClassicAll	8	$9.2027 \times 10^{-13}$	1	$3.215 \times 10^{-14}$	$1.9936 \times 10^{-3}$	
	QuaternionAll	8	$9.2208 \times 10^{-13}$	1	$3.967 \times 10^{-14}$	$1.2568 \times 10^{-3}$	58.626
pdb2kuh 404	ClassicAll	8	$1.1667 \times 10^{-3}$	6	$2.015 \times 10^{-14}$	$2.8811 \times 10^{-3}$	
	QuaternionAll	8	$1.1667 \times 10^{-3}$	6	$2.491 \times 10^{-14}$	$1.8443 \times 10^{-3}$	56.215
pdb2kwh 338	ClassicAll	16	$2.0587 \times 10^{-3}$	6	$1.408 \times 10^{-13}$	$5.4492 \times 10^{-3}$	
	QuaternionAll	16	$2.0587 \times 10^{-3}$	6	$1.825 \times 10^{-13}$	$3.3426 \times 10^{-3}$	63.020
pdb2kxa 144	ClassicAll	16	$3.9712 \times 10^{-12}$	8	$1.325 \times 10^{-12}$	$1.3758 \times 10^{-3}$	
	QuaternionAll	16	$3.7392 \times 10^{-12}$	8	$1.351 \times 10^{-12}$	$9.7643 \times 10^{-4}$	40.899
pdb2l3m 428	ClassicAll	8	$1.5178 \times 10^{-3}$	1	$1.028 \times 10^{-12}$	$9.4920 \times 10^{-3}$	
	QuaternionAll	8	$1.5178 \times 10^{-3}$	1	$9.340 \times 10^{-13}$	$4.5640 \times 10^{-3}$	107.977
pdb2l3n 626	ClassicAll	128	$3.5629 \times 10^{-4}$	109	$2.376 \times 10^{-7}$	1.7057	
	QuaternionAll	128	$3.5629 \times 10^{-4}$	109	$2.376 \times 10^{-7}$	$8.2475 \times 10^{-1}$	106.816
pdb2l45 116	ClassicAll	8	$5.9466 \times 10^{-13}$	1	$2.236 \times 10^{-14}$	$9.4055 \times 10^{-4}$	
	QuaternionAll	8	$6.7808 \times 10^{-13}$	1	$3.033 \times 10^{-14}$	$5.8855 \times 10^{-4}$	59.808
pdb2l5r 138	ClassicAll	2	$3.0491 \times 10^{-13}$	2	$3.535 \times 10^{-14}$	$7.5098 \times 10^{-4}$	
	QuaternionAll	2	$3.0031 \times 10^{-13}$	2	$4.436 \times 10^{-14}$	$4.2098 \times 10^{-4}$	78.388
pdb2l98 434	ClassicAll	608	$5.6413 \times 10^{-12}$	154	$3.273 \times 10^{-13}$	1.0512	
	QuaternionAll	608	$6.2089 \times 10^{-12}$	154	$3.637 \times 10^{-13}$	$5.6327 \times 10^{-1}$	86.629
pdb2lci 806	ClassicAll	128	$1.2015 \times 10^{-12}$	29	$2.579 \times 10^{-13}$	$1.1149 \times 10^{-1}$	
	QuaternionAll	128	$1.1830 \times 10^{-12}$	29	$2.404 \times 10^{-13}$	$7.1232 \times 10^{-2}$	56.511

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	32	$6.0282 \times 10^{-3}$	14	$3.047 \times 10^{-7}$	$2.6048 \times 10^{-3}$	
	QuaternionAll	32	$6.0282 \times 10^{-3}$	14	$3.047 \times 10^{-7}$	$1.8393 \times 10^{-3}$	41.618
pdb2le2 676	ClassicAll	16	$1.5317 \times 10^{-12}$	2	$2.064 \times 10^{-13}$	$4.2776 \times 10^{-1}$	
	QuaternionAll	16	$1.4989 \times 10^{-12}$	2	$2.042 \times 10^{-13}$	$2.0895 \times 10^{-1}$	104.716
pdb2le7 122	ClassicAll	8	$8.8940 \times 10^{-14}$	2	$2.111 \times 10^{-14}$	$7.9459 \times 10^{-4}$	
	QuaternionAll	8	$1.1008 \times 10^{-13}$	2	$2.749 \times 10^{-14}$	$5.1307 \times 10^{-4}$	54.868
pdb2ler 68	ClassicAll	8	$5.1096 \times 10^{-14}$	2	$1.314 \times 10^{-14}$	$4.2740 \times 10^{-4}$	
	QuaternionAll	8	$6.2001 \times 10^{-14}$	2	$1.532 \times 10^{-14}$	$2.7520 \times 10^{-4}$	55.305
pdb2lgi 338	ClassicAll	16	$9.7255 \times 10^{-12}$	6	$1.068 \times 10^{-12}$	$4.1270 \times 10^{-2}$	
	QuaternionAll	16	$9.6518 \times 10^{-12}$	6	$1.052 \times 10^{-12}$	$2.1800 \times 10^{-2}$	89.307
pdb2lhe 338	ClassicAll	704	$9.7862 \times 10^{-10}$	54	$4.963 \times 10^{-11}$	$1.8045 \times 10^1$	
	QuaternionAll	704	$9.7867 \times 10^{-10}$	54	$4.967 \times 10^{-11}$	8.6584	108.405
pdb2lhg 338	ClassicAll	16	$5.0995 \times 10^{-13}$	14	$6.485 \times 10^{-14}$	$3.1087 \times 10^{-3}$	
	QuaternionAll	16	$5.4683 \times 10^{-13}$	14	$7.343 \times 10^{-14}$	$2.1955 \times 10^{-3}$	41.590
pdb2lix 162	ClassicAll	2	$4.9988 \times 10^{-13}$	1	$4.842 \times 10^{-14}$	$1.4134 \times 10^{-3}$	
	QuaternionAll	2	$5.1517 \times 10^{-13}$	1	$5.614 \times 10^{-14}$	$7.7418 \times 10^{-4}$	82.565
pdb2lld 242	ClassicAll	16	$3.3970 \times 10^{-3}$	9	$4.630 \times 10^{-7}$	$4.5922 \times 10^{-3}$	
	QuaternionAll	16	$3.3970 \times 10^{-3}$	9	$4.630 \times 10^{-7}$	$2.8003 \times 10^{-3}$	63.990
pdb2lm9 578	ClassicAll	8	$2.2967 \times 10^{-3}$	2	$6.254 \times 10^{-14}$	$4.0805 \times 10^{-3}$	
	QuaternionAll	8	$2.2967 \times 10^{-3}$	2	$7.713 \times 10^{-14}$	$2.6141 \times 10^{-3}$	56.093
pdb2lmf 140	ClassicAll	5376	$1.3912 \times 10^{-5}$	1613	$2.554 \times 10^{-6}$	$4.4378 \times 10^{-1}$	
	QuaternionAll	5376	$1.3912 \times 10^{-5}$	1613	$2.554 \times 10^{-6}$	$4.4877 \times 10^{-1}$	-1.112
pdb2ln3 500	ClassicAll	8	$2.5821 \times 10^{-13}$	1	$1.292 \times 10^{-13}$	$6.6050 \times 10^{-3}$	
	QuaternionAll	8	$2.9987 \times 10^{-13}$	1	$1.359 \times 10^{-13}$	$3.8591 \times 10^{-3}$	71.152
pdb2lo2 230	ClassicAll	64	$1.4016 \times 10^{-2}$	26	$1.353 \times 10^{-7}$	$1.3196 \times 10^{-2}$	
	QuaternionAll	64	$1.4016 \times 10^{-2}$	26	$1.353 \times 10^{-7}$	$7.4255 \times 10^{-3}$	77.715
pdb2lqp 428	ClassicAll	2304	$5.7598 \times 10^{-4}$	222	$8.247 \times 10^{-8}$	$6.5259 \times 10^{-1}$	
	QuaternionAll	2304	$5.7598 \times 10^{-4}$	222	$8.247 \times 10^{-8}$	$5.9247 \times 10^{-1}$	10.149
pdb2lr0 806	ClassicAll	16	$1.2202 \times 10^{-11}$	5	$3.549 \times 10^{-12}$	$3.2315 \times 10^{-1}$	
	QuaternionAll	16	$1.1747 \times 10^{-11}$	5	$3.440 \times 10^{-12}$	$1.6220 \times 10^{-1}$	99.236
pdb2lrh 806	ClassicAll	384	$2.9721 \times 10^{-12}$	189	$5.631 \times 10^{-13}$	$8.9441 \times 10^{-1}$	
	QuaternionAll	384	$2.9099 \times 10^{-12}$	189	$6.564 \times 10^{-13}$	$4.8708 \times 10^{-1}$	83.629
pdb2ls9 152	ClassicAll	16	$2.7045 \times 10^{-12}$	5	$1.122 \times 10^{-13}$	$1.6481 \times 10^{-3}$	
	QuaternionAll	16	$3.0425 \times 10^{-12}$	5	$1.471 \times 10^{-13}$	$1.1036 \times 10^{-3}$	49.336
pdb2lsa 140	ClassicAll	8	$2.5535 \times 10^{-3}$	2	$5.235 \times 10^{-14}$	$9.4580 \times 10^{-4}$	
	QuaternionAll	8	$2.5535 \times 10^{-3}$	2	$6.998 \times 10^{-14}$	$6.1781 \times 10^{-4}$	53.090
pdb2lss 422	ClassicAll	8	$1.2372 \times 10^{-3}$	1	$1.230 \times 10^{-13}$	$5.1730 \times 10^{-3}$	
	QuaternionAll	8	$1.2372 \times 10^{-3}$	1	$1.455 \times 10^{-13}$	$3.0589 \times 10^{-3}$	69.115
pdb2lt3 680	ClassicAll	8	$9.6961 \times 10^{-13}$	6	$7.245 \times 10^{-14}$	$6.6260 \times 10^{-3}$	
	QuaternionAll	8	$1.0253 \times 10^{-12}$	6	$7.760 \times 10^{-14}$	$3.9988 \times 10^{-3}$	65.699
pdb2lu6 86	ClassicAll	8	$7.7550 \times 10^{-3}$	1	$5.356 \times 10^{-15}$	$5.3252 \times 10^{-4}$	
	QuaternionAll	8	$7.7550 \times 10^{-3}$	1	$6.922 \times 10^{-15}$	$3.4349 \times 10^{-4}$	55.034
pdb2lx0 194	ClassicAll	24576	$7.4851 \times 10^{-12}$	3285	$3.569 \times 10^{-13}$	3.7916	
	QuaternionAll	24576	$7.5304 \times 10^{-12}$	3285	$4.035 \times 10^{-13}$	3.4710	9.238
pdb2lxb 892	ClassicAll	16	$9.0172 \times 10^{-13}$	5	$1.542 \times 10^{-13}$	$2.6833 \times 10^{-2}$	
	QuaternionAll	16	$8.6577 \times 10^{-13}$	5	$1.585 \times 10^{-13}$	$1.3296 \times 10^{-2}$	101.818
pdb2lzf 820	ClassicAll	8	$5.9653 \times 10^{-4}$	2	$3.217 \times 10^{-14}$	$8.1541 \times 10^{-1}$	
	QuaternionAll	8	$5.9653 \times 10^{-4}$	2	$3.959 \times 10^{-14}$	$3.9900 \times 10^{-1}$	104.361
pdb2m1a 158	ClassicAll	8	$9.1771 \times 10^{-14}$	1	$6.346 \times 10^{-15}$	$1.0487 \times 10^{-3}$	
	QuaternionAll	8	$9.0451 \times 10^{-14}$	1	$7.612 \times 10^{-15}$	$6.7610 \times 10^{-4}$	55.111
pdb2m1j 182	ClassicAll	32	$1.5890 \times 10^{-13}$	10	$1.865 \times 10^{-14}$	$4.6872 \times 10^{-3}$	
	QuaternionAll	32	$1.6894 \times 10^{-13}$	10	$2.212 \times 10^{-14}$	$3.0380 \times 10^{-3}$	54.286
pdb2m2y 110	ClassicAll	8	$1.8177 \times 10^{-3}$	1	$2.699 \times 10^{-13}$	$9.8928 \times 10^{-4}$	
	QuaternionAll	8	$1.8177 \times 10^{-3}$	1	$2.808 \times 10^{-13}$	$6.0391 \times 10^{-4}$	63.811

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
pdb2m3f 134	ClassicAll	16	$9.5240 \times 10^{-14}$	5	$3.629 \times 10^{-14}$	$1.1373 \times 10^{-3}$	39.873
	QuaternionAll	16	$5.7597 \times 10^{-14}$	5	$4.641 \times 10^{-14}$	$8.1308 \times 10^{-4}$	
pdb2m8m 170	ClassicAll	8	$6.9769 \times 10^{-3}$	5	$2.424 \times 10^{-14}$	$1.1476 \times 10^{-3}$	56.679
	QuaternionAll	8	$6.9769 \times 10^{-3}$	5	$3.058 \times 10^{-14}$	$7.3245 \times 10^{-4}$	
pdb2m8o 170	ClassicAll	16	$4.6389 \times 10^{-3}$	9	$1.337 \times 10^{-7}$	$1.4163 \times 10^{-3}$	39.702
	QuaternionAll	16	$4.6389 \times 10^{-3}$	9	$1.337 \times 10^{-7}$	$1.0138 \times 10^{-3}$	
pdb2m97 416	ClassicAll	8	$2.4560 \times 10^{-12}$	6	$4.654 \times 10^{-14}$	$2.9164 \times 10^{-3}$	56.747
	QuaternionAll	8	$2.4592 \times 10^{-12}$	6	$5.847 \times 10^{-14}$	$1.8606 \times 10^{-3}$	
pdb2m9g 1108	ClassicAll	24	$4.9692 \times 10^{-12}$	9	$2.939 \times 10^{-13}$	$4.0916 \times 10^{-2}$	66.833
	QuaternionAll	24	$4.9567 \times 10^{-12}$	9	$3.170 \times 10^{-13}$	$2.4525 \times 10^{-2}$	
pdb2m9r 242	ClassicAll	65536	$3.7505 \times 10^{-12}$	7301	$3.537 \times 10^{-14}$	$3.1853 \times 10^1$	37.069
	QuaternionAll	65536	$3.6480 \times 10^{-12}$	7301	$4.406 \times 10^{-14}$	$2.3239 \times 10^1$	
pdb2mdv 460	ClassicAll	16	$4.7210 \times 10^{-4}$	6	$3.178 \times 10^{-12}$	$2.7738 \times 10^{-1}$	101.182
	QuaternionAll	16	$4.7210 \times 10^{-4}$	6	$3.178 \times 10^{-12}$	$1.3787 \times 10^{-1}$	
pdb2me1 164	ClassicAll	30720	$2.7384 \times 10^{-5}$	14030	$1.477 \times 10^{-6}$	4.8603	10.305
	QuaternionAll	30720	$2.7384 \times 10^{-5}$	14030	$1.477 \times 10^{-6}$	4.4062	
pdb2me3 164	ClassicAll	8192	$1.1059 \times 10^{-5}$	2542	$2.347 \times 10^{-7}$	$8.2984 \times 10^{-1}$	8.206
	QuaternionAll	8192	$1.1059 \times 10^{-5}$	2542	$2.347 \times 10^{-7}$	$7.6690 \times 10^{-1}$	
pdb2me4 164	ClassicAll	32768	$2.9241 \times 10^{-5}$	854	$2.758 \times 10^{-7}$	4.9982	17.888
	QuaternionAll	32768	$2.9241 \times 10^{-5}$	854	$2.758 \times 10^{-7}$	4.2398	
pdb2mg1 164	ClassicAll	8	$4.4954 \times 10^{-13}$	6	$4.400 \times 10^{-14}$	$1.1133 \times 10^{-3}$	55.501
	QuaternionAll	8	$5.4976 \times 10^{-13}$	6	$5.374 \times 10^{-14}$	$7.1597 \times 10^{-4}$	
pdb2mg2 170	ClassicAll	16	$1.0745 \times 10^{-3}$	10	$1.831 \times 10^{-14}$	$1.5972 \times 10^{-3}$	44.026
	QuaternionAll	16	$1.0745 \times 10^{-3}$	10	$2.481 \times 10^{-14}$	$1.1089 \times 10^{-3}$	
pdb2mg3 170	ClassicAll	16	$6.2977 \times 10^{-13}$	14	$3.542 \times 10^{-14}$	$1.9385 \times 10^{-3}$	51.199
	QuaternionAll	16	$6.7812 \times 10^{-13}$	14	$4.459 \times 10^{-14}$	$1.2821 \times 10^{-3}$	
pdb2mh8 338	ClassicAll	40	$4.2246 \times 10^{-12}$	26	$1.547 \times 10^{-13}$	$5.3693 \times 10^{-3}$	26.731
	QuaternionAll	40	$4.0208 \times 10^{-12}$	26	$1.883 \times 10^{-13}$	$4.2367 \times 10^{-3}$	
pdb2mhw 164	ClassicAll	8	$3.6932 \times 10^{-3}$	2	$6.229 \times 10^{-14}$	$1.1186 \times 10^{-3}$	54.037
	QuaternionAll	8	$3.6932 \times 10^{-3}$	2	$7.130 \times 10^{-14}$	$7.2620 \times 10^{-4}$	
pdb2mij 224	ClassicAll	16	$1.2077 \times 10^{-12}$	1	$1.244 \times 10^{-13}$	$5.3586 \times 10^{-3}$	71.501
	QuaternionAll	16	$1.2294 \times 10^{-12}$	1	$1.522 \times 10^{-13}$	$3.1245 \times 10^{-3}$	
pdb2mix 128	ClassicAll	8	$3.7545 \times 10^{-13}$	1	$4.816 \times 10^{-14}$	$1.4998 \times 10^{-3}$	70.536
	QuaternionAll	8	$3.4098 \times 10^{-13}$	1	$4.684 \times 10^{-14}$	$8.7949 \times 10^{-4}$	
pdb2mj1 110	ClassicAll	168	$8.6589 \times 10^{-4}$	45	$4.712 \times 10^{-7}$	$7.9187 \times 10^{-3}$	29.487
	QuaternionAll	168	$8.6589 \times 10^{-4}$	45	$4.712 \times 10^{-7}$	$6.1154 \times 10^{-3}$	
pdb2mj2 218	ClassicAll	32	$3.7278 \times 10^{-3}$	2	$1.591 \times 10^{-7}$	$3.2246 \times 10^{-3}$	36.475
	QuaternionAll	32	$3.7278 \times 10^{-3}$	2	$1.591 \times 10^{-7}$	$2.3628 \times 10^{-3}$	
pdb2mjg 556	ClassicAll	256	$1.4274 \times 10^{-3}$	94	$9.193 \times 10^{-9}$	$7.6677 \times 10^{-1}$	89.651
	QuaternionAll	256	$1.4274 \times 10^{-3}$	94	$9.193 \times 10^{-9}$	$4.0430 \times 10^{-1}$	
pdb2mle 434	ClassicAll	16	$1.6719 \times 10^{-3}$	6	$1.491 \times 10^{-13}$	$1.0910 \times 10^{-1}$	108.158
	QuaternionAll	16	$1.6719 \times 10^{-3}$	6	$1.535 \times 10^{-13}$	$5.2413 \times 10^{-2}$	
pdb2mlf 434	ClassicAll	16	$8.3036 \times 10^{-13}$	6	$9.918 \times 10^{-14}$	$7.1563 \times 10^{-3}$	62.937
	QuaternionAll	16	$8.8493 \times 10^{-13}$	6	$1.127 \times 10^{-13}$	$4.3921 \times 10^{-3}$	
pdb2mpu 554	ClassicAll	8	$2.5305 \times 10^{-12}$	1	$9.785 \times 10^{-14}$	$1.7354 \times 10^{-2}$	101.834
	QuaternionAll	8	$2.5592 \times 10^{-12}$	1	$1.016 \times 10^{-13}$	$8.5980 \times 10^{-3}$	
pdb2mra 704	ClassicAll	40	$4.3616 \times 10^{-12}$	9	$2.632 \times 10^{-13}$	$8.2104 \times 10^{-2}$	89.047
	QuaternionAll	40	$4.3117 \times 10^{-12}$	9	$2.768 \times 10^{-13}$	$4.3431 \times 10^{-2}$	
pdb2msu 122	ClassicAll	1152	$3.6237 \times 10^{-12}$	29	$7.813 \times 10^{-14}$	$7.9977 \times 10^{-2}$	22.074
	QuaternionAll	1152	$3.6441 \times 10^{-12}$	29	$8.765 \times 10^{-14}$	$6.5515 \times 10^{-2}$	
pdb2mty 120	ClassicAll	16	$5.1232 \times 10^{-12}$	16	$1.848 \times 10^{-14}$	$1.7035 \times 10^{-3}$	58.793
	QuaternionAll	16	$5.2129 \times 10^{-12}$	16	$2.363 \times 10^{-14}$	$1.0728 \times 10^{-3}$	
pdb2muh 98	ClassicAll	18432	$1.3995 \times 10^{-5}$	5070	$4.190 \times 10^{-7}$	$1.5133 \times 10^1$	84.741
	QuaternionAll	18432	$1.3995 \times 10^{-5}$	5070	$4.190 \times 10^{-7}$	8.1914	

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
pdb2mvj 156	ClassicAll	64	$6.1752 \times 10^{-12}$	3	$1.534 \times 10^{-13}$	$6.0424 \times 10^{-3}$	
	QuaternionAll	64	$6.1858 \times 10^{-12}$	3	$1.647 \times 10^{-13}$	$4.1485 \times 10^{-3}$	45.652
pdb2n00 572	ClassicAll	1024	$9.6419 \times 10^{-5}$	342	$3.910 \times 10^{-7}$	1.0703	
	QuaternionAll	1024	$9.6419 \times 10^{-5}$	342	$3.910 \times 10^{-7}$	$7.0664 \times 10^{-1}$	51.460
pdb2n0b 60	ClassicAll	573440	$1.0219 \times 10^{-11}$	516662	$7.123 \times 10^{-13}$	$1.3982 \times 10^2$	
	QuaternionAll	573440	$1.0781 \times 10^{-11}$	516662	$9.477 \times 10^{-13}$	$1.1558 \times 10^2$	20.970
pdb2n0c 60	ClassicAll	409600	$1.0471 \times 10^{-12}$	136912	$1.293 \times 10^{-13}$	$8.1007 \times 10^1$	
	QuaternionAll	409600	$9.1394 \times 10^{-13}$	136912	$1.682 \times 10^{-13}$	$6.7311 \times 10^1$	20.347
pdb2n0d 60	ClassicAll	73728	$5.2061 \times 10^{-11}$	61516	$3.639 \times 10^{-12}$	5.1307	
	QuaternionAll	73728	$5.7645 \times 10^{-11}$	61516	$4.540 \times 10^{-12}$	4.5411	12.983
pdb2n0e 60	ClassicAll	448	$1.1503 \times 10^{-11}$	250	$3.314 \times 10^{-12}$	$2.2131 \times 10^{-2}$	
	QuaternionAll	448	$1.8786 \times 10^{-11}$	250	$4.286 \times 10^{-12}$	$1.2801 \times 10^{-2}$	72.891
pdb2n0f 60	ClassicAll	24	$2.2697 \times 10^{-12}$	8	$3.185 \times 10^{-13}$	$2.3725 \times 10^{-3}$	
	QuaternionAll	24	$2.7490 \times 10^{-12}$	8	$4.023 \times 10^{-13}$	$1.3768 \times 10^{-3}$	72.326
pdb2n0g 60	ClassicAll	2048	$1.4896 \times 10^{-11}$	1022	$8.315 \times 10^{-13}$	$5.8145 \times 10^{-2}$	
	QuaternionAll	2048	$1.4974 \times 10^{-11}$	1022	$9.618 \times 10^{-13}$	$5.7030 \times 10^{-2}$	1.955
pdb2n0h 60	ClassicAll	2048	$4.1935 \times 10^{-12}$	2022	$7.716 \times 10^{-13}$	$5.1485 \times 10^{-2}$	
	QuaternionAll	2048	$4.1379 \times 10^{-12}$	2022	$8.755 \times 10^{-13}$	$5.4972 \times 10^{-2}$	-6.344
pdb2n35 314	ClassicAll	256	$1.4234 \times 10^{-4}$	202	$4.067 \times 10^{-8}$	$3.9782 \times 10^{-2}$	
	QuaternionAll	256	$1.4234 \times 10^{-4}$	202	$4.067 \times 10^{-8}$	$2.9834 \times 10^{-2}$	33.346
pdb2n3a 574	ClassicAll	64	$2.1457 \times 10^{-3}$	45	$8.770 \times 10^{-14}$	$6.4307 \times 10^{-1}$	
	QuaternionAll	64	$2.1457 \times 10^{-3}$	45	$1.049 \times 10^{-13}$	$3.1953 \times 10^{-1}$	101.256
pdb2n41 638	ClassicAll	384	$3.6179 \times 10^{-3}$	374	$1.067 \times 10^{-7}$	$4.6591 \times 10^{-1}$	
	QuaternionAll	384	$3.6179 \times 10^{-3}$	374	$1.067 \times 10^{-7}$	$2.6788 \times 10^{-1}$	73.925
pdb2n4e 638	ClassicAll	64	$4.6757 \times 10^{-3}$	18	$1.081 \times 10^{-7}$	$5.5445 \times 10^{-2}$	
	QuaternionAll	64	$4.6757 \times 10^{-3}$	18	$1.081 \times 10^{-7}$	$3.2210 \times 10^{-2}$	72.139
pdb2n67 566	ClassicAll	16	$2.0736 \times 10^{-12}$	1	$4.443 \times 10^{-13}$	$7.6106 \times 10^{-3}$	
	QuaternionAll	16	$2.0936 \times 10^{-12}$	1	$4.465 \times 10^{-13}$	$4.8955 \times 10^{-3}$	55.460
pdb2n7j 336	ClassicAll	2	$2.5110 \times 10^{-12}$	1	$5.969 \times 10^{-13}$	$9.3849 \times 10^{-2}$	
	QuaternionAll	2	$2.6436 \times 10^{-12}$	1	$6.094 \times 10^{-13}$	$4.3939 \times 10^{-2}$	113.589
pdb2na9 266	ClassicAll	96	$2.3390 \times 10^{-12}$	33	$5.440 \times 10^{-14}$	$2.0714 \times 10^{-2}$	
	QuaternionAll	96	$2.3721 \times 10^{-12}$	33	$6.690 \times 10^{-14}$	$1.2074 \times 10^{-2}$	71.554
pdb2ndc 110	ClassicAll	8	$3.1313 \times 10^{-3}$	2	$3.365 \times 10^{-14}$	$7.2414 \times 10^{-4}$	
	QuaternionAll	8	$3.1313 \times 10^{-3}$	2	$4.481 \times 10^{-14}$	$4.7306 \times 10^{-4}$	53.077
pdb2nde 110	ClassicAll	8	$8.5286 \times 10^{-5}$	2	$7.022 \times 10^{-14}$	$7.2508 \times 10^{-4}$	
	QuaternionAll	8	$8.5286 \times 10^{-5}$	2	$8.855 \times 10^{-14}$	$4.6803 \times 10^{-4}$	54.924
pdb2nvj 152	ClassicAll	8	$6.7520 \times 10^{-3}$	7	$2.082 \times 10^{-14}$	$1.0214 \times 10^{-3}$	
	QuaternionAll	8	$6.7520 \times 10^{-3}$	7	$2.293 \times 10^{-14}$	$6.6588 \times 10^{-4}$	53.387
pdb2p6j 314	ClassicAll	8	$3.2640 \times 10^{-13}$	1	$4.795 \times 10^{-14}$	$2.1989 \times 10^{-3}$	
	QuaternionAll	8	$3.5480 \times 10^{-13}$	1	$6.389 \times 10^{-14}$	$1.4052 \times 10^{-3}$	56.475
pdb2rlg 108	ClassicAll	8	$4.8140 \times 10^{-13}$	2	$5.501 \times 10^{-14}$	$2.2010 \times 10^{-3}$	
	QuaternionAll	8	$5.3066 \times 10^{-13}$	2	$6.973 \times 10^{-14}$	$1.2342 \times 10^{-3}$	78.342
pdb2rlh 108	ClassicAll	8	$1.0750 \times 10^{-12}$	3	$4.772 \times 10^{-14}$	$1.5218 \times 10^{-3}$	
	QuaternionAll	8	$1.0423 \times 10^{-12}$	3	$5.801 \times 10^{-14}$	$8.8788 \times 10^{-4}$	71.391
pdb2rmy 206	ClassicAll	10240	$1.1655 \times 10^{-4}$	2805	$1.609 \times 10^{-7}$	1.5063	
	QuaternionAll	10240	$1.1655 \times 10^{-4}$	2805	$1.609 \times 10^{-7}$	1.3421	12.235
pdb2roo 260	ClassicAll	16	$3.0591 \times 10^{-4}$	14	$3.610 \times 10^{-6}$	$4.2128 \times 10^{-2}$	
	QuaternionAll	16	$3.0591 \times 10^{-4}$	14	$3.610 \times 10^{-6}$	$2.2029 \times 10^{-2}$	91.237
pdb2rut 218	ClassicAll	96	$2.0579 \times 10^{-13}$	26	$4.389 \times 10^{-14}$	$1.9890 \times 10^{-2}$	
	QuaternionAll	96	$4.0546 \times 10^{-13}$	26	$5.013 \times 10^{-14}$	$1.1147 \times 10^{-2}$	78.435
pdb2ruv 224	ClassicAll	32	$5.4278 \times 10^{-13}$	6	$5.775 \times 10^{-14}$	$4.8844 \times 10^{-3}$	
	QuaternionAll	32	$6.5510 \times 10^{-13}$	6	$7.404 \times 10^{-14}$	$3.2191 \times 10^{-3}$	51.730
pdb2rux 218	ClassicAll	192	$3.4373 \times 10^{-3}$	49	$3.717 \times 10^{-7}$	$2.7441 \times 10^{-2}$	
	QuaternionAll	192	$3.4373 \times 10^{-3}$	49	$3.717 \times 10^{-7}$	$1.9435 \times 10^{-2}$	41.195

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
pdb2ruy 224	ClassicAll	384	$4.1535 \times 10^{-13}$	17	$1.968 \times 10^{-14}$	$2.8761 \times 10^{-2}$	
	QuaternionAll	384	$3.5904 \times 10^{-13}$	17	$2.387 \times 10^{-14}$	$2.5472 \times 10^{-2}$	12.910
pdb2rv3 218	ClassicAll	16	$3.0630 \times 10^{-4}$	5	$3.656 \times 10^{-14}$	$3.3604 \times 10^{-3}$	
	QuaternionAll	16	$3.0630 \times 10^{-4}$	5	$4.118 \times 10^{-14}$	$2.0977 \times 10^{-3}$	60.197
pdb2rv5 212	ClassicAll	192	$7.5780 \times 10^{-4}$	29	$1.857 \times 10^{-7}$	$3.7516 \times 10^{-2}$	
	QuaternionAll	192	$7.5780 \times 10^{-4}$	29	$1.857 \times 10^{-7}$	$2.3951 \times 10^{-2}$	56.635