

KIC with the new sp2 corrections and smooth hbonds

Amelie Stein & Tanja Kortemme

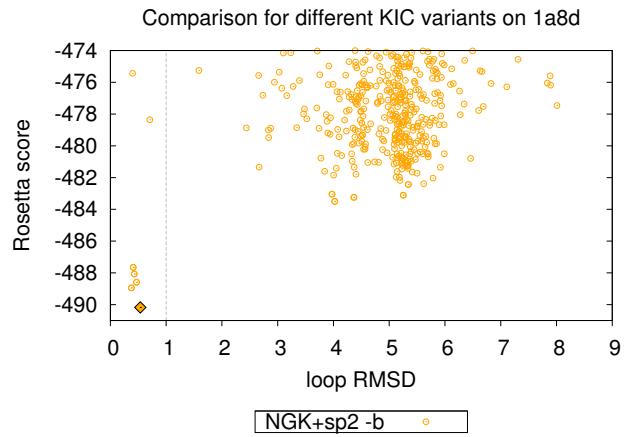
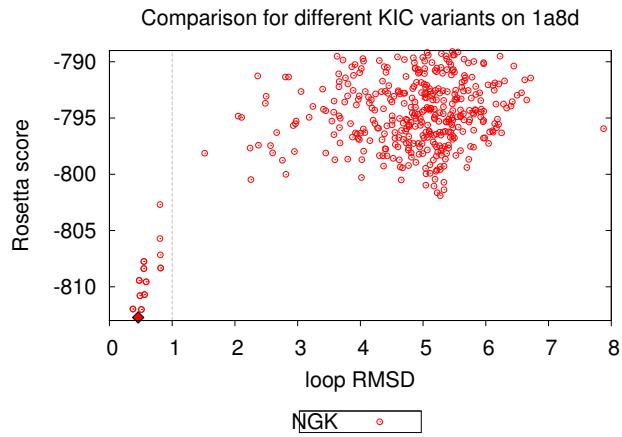
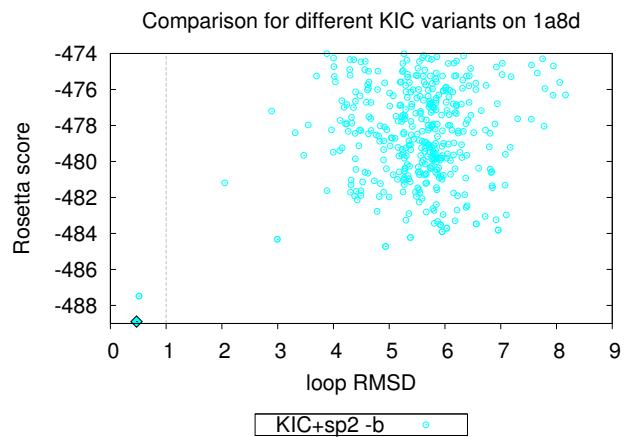
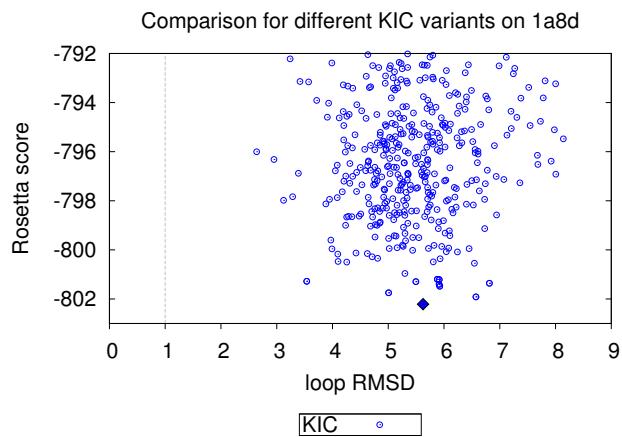
April 30, 2013

- r54685-based
- standard (score12) runs were done with 5 outer cycles, bicubic interpolation switched off⁽¹⁾, and a bumpfix value of 0.36, which clearly boosts NGK performance though there doesn't seem to be a measurable effect on KIC
- sp2 runs were done on structures that were pre-min-packed with sp2 weights and flags. The runs shown here were done with bicubic disabled.

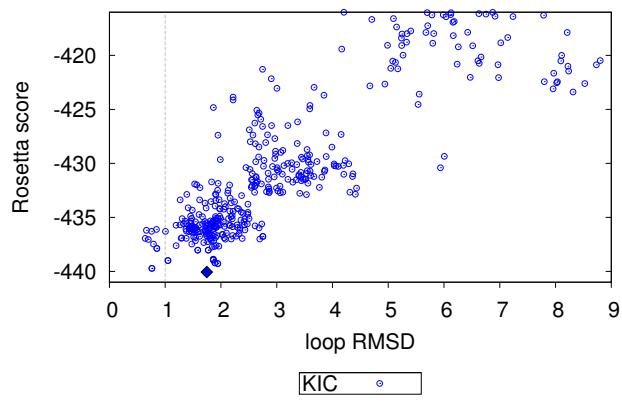
⁽¹⁾performs badly with KIC and especially NGK, for not really understood reasons – may have to do with accepting too many poor initial conformations and/or lack of adaptation of bicubic to rama2b, which in turn may depend on the bumpfix factor – trials to explore which bumpfix works best with bicubic are planned...

	KIC		KIC+sp2 -b		NGK		NGK+sp2 -b	
1a8d (2)	0.0	-	0.4	1	2.6	1	1.4	1
1arb (2)	1.6	2	10.2	1	23.6	2	17.2	1
1bhe (2)	3.8	1	3.6	2	20.0	1	28.0	1
1bn8 (2)	25.4	1	39.0	1	4.6	4	9.0	1
1c5e (2)	47.0	1	50.0	1	49.8	1	61.2	1
1cb0 (2)	36.0	1	44.6	1	40.6	1	55.4	1
1cnv (2)	0.0	-	0.0	-	0.2	243	0.0	-
1cs6 (2)	0.0	-	0.0	-	0.0	-	0.0	-
1cyo	16.2	56	11.6	1	20.6	16	14.2	14
1dqz (2)	24.2	1	38.8	1	25.4	1	33.8	1
1dts	0.0	-	0.0	-	0.8	10	3.4	144
1eco	54.4	1	50.8	1	77.4	1	73.8	1
1ede	3.0	1	15.8	1	6.2	1	8.0	1
1exm (2)	9.2	8	43.0	1	40.0	1	72.8	2
1ezm	0.0	-	0.0	-	0.0	-	0.2	8
1f46 (2)	0.0	-	0.0	-	29.6	1	17.4	91
1i7p (2)	16.0	6	15.6	1	38.2	1	27.4	4
1m3s (2)	7.4	21	9.8	67	17.6	18	21.0	68
1ms9 (2)	66.0	3	79.2	1	36.2	2	52.4	1
1msc	0.0	-	0.0	-	0.0	-	0.0	-
1my7 (2)	45.4	1	67.0	1	72.6	1	78.2	1
1onc	0.0	-	0.6	27	0.4	10	0.6	6
1oth (2)	34.0	1	49.2	1	50.2	1	53.0	1
1oyc (2)	0.0	-	0.2	1	5.6	1	18.2	1
1pbe	3.4	1	1.4	112	12.2	1	13.8	7
1qlw (2)	1.8	5	3.2	1	6.2	1	13.8	1
1rro	12.8	1	10.4	1	34.4	1	23.4	1
1srp	95.6	1	98.6	1	93.0	1	94.6	1
1t1d (2)	8.2	1	4.0	7	17.2	1	13.6	2
1tca	0.0	-	0.6	1	0.2	2	1.8	1
1thg	2.4	39	1.0	53	0.6	2	0.8	1
1thw	0.0	-	0.2	250	2.0	1	2.0	1
1tib	0.8	272	1.8	35	2.0	2	10.4	1
1tml	23.0	1	33.2	1	34.6	1	44.8	1
1xif	23.0	1	58.0	1	67.6	1	86.0	1
2cpl	23.2	1	36.0	1	15.0	1	30.8	3
2ebn	0.0	-	2.2	41	0.4	1	0.2	98
2exo	5.2	1	10.4	1	20.8	1	29.2	1
2pia (2)	86.4	1	95.6	1	94.6	1	99.2	1
2rn2	2.8	1	6.8	1	14.0	1	20.4	1
2sil	1.2	13	1.2	56	4.0	1	2.6	2
2tgi	0.0	-	0.0	-	0.0	-	0.4	1
3cla	11.2	1	21.4	1	3.6	4	7.6	3
3hsc	21.4	1	17.2	1	65.0	1	60.8	1
4i1b	0.0	-	0.0	-	0.0	-	0.2	37
median	3.8	14 × -	9.8	8 × -	15.0	5 × -	17.2	3 × -
non-cis-pro	5.2		10.2		15.0		17.2	
dataset 2 only	8.2	5 × -	10.2	3 × -	23.6	1 × -	21.0	2 × -
d2 non-cis-pro	9.2		15.6		23.6		27.4	

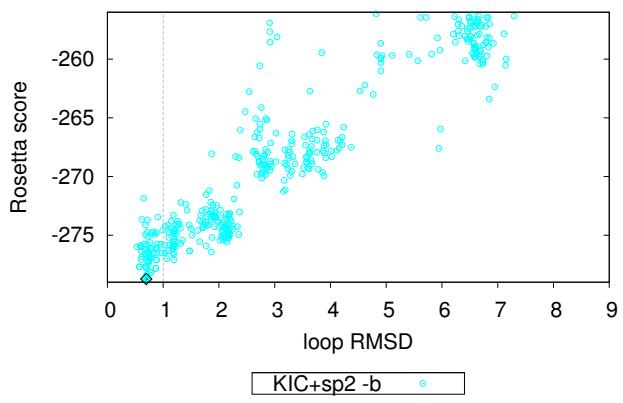
1 Full-atom stage results for each individual loop and parameter set



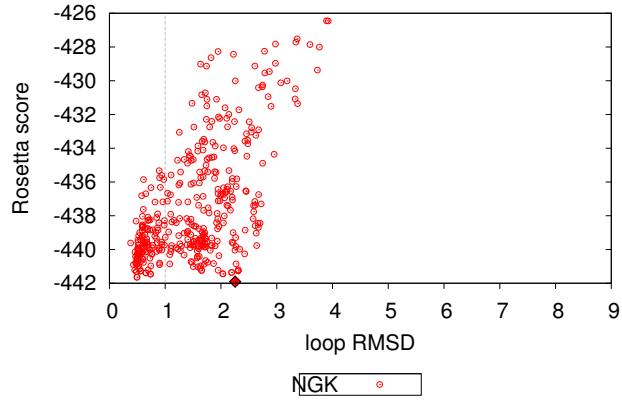
Comparison for different KIC variants on 1arb



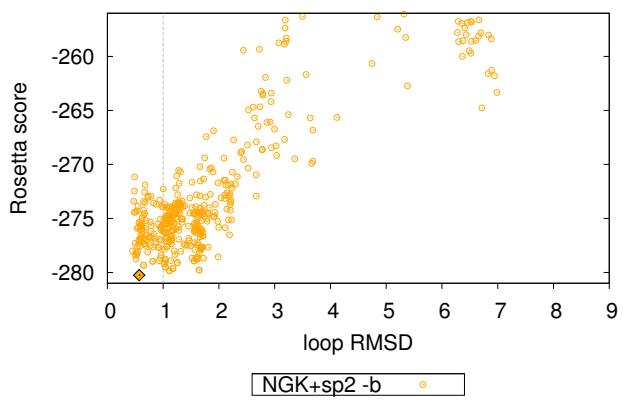
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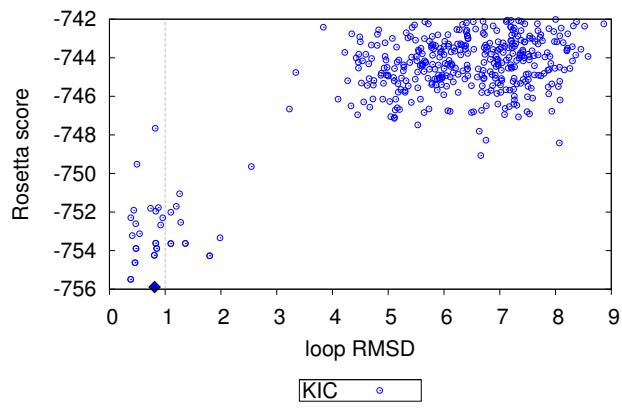
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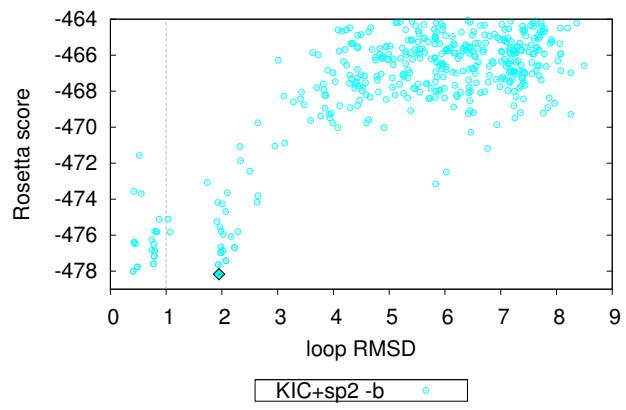
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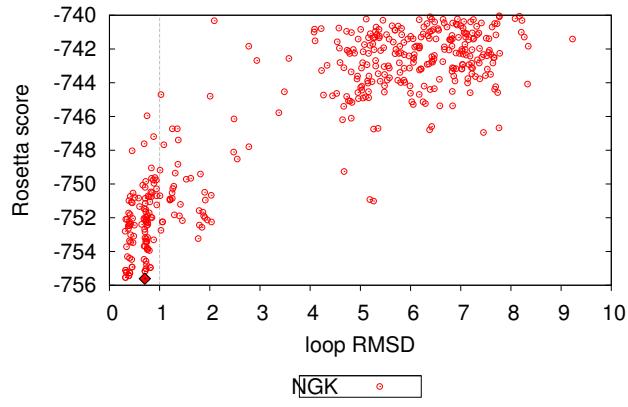
Comparison for different KIC variants on 1bhe



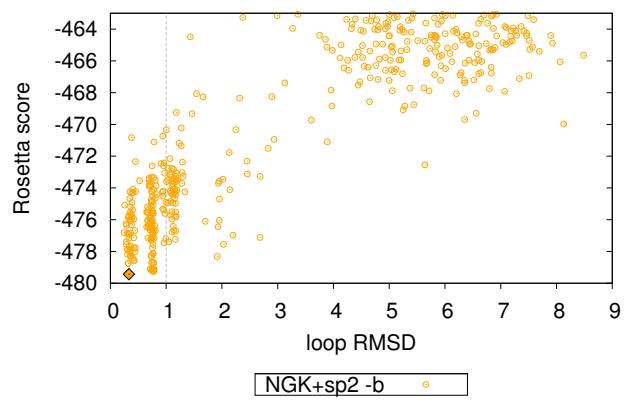
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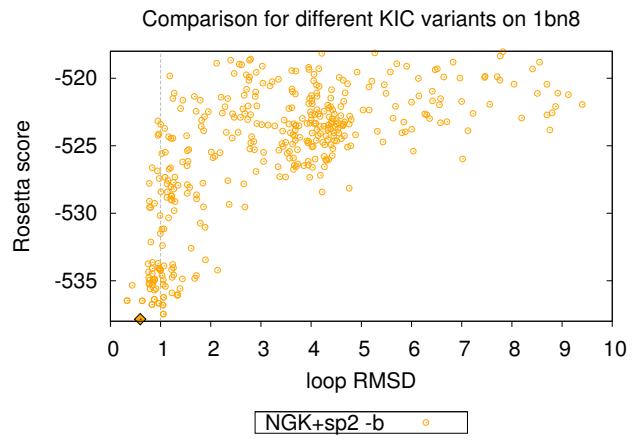
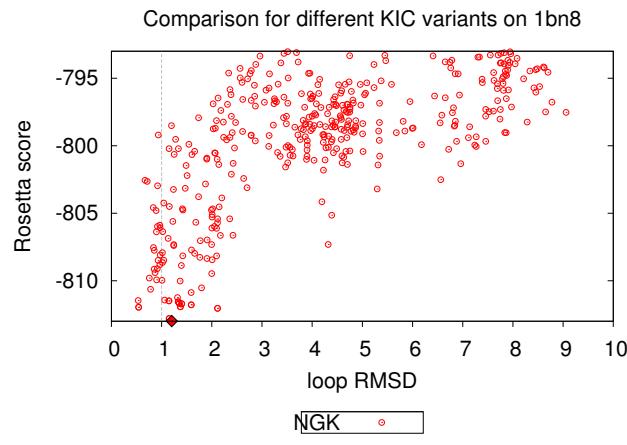
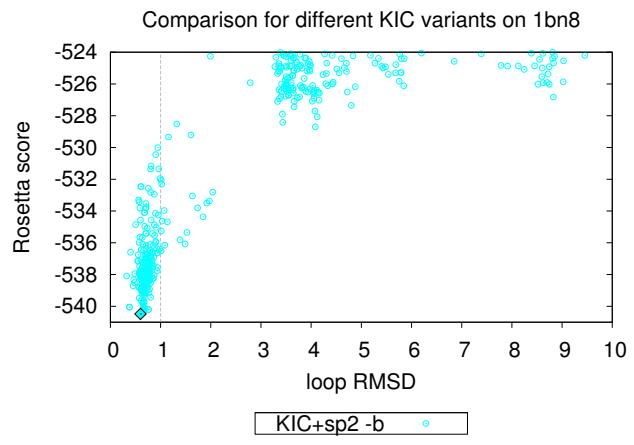
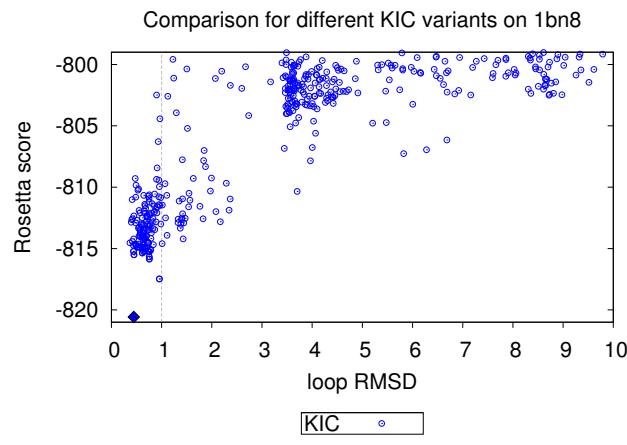


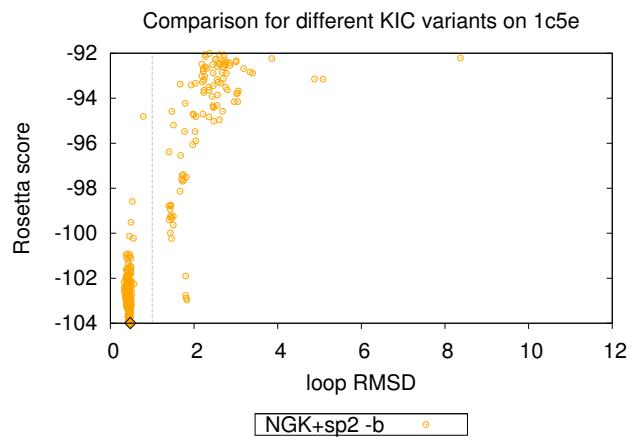
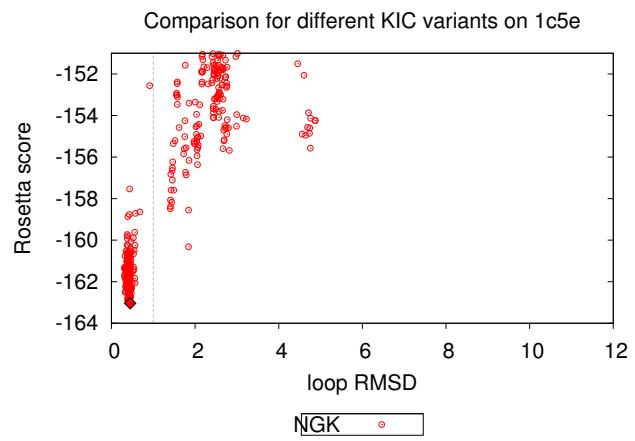
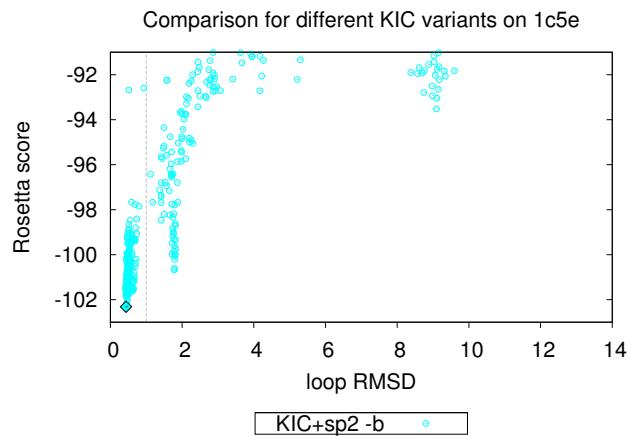
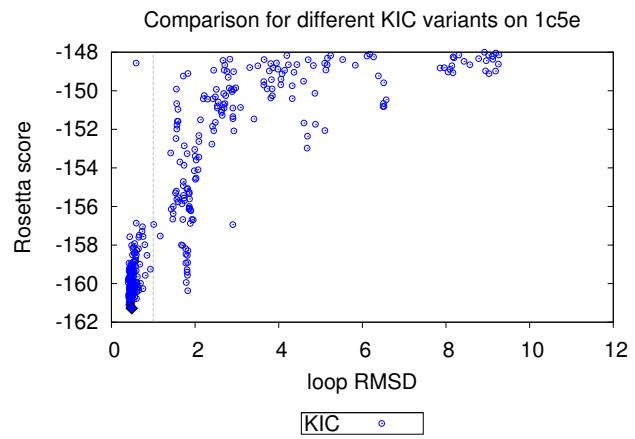
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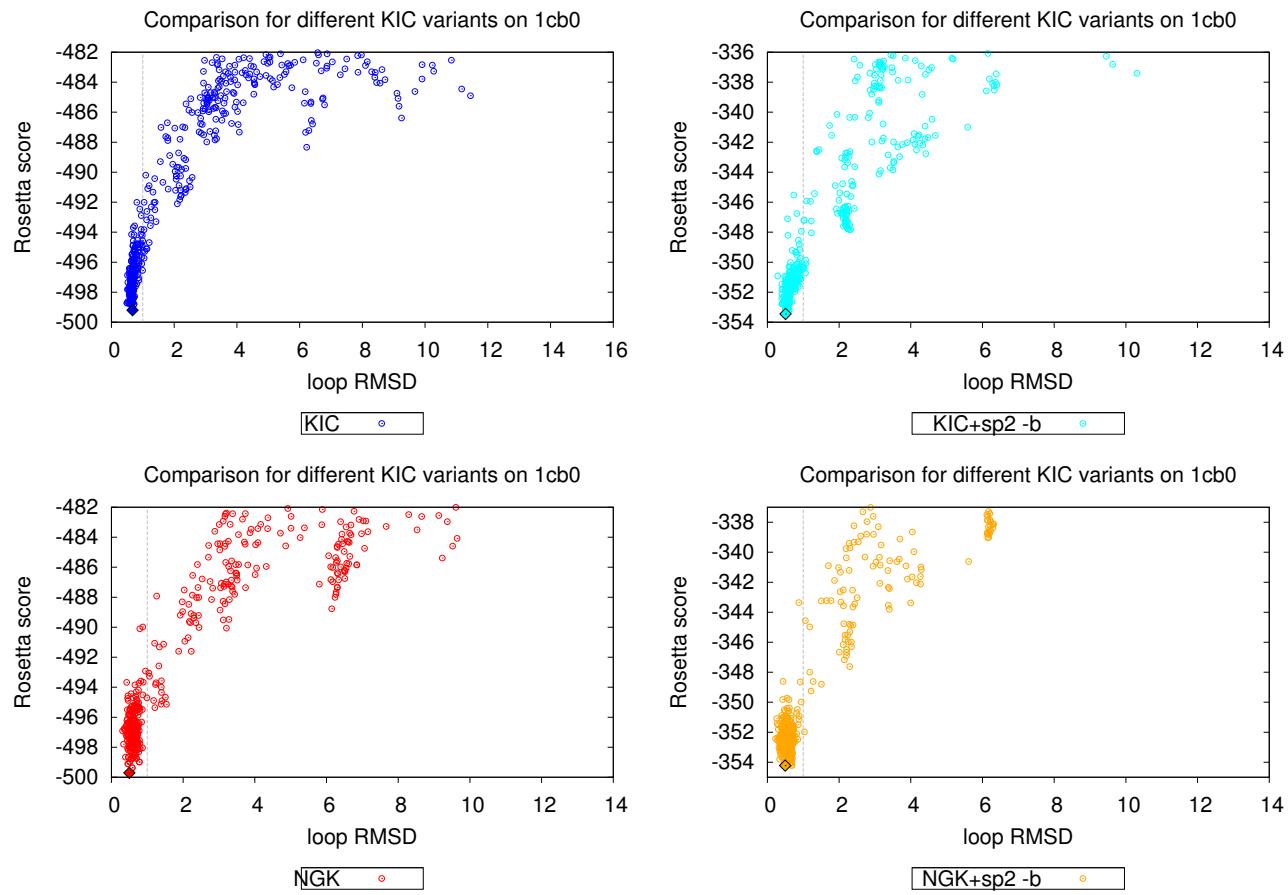


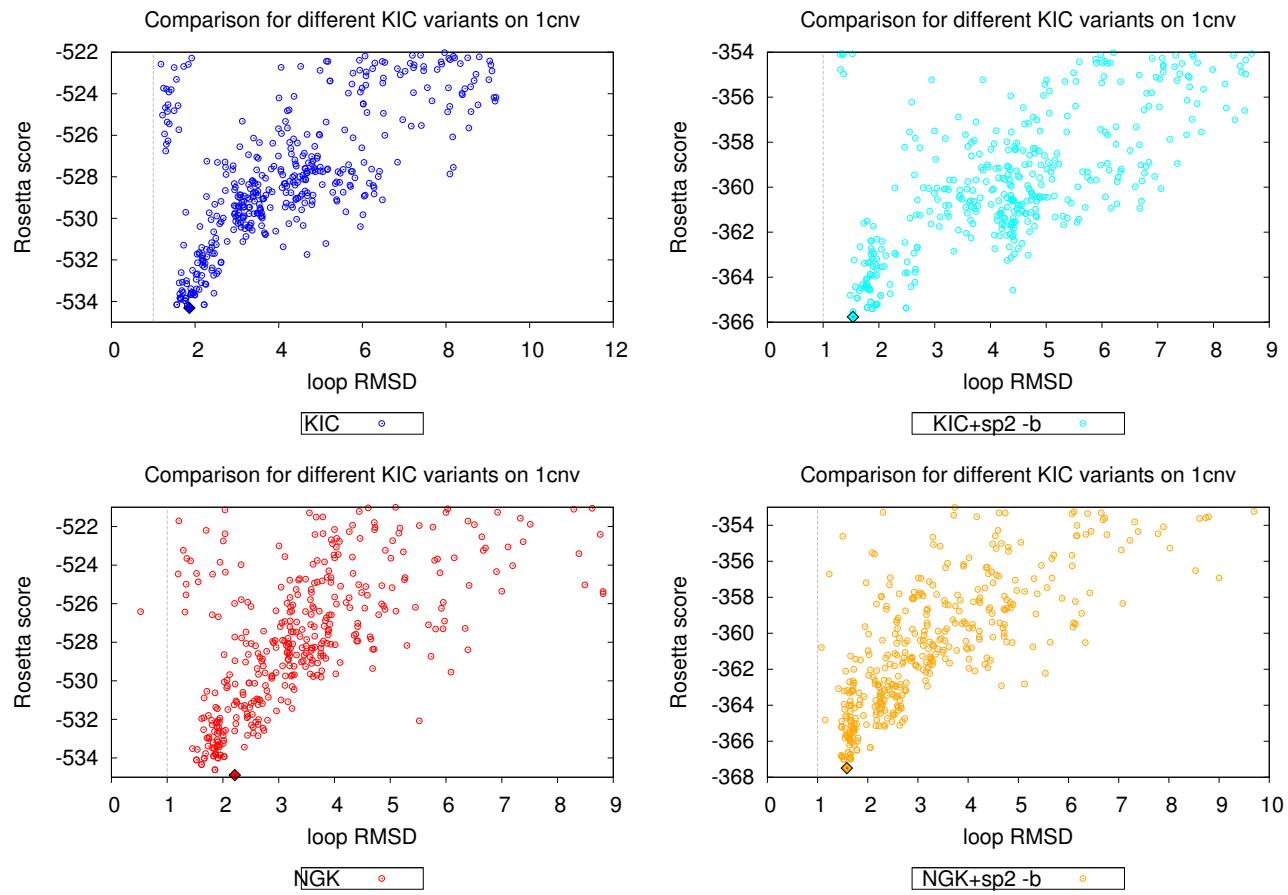
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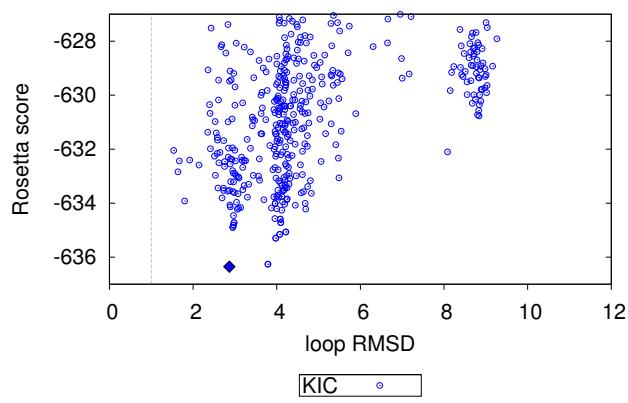




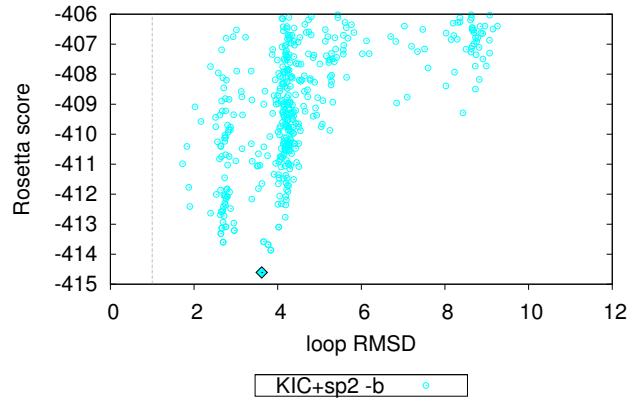




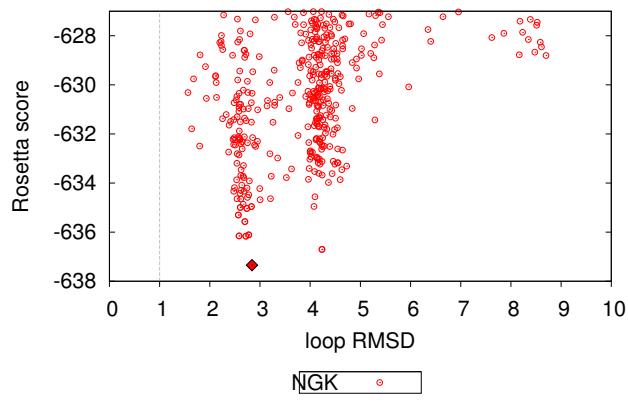
Comparison for different KIC variants on 1cs6



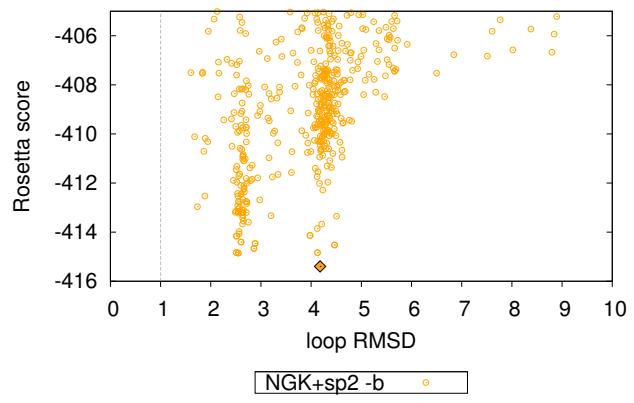
Comparison for different KIC variants on 1cs6

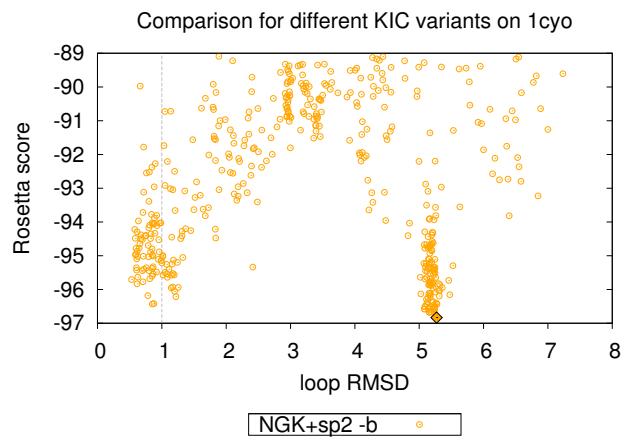
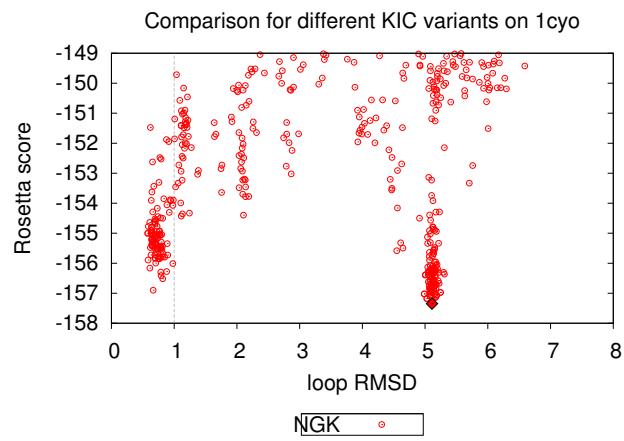
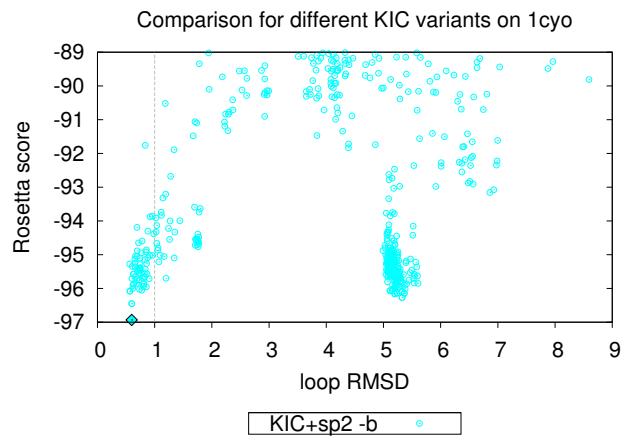
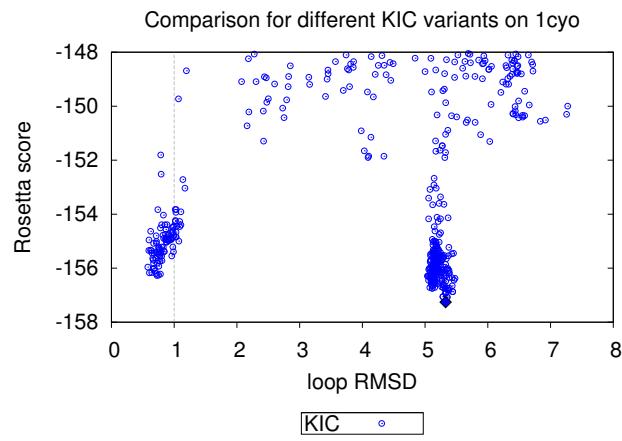


Comparison for different KIC variants on 1cs6

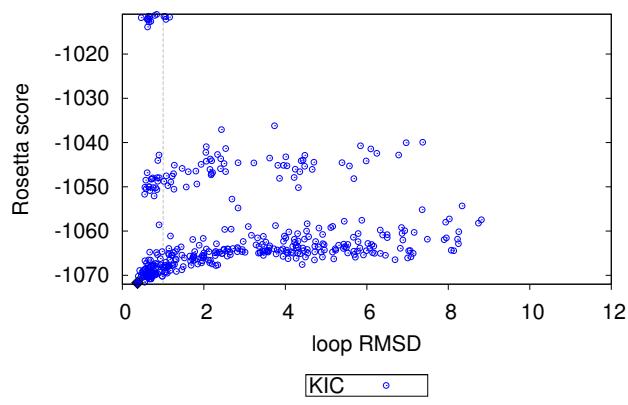


Comparison for different KIC variants on 1cs6

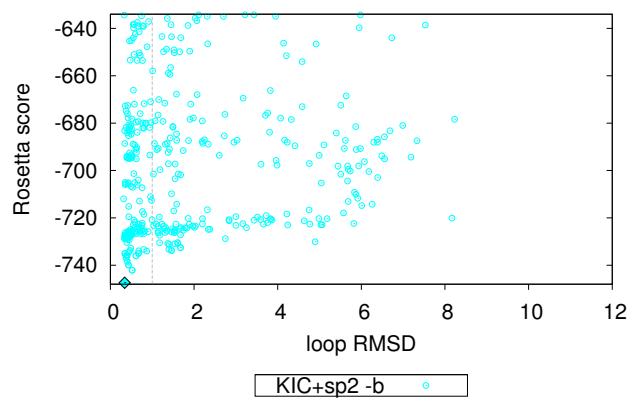




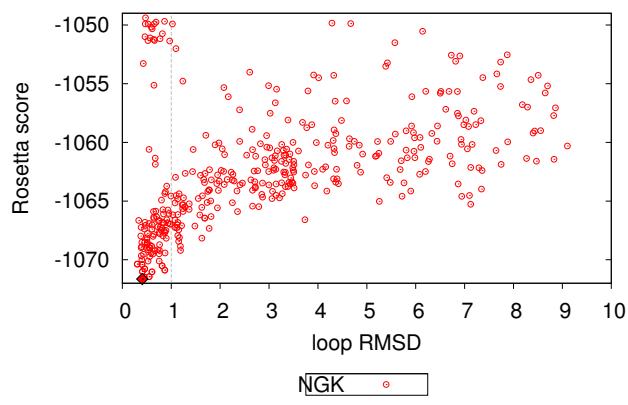
Comparison for different KIC variants on 1dqz



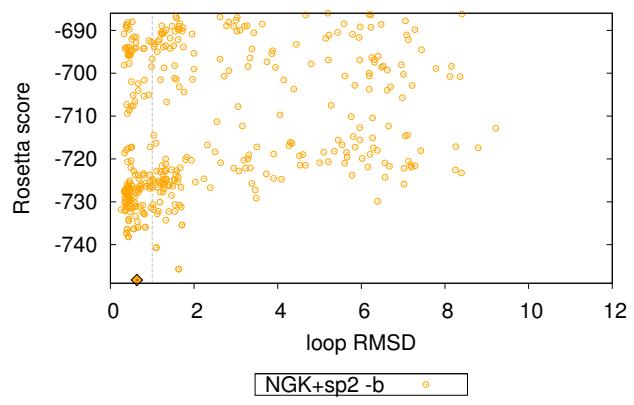
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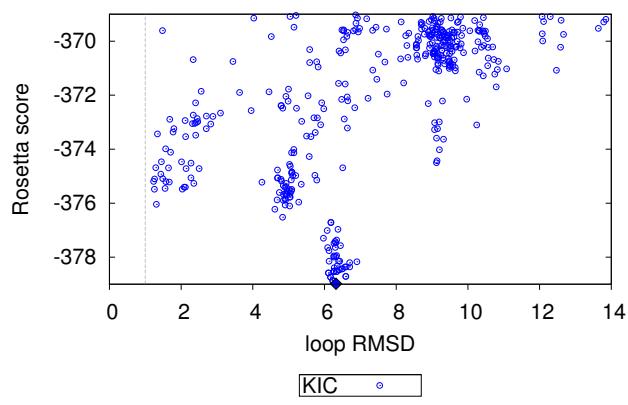
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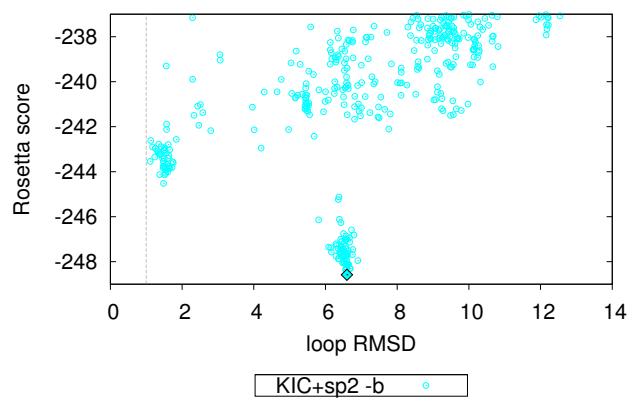
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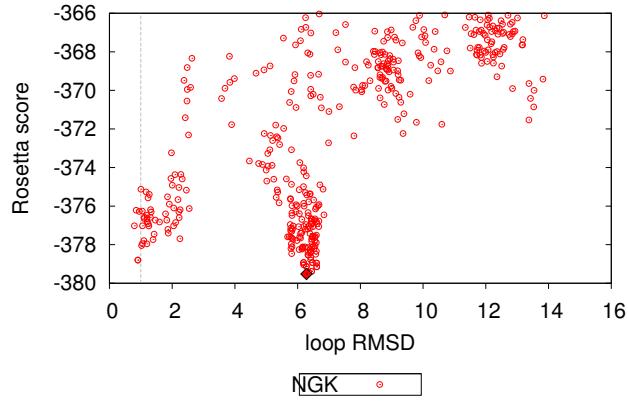
Comparison for different KIC variants on 1dts



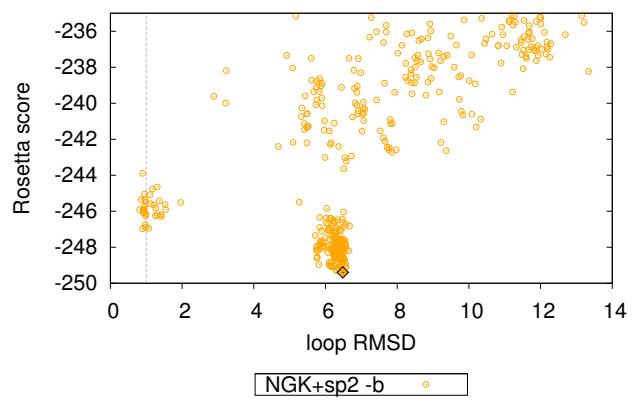
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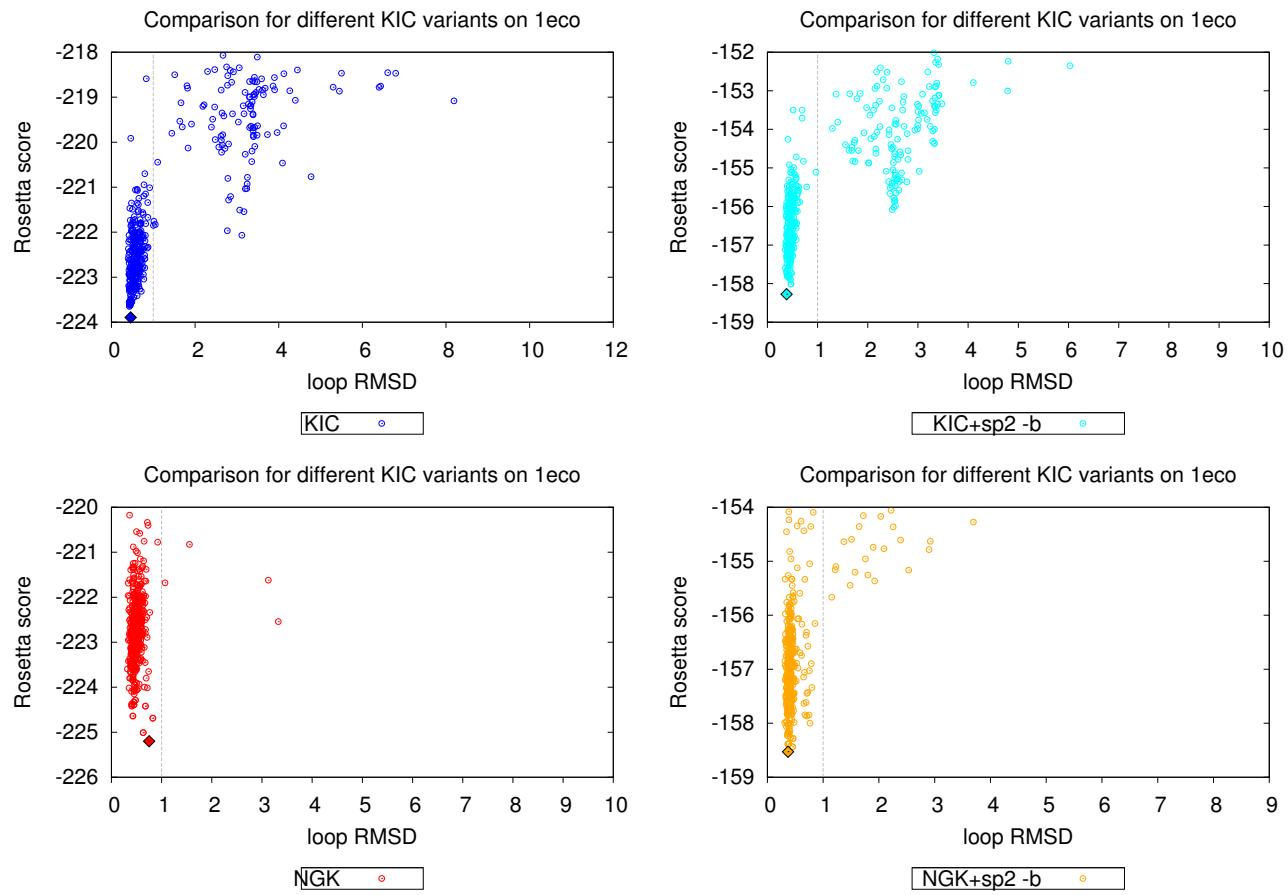


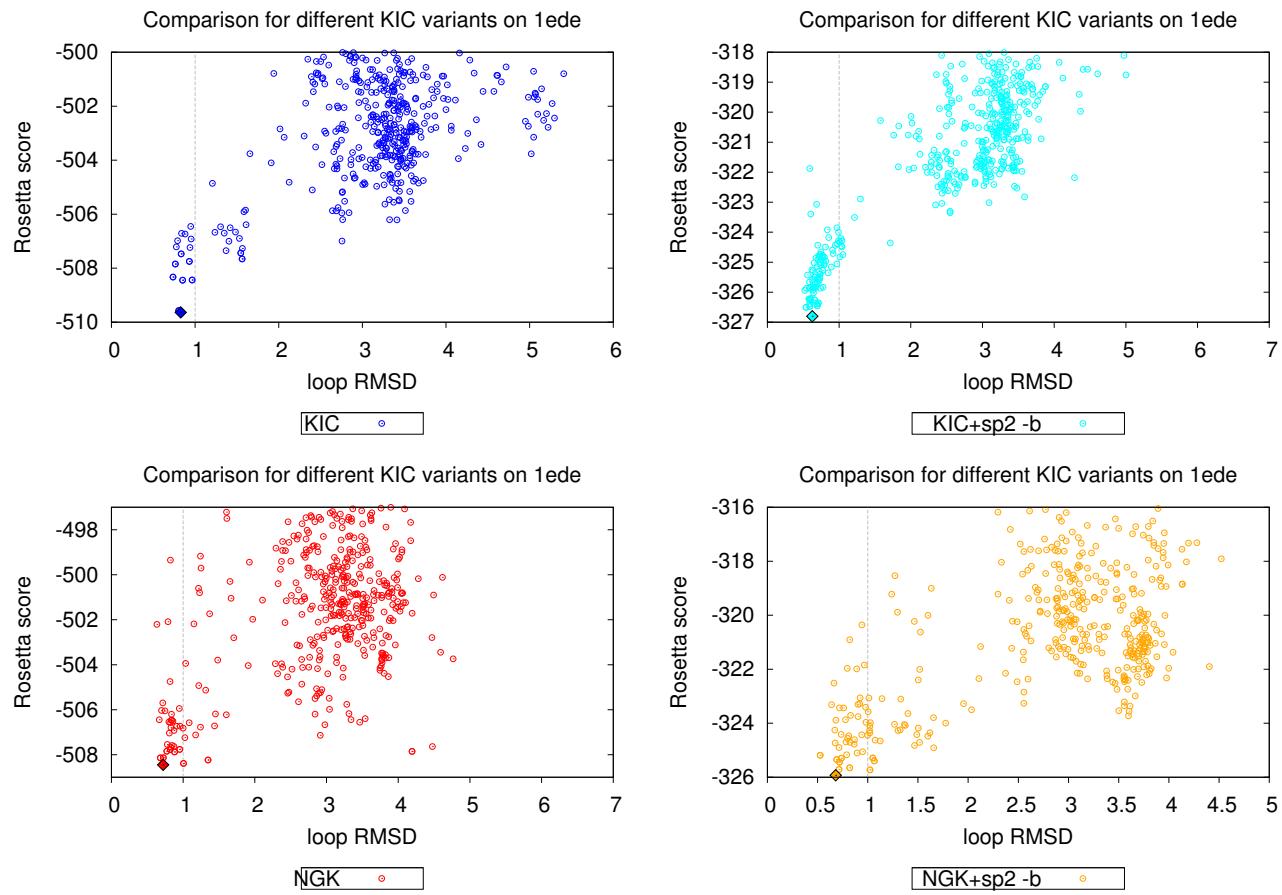
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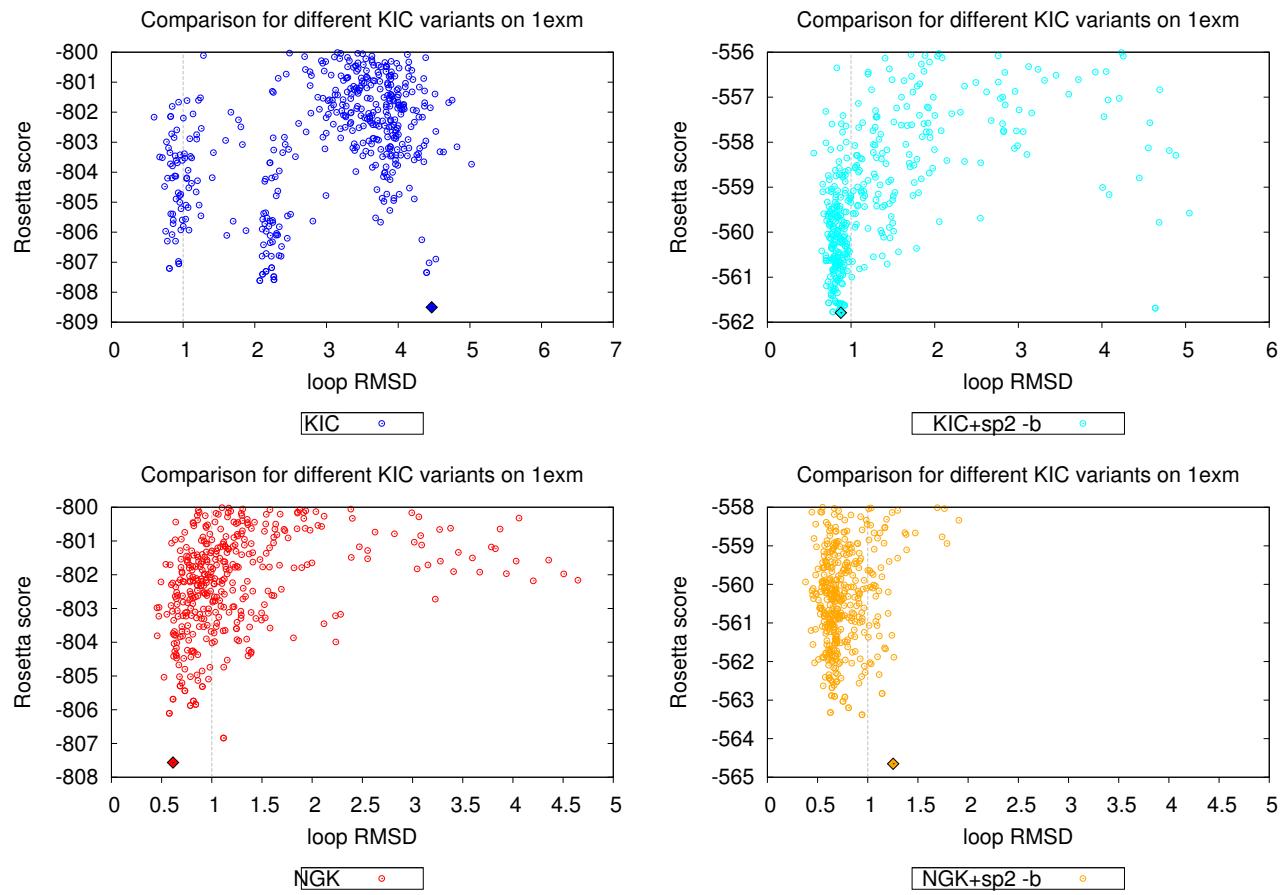


Comparison for different KIC variants on 1dts

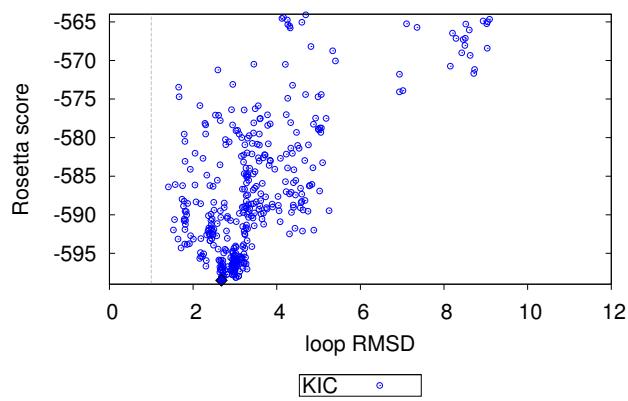




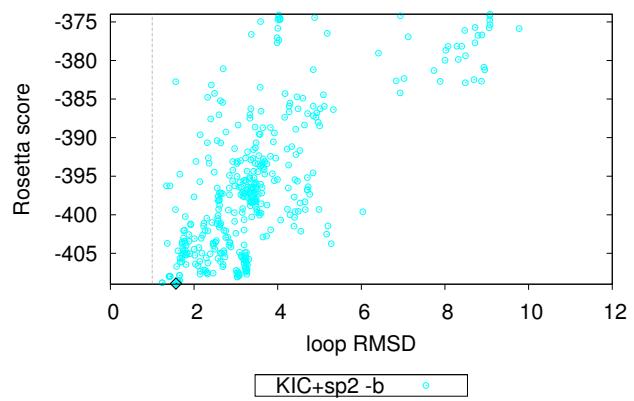




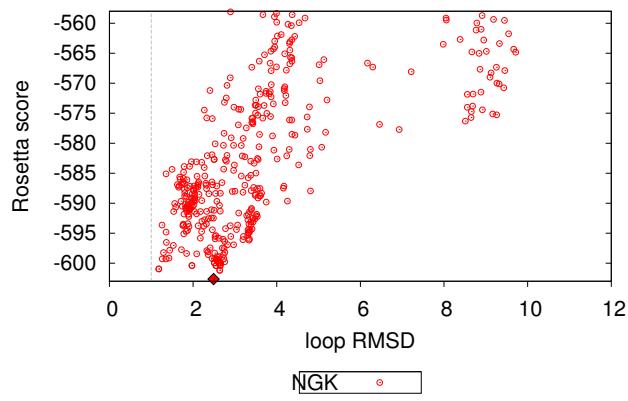
Comparison for different KIC variants on 1ezm



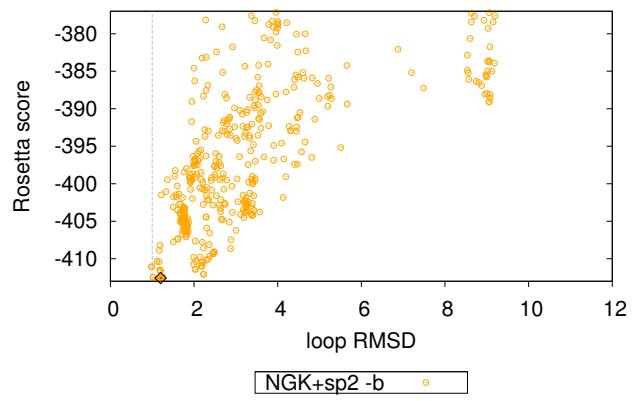
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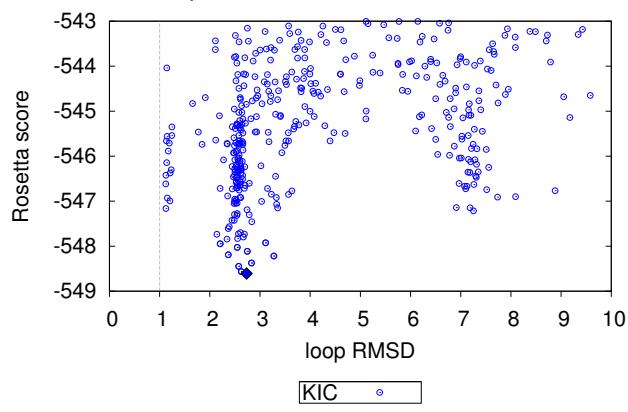
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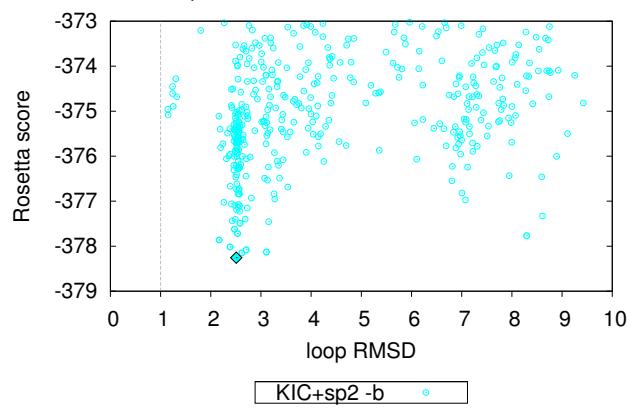
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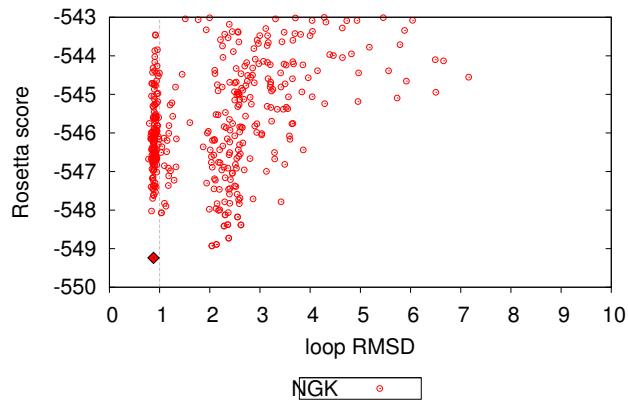
Comparison for different KIC variants on 1f46



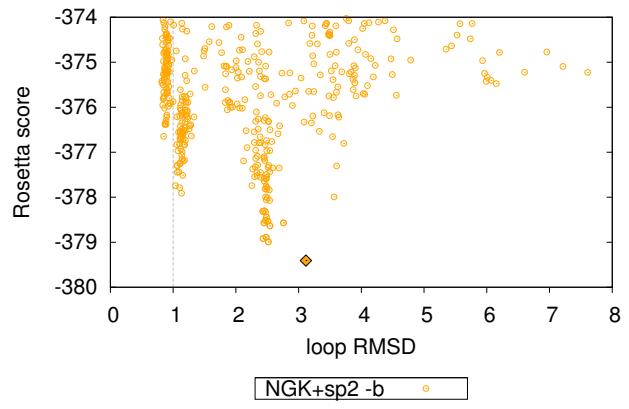
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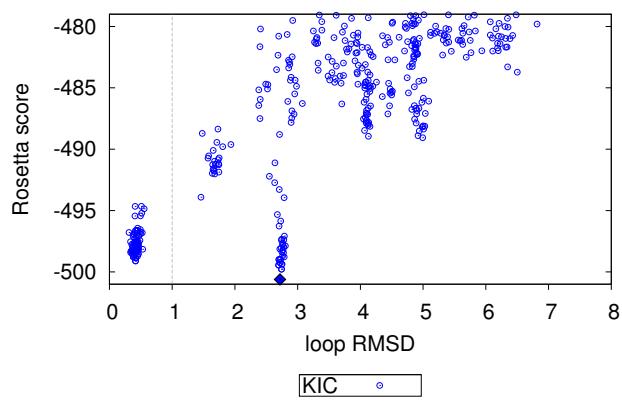
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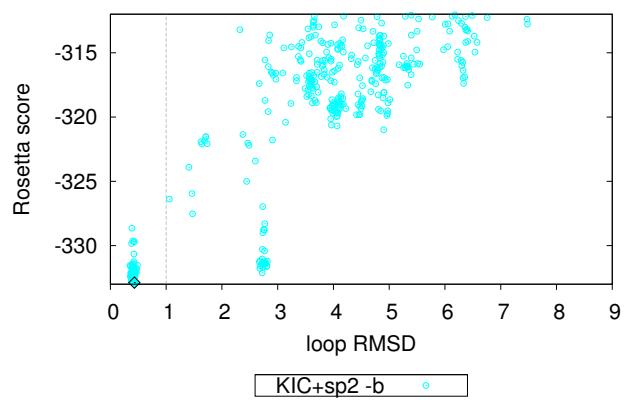
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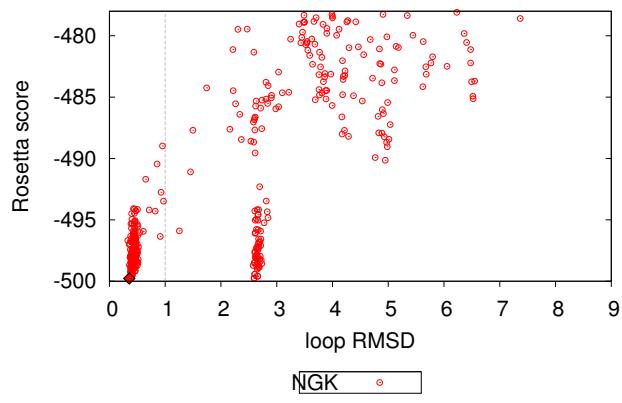
Comparison for different KIC variants on 1i7p



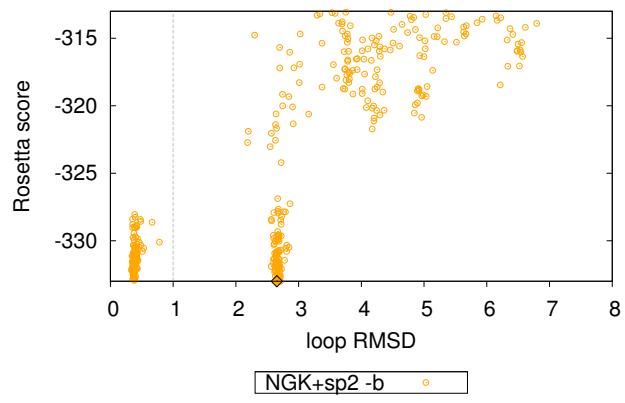
Comparison for different KIC variants on 1i7p



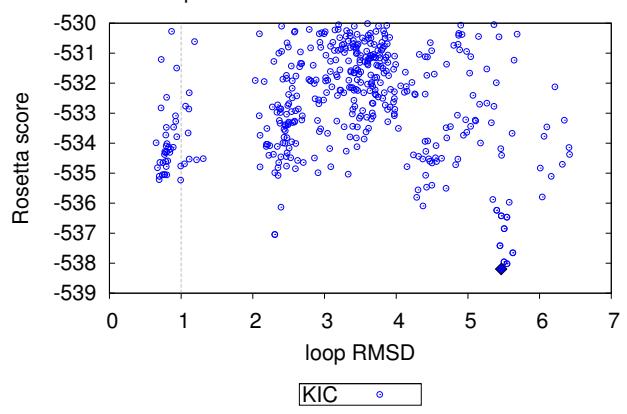
Comparison for different KIC variants on 1i7p



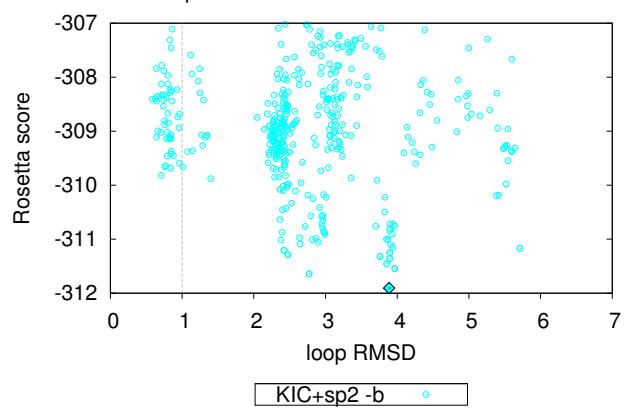
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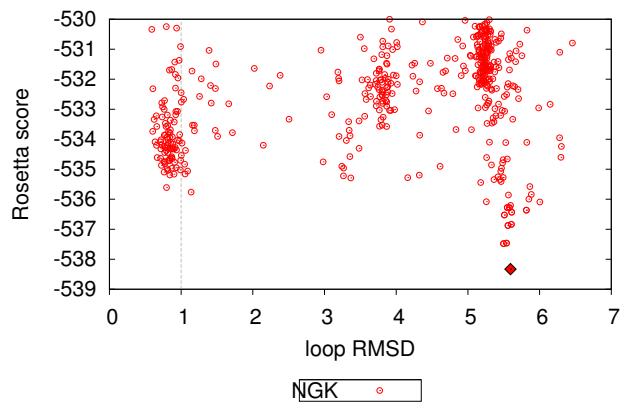
Comparison for different KIC variants on 1m3s



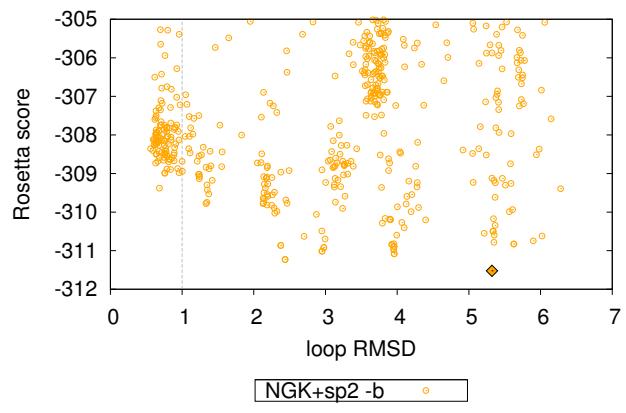
Comparison for different KIC variants on 1m3s

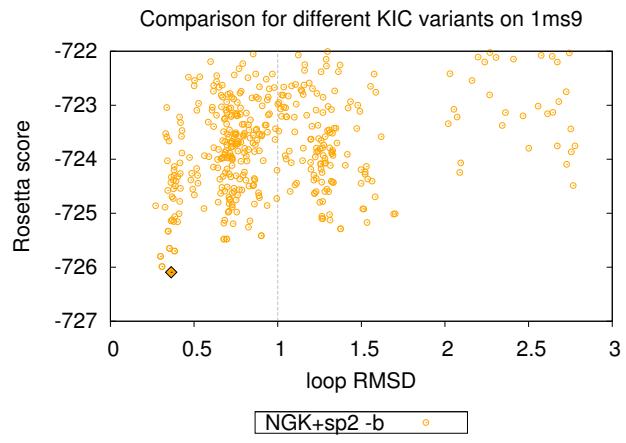
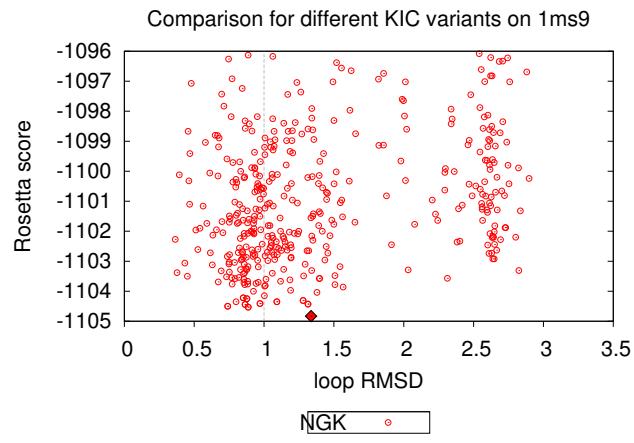
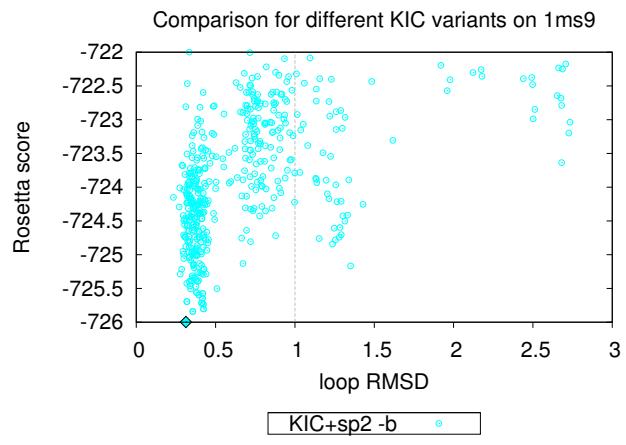
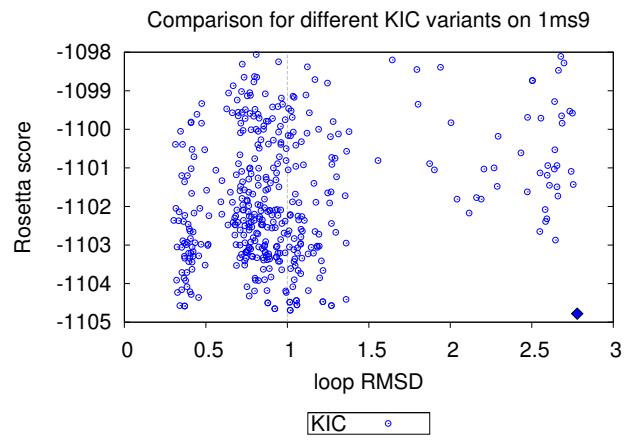


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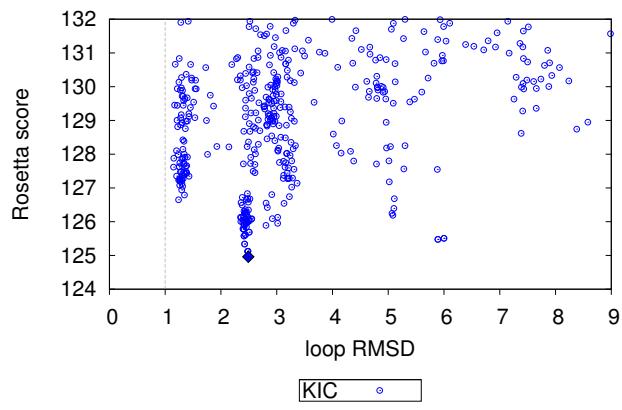


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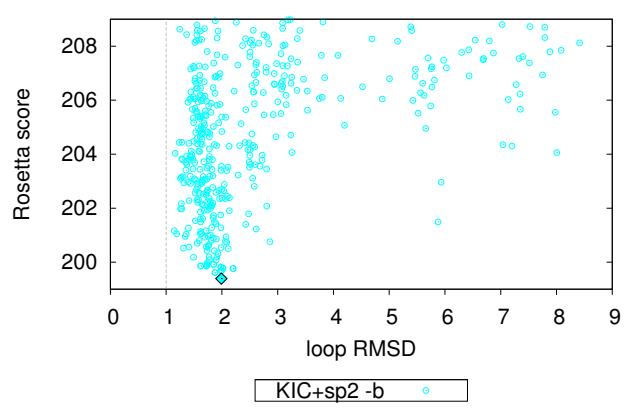




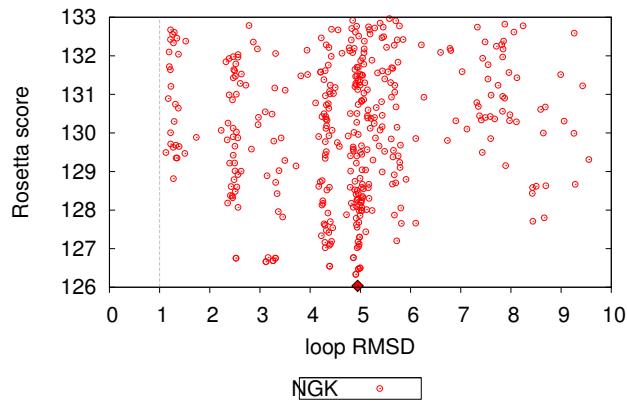
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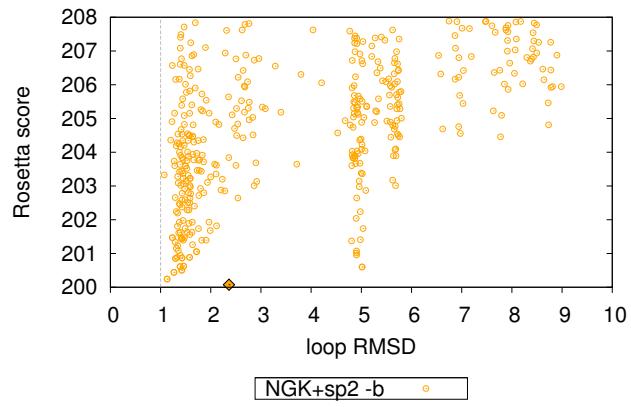
Comparison for different KIC variants on 1msc

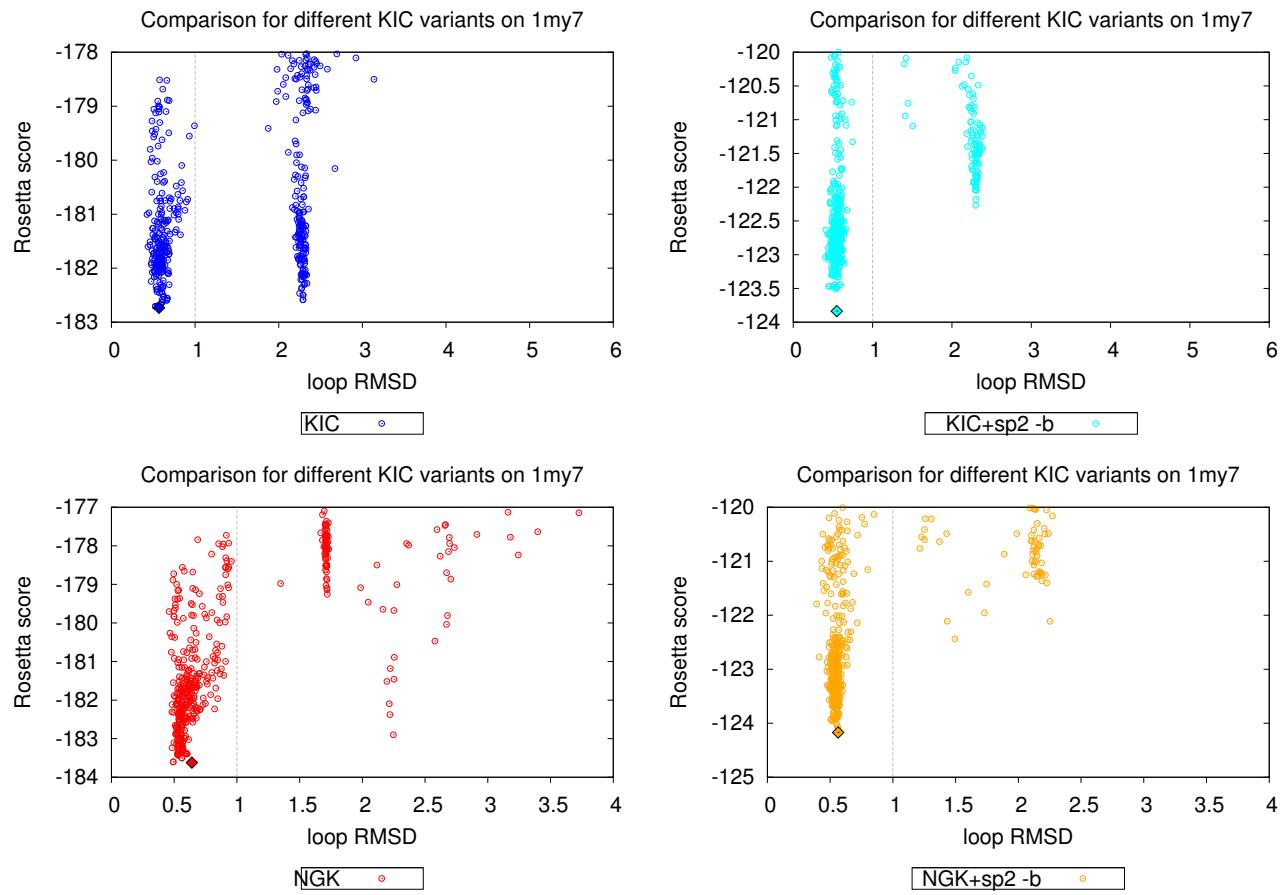


Comparison for different KIC variants on 1msc

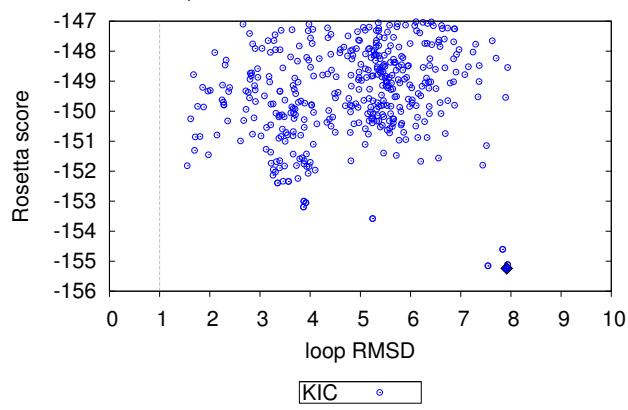


Comparison for different KIC variants on 1msc

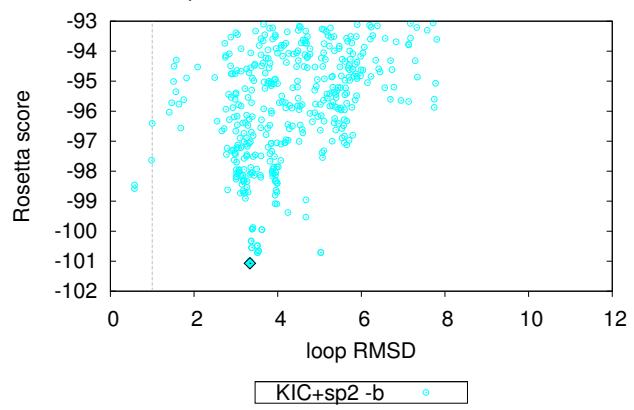




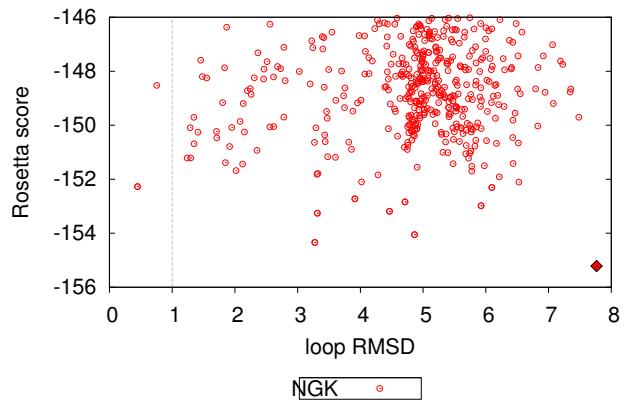
Comparison for different KIC variants on 1onc



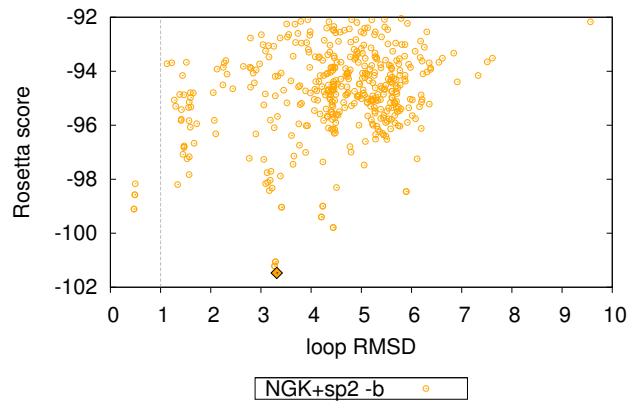
Comparison for different KIC variants on 1onc



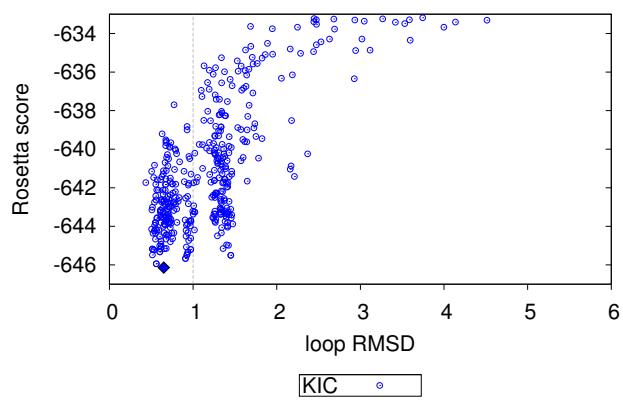
Comparison for different KIC variants on 1onc



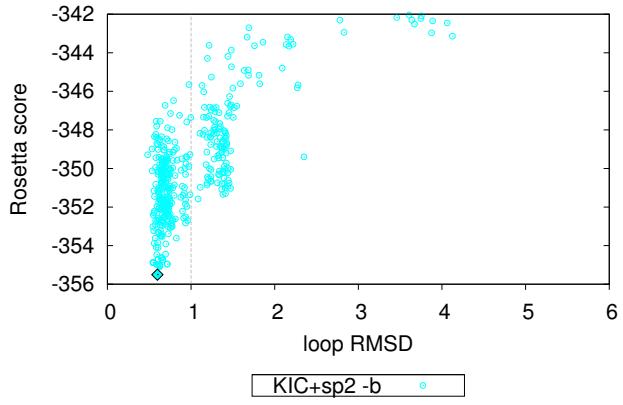
Comparison for different KIC variants on 1onc



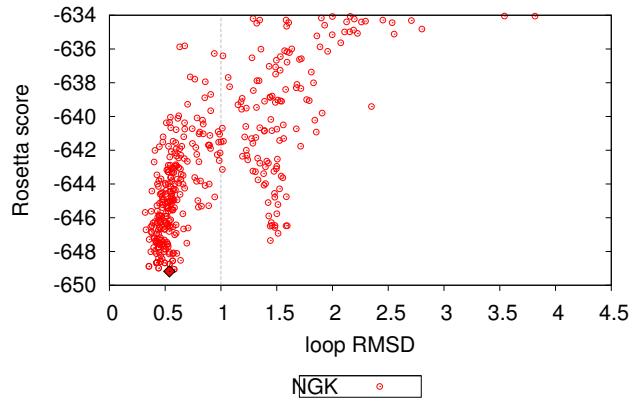
Comparison for different KIC variants on 10th



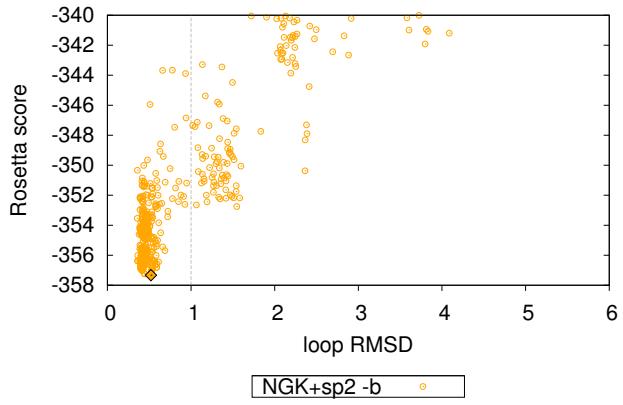
Comparison for different KIC variants on 10th



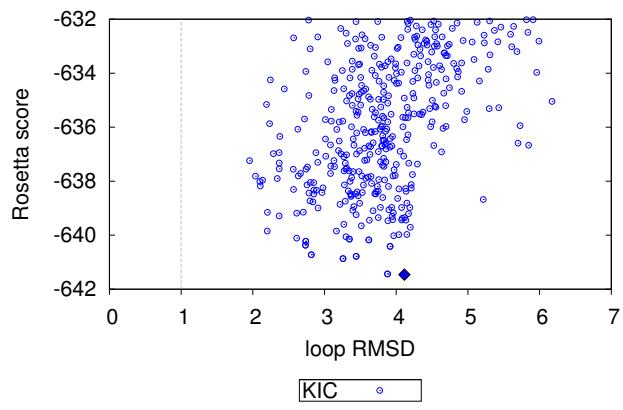
Comparison for different KIC variants on 10th



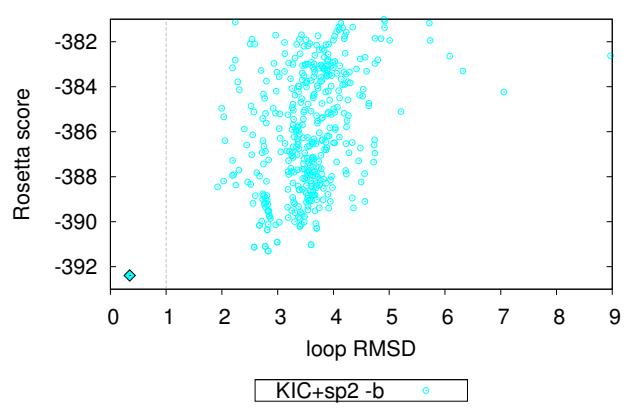
Comparison for different KIC variants on 10th



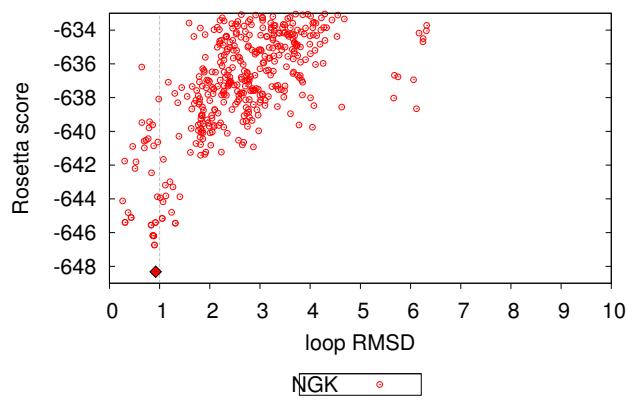
Comparison for different KIC variants on 1oyc



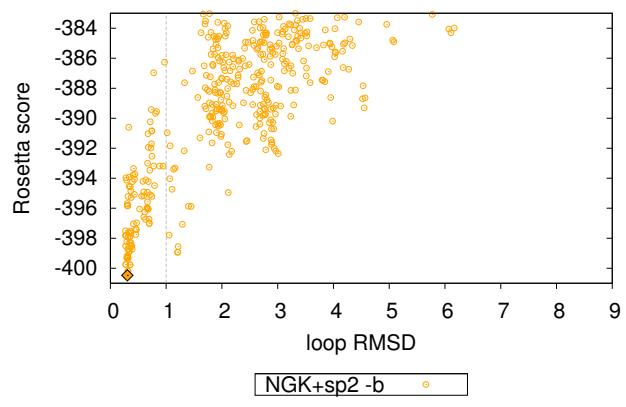
Comparison for different KIC variants on 1oyc



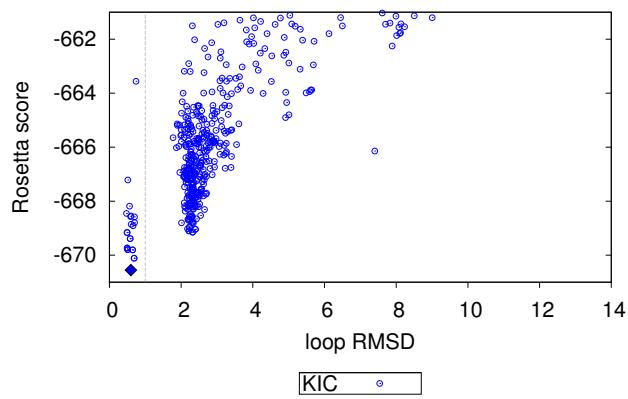
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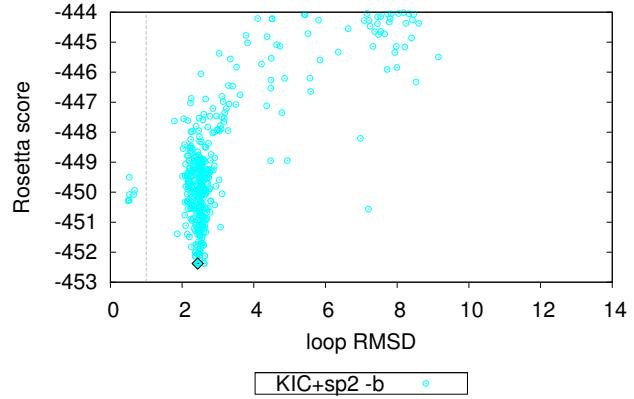
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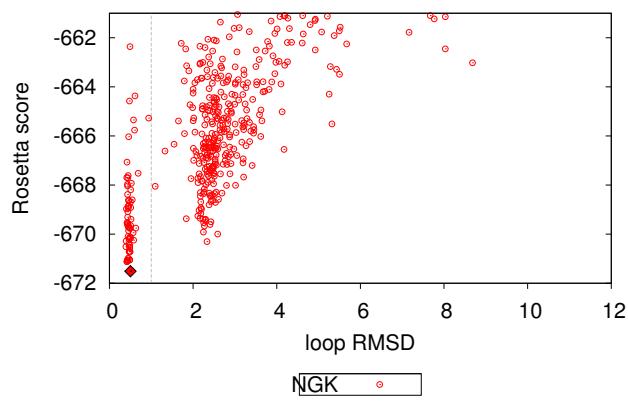
Comparison for different KIC variants on 1pbe



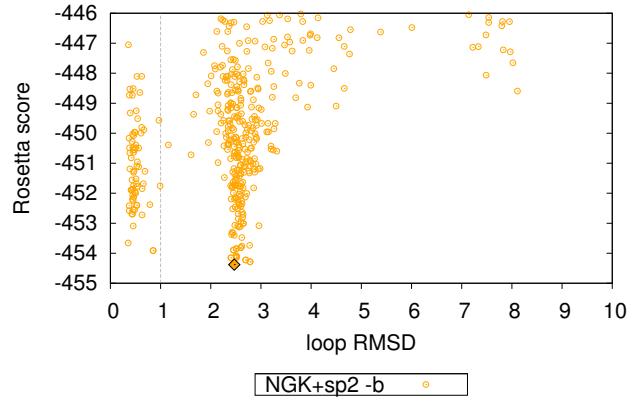
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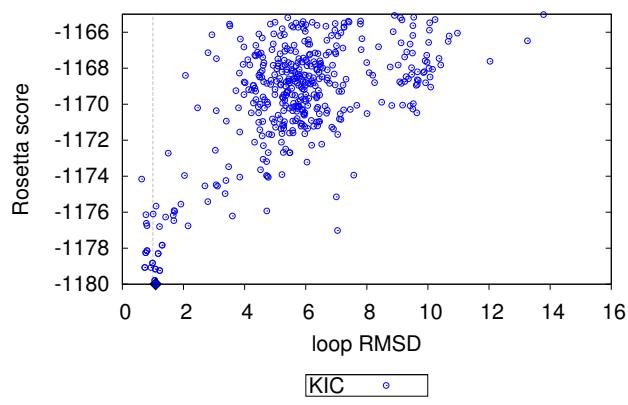
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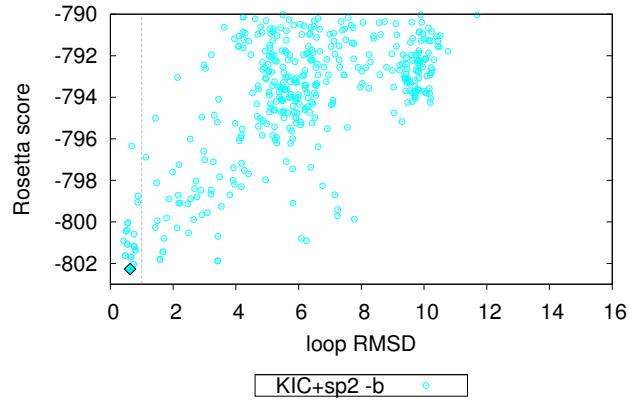
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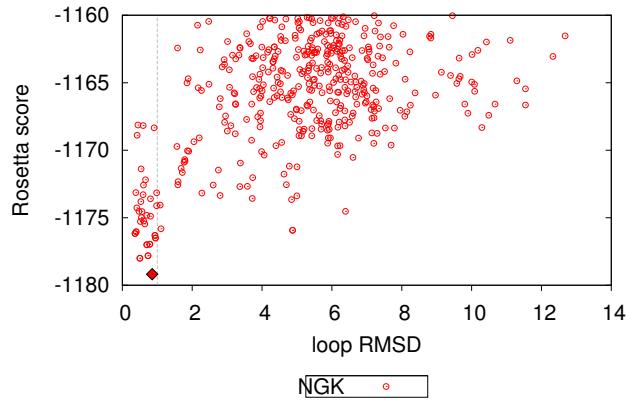
Comparison for different KIC variants on 1qlw



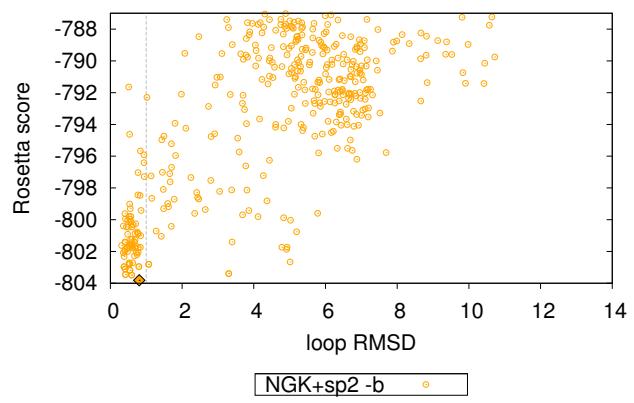
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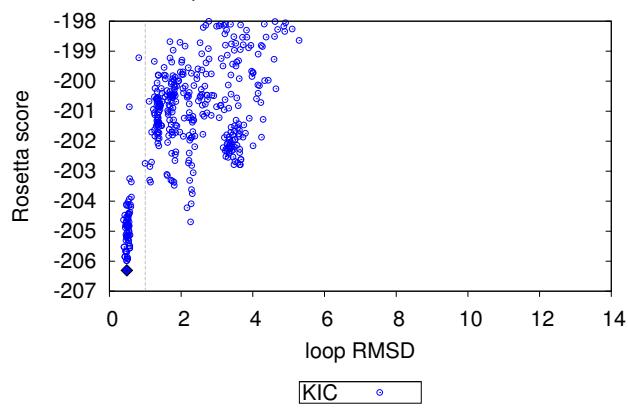
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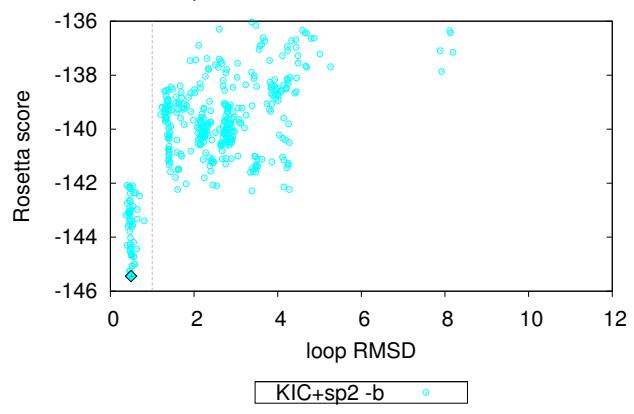
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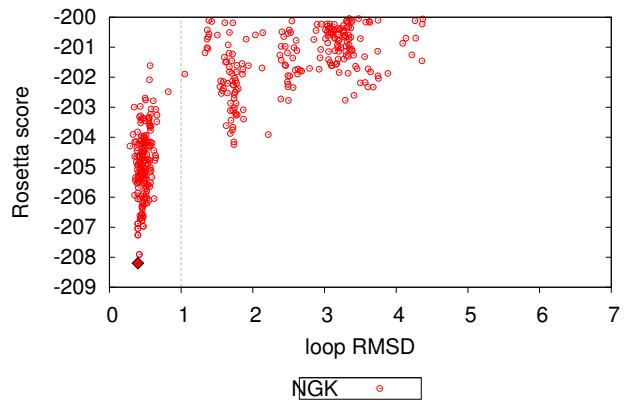
Comparison for different KIC variants on 1rro



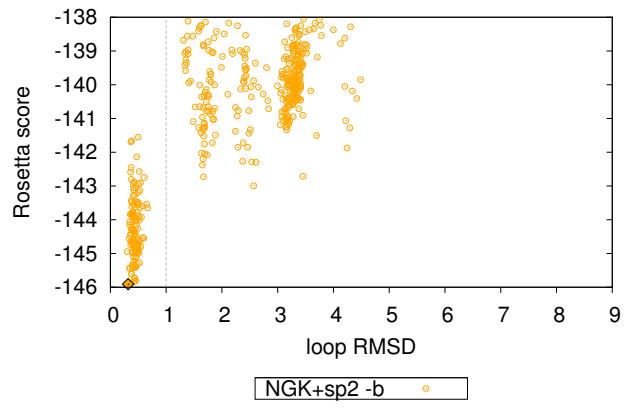
Comparison for different KIC variants on 1rro



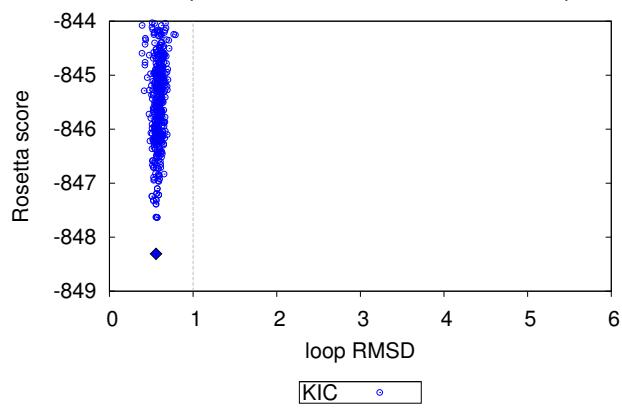
Comparison for different KIC variants on 1rro



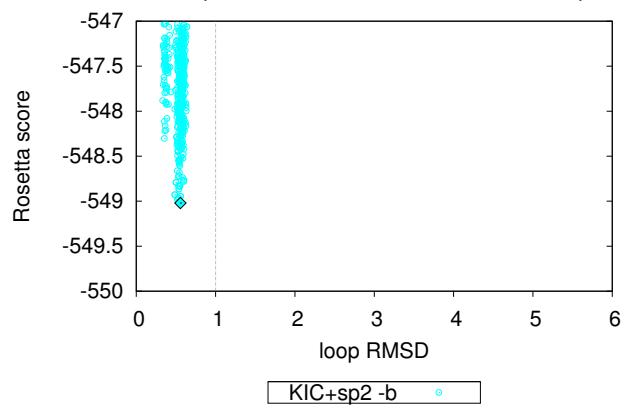
Comparison for different KIC variants on 1rro



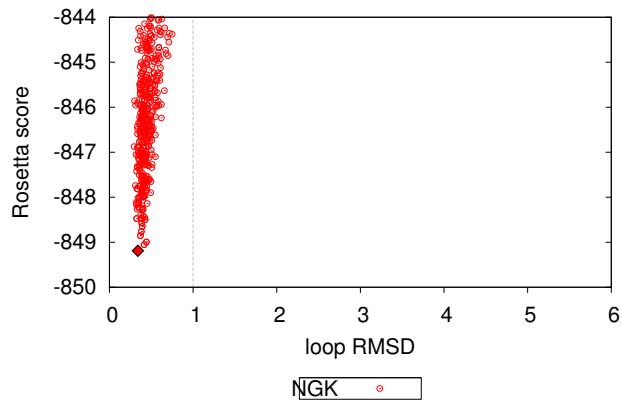
Comparison for different KIC variants on 1srp



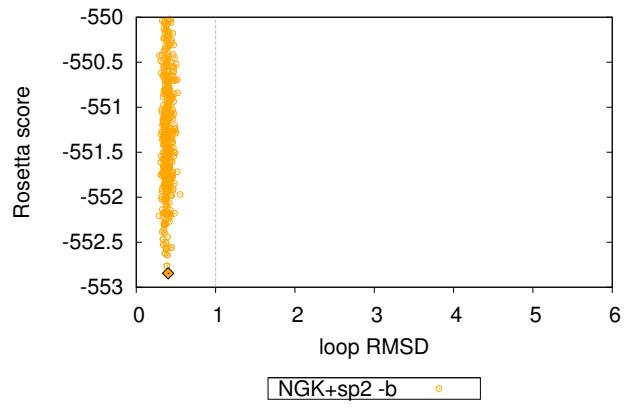
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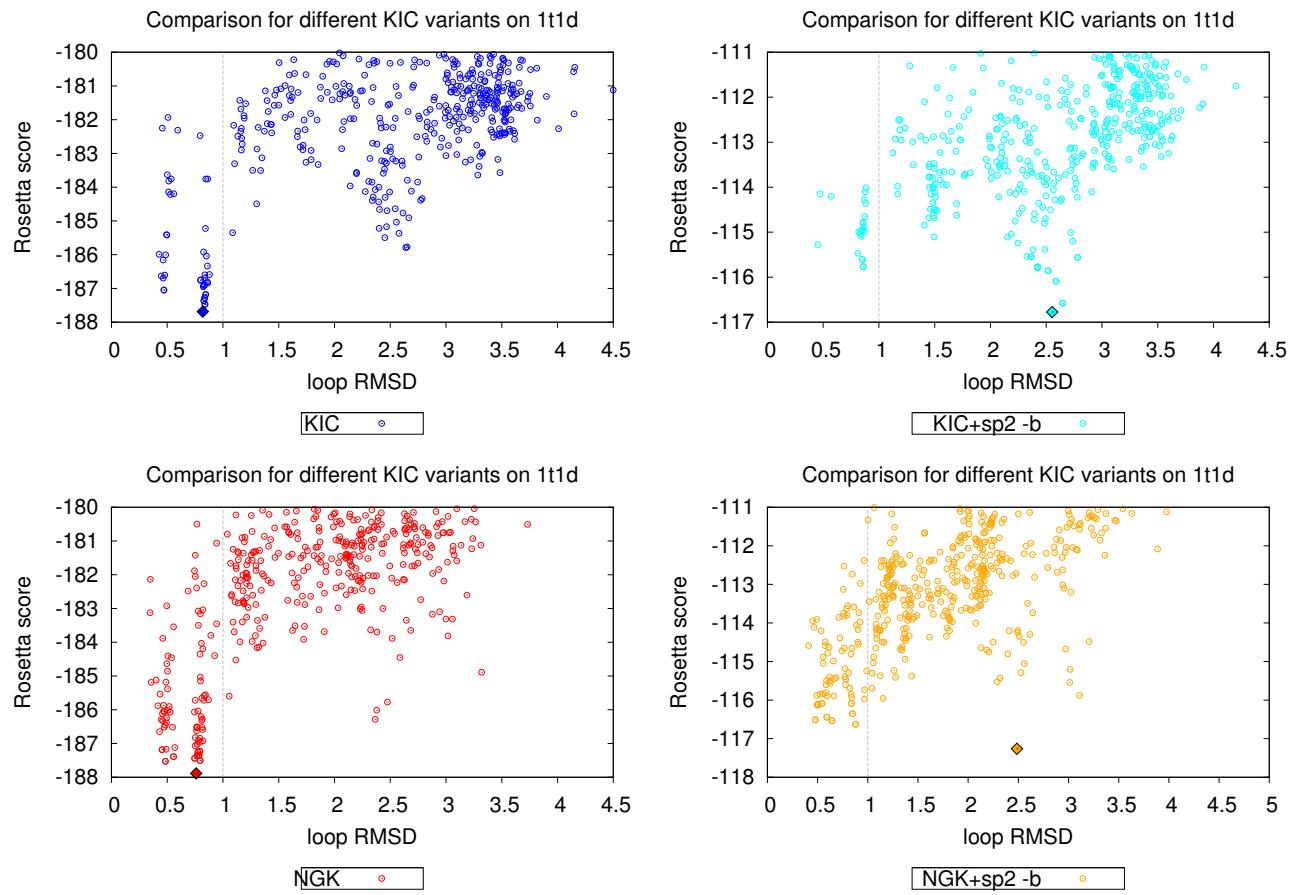


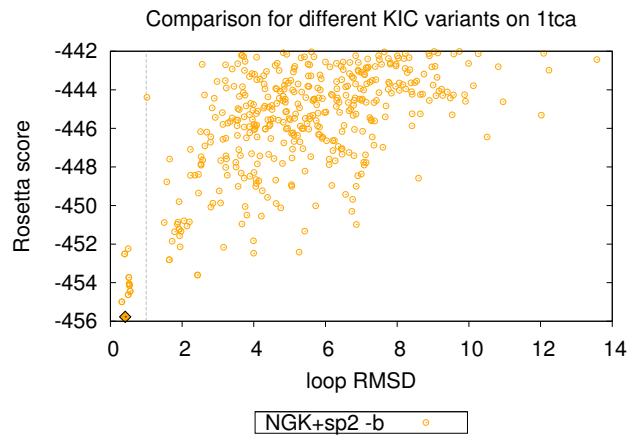
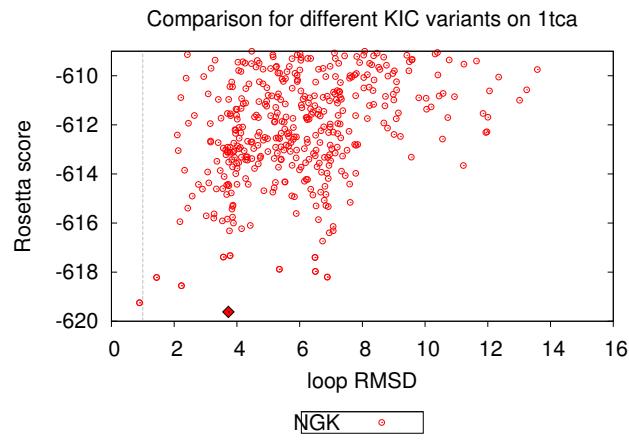
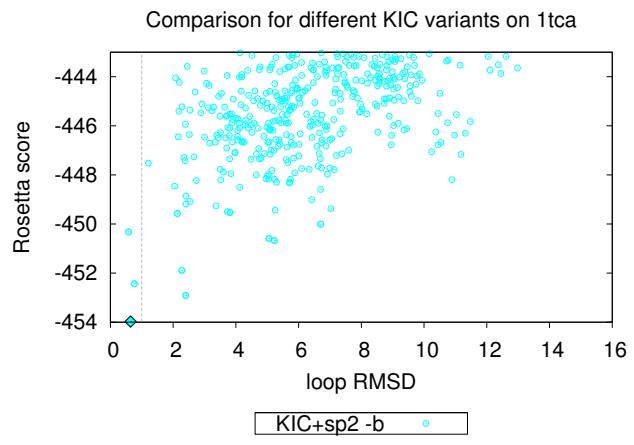
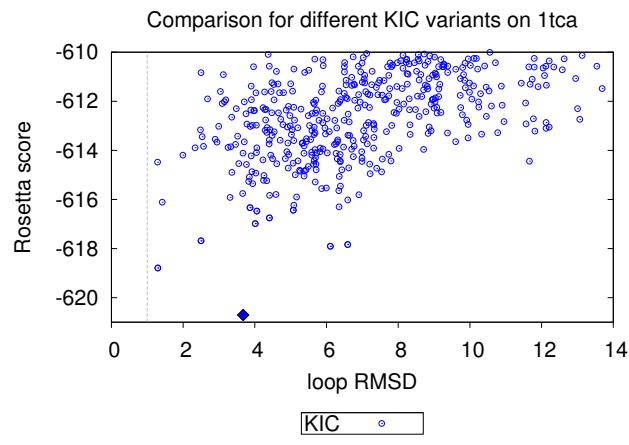
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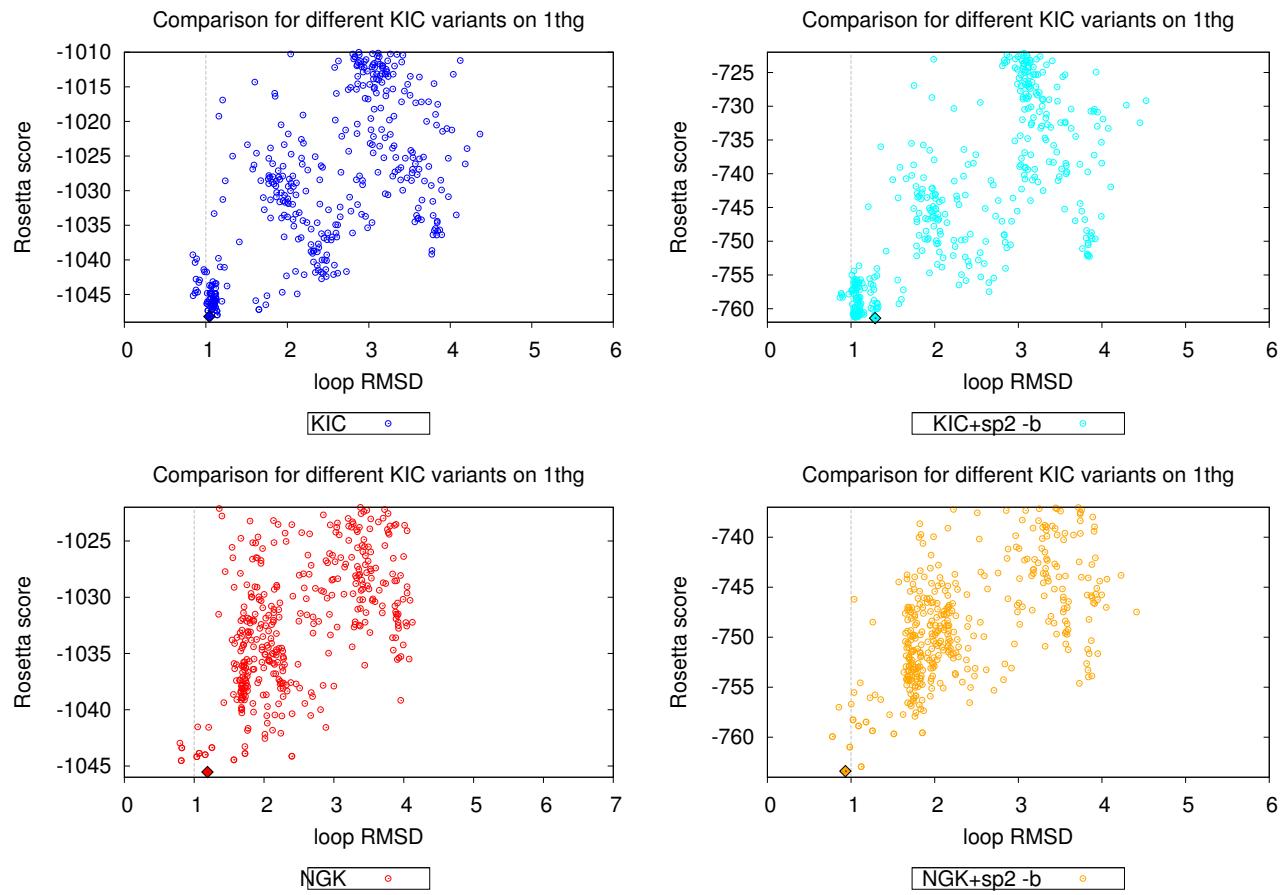


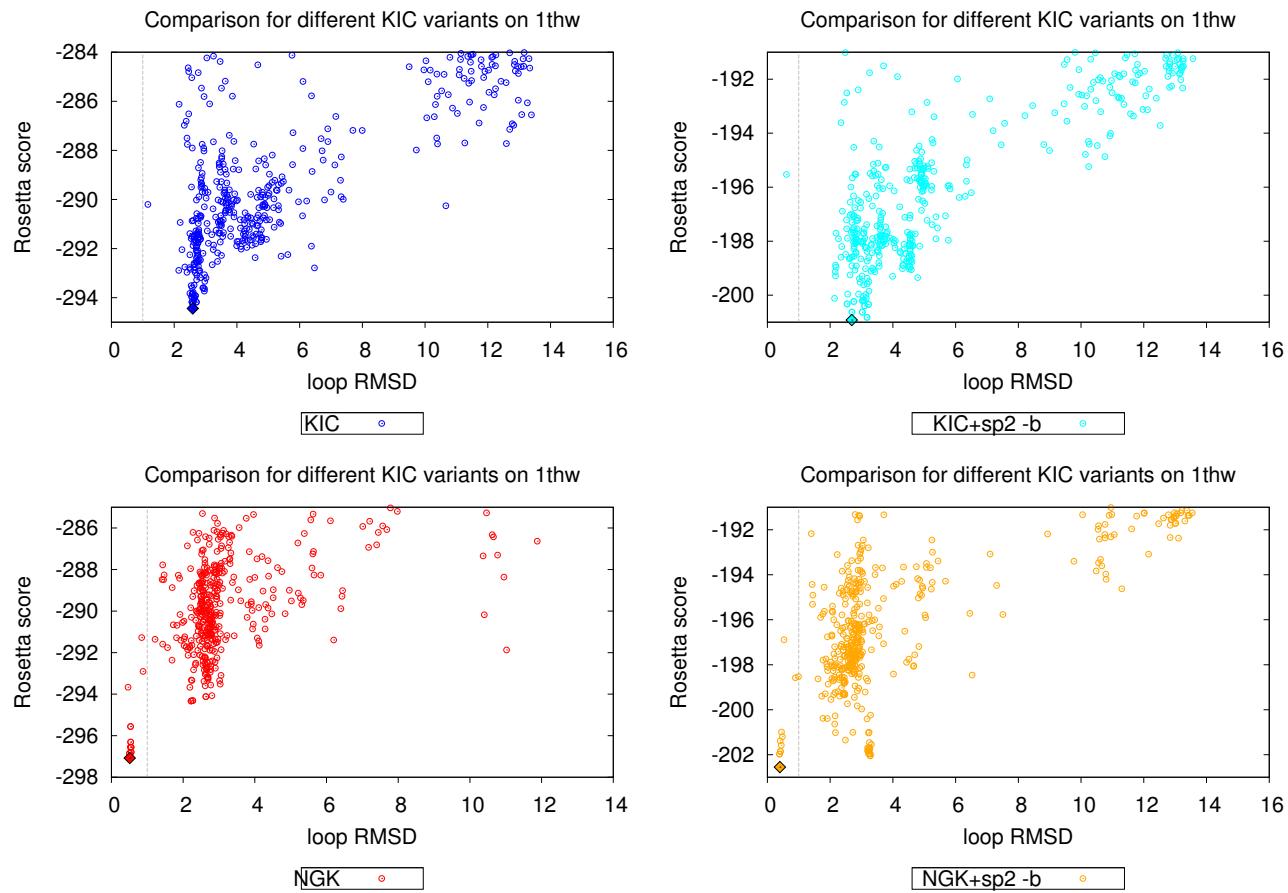
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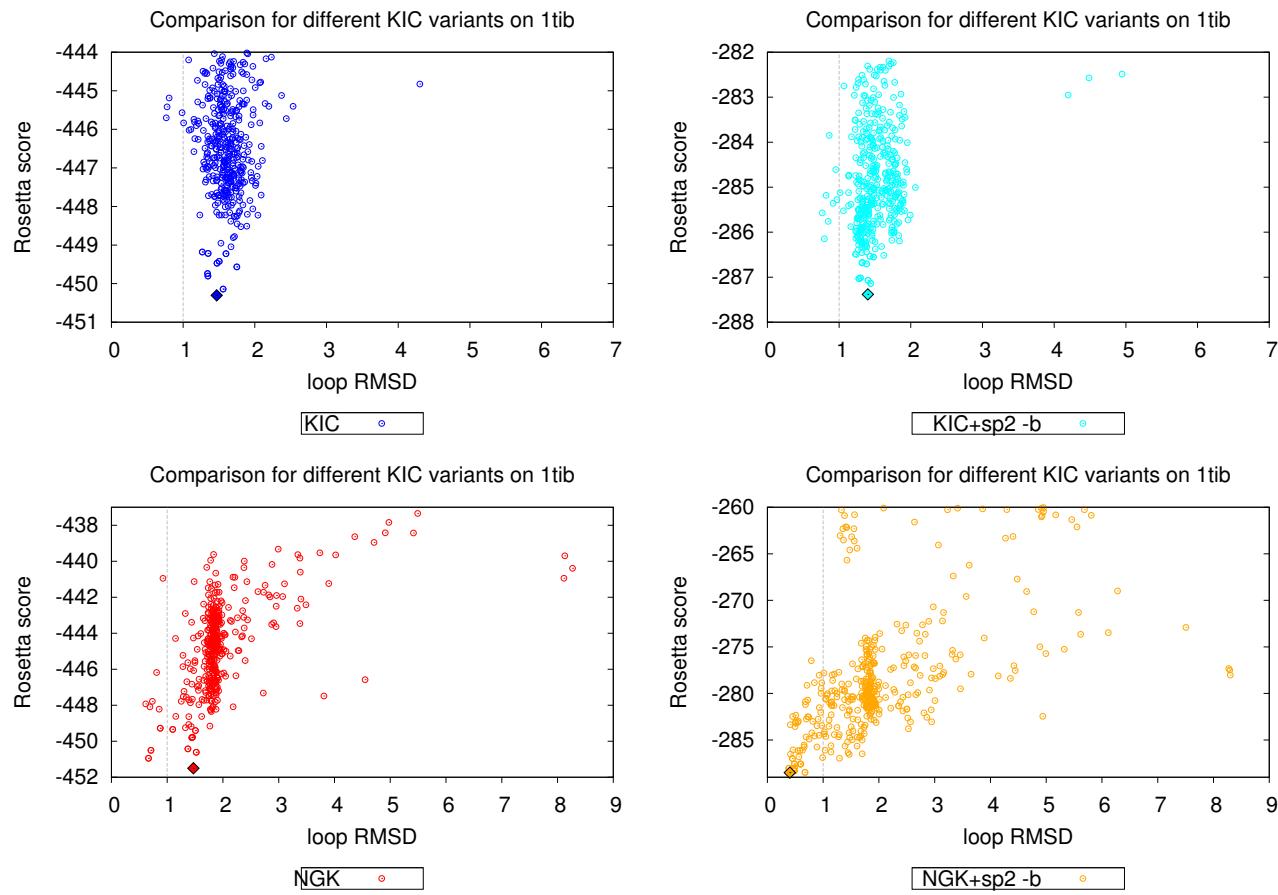


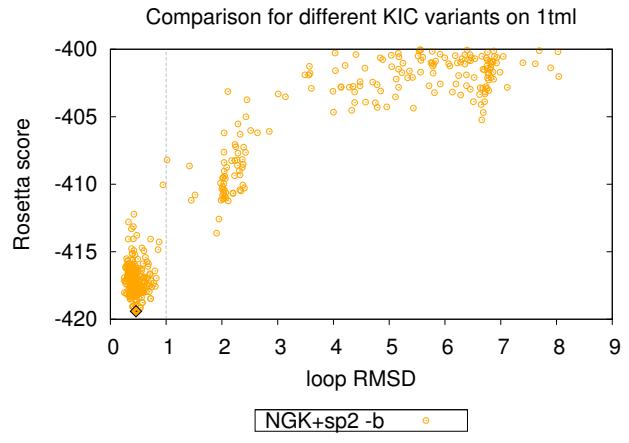
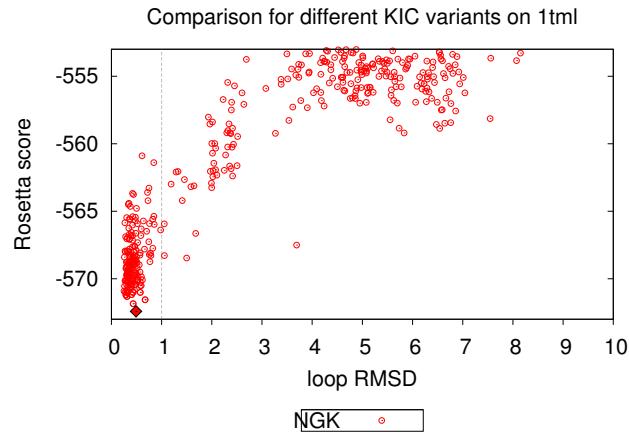
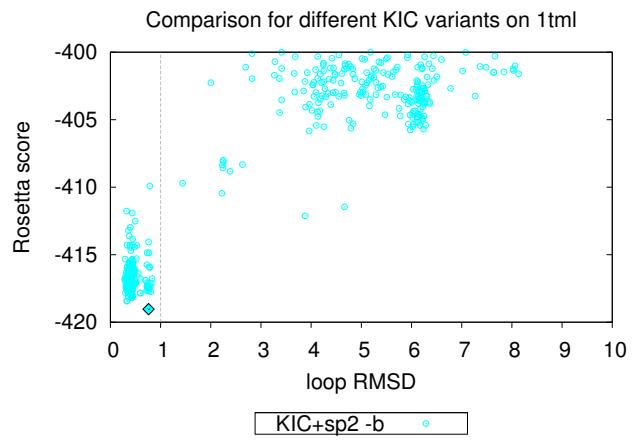
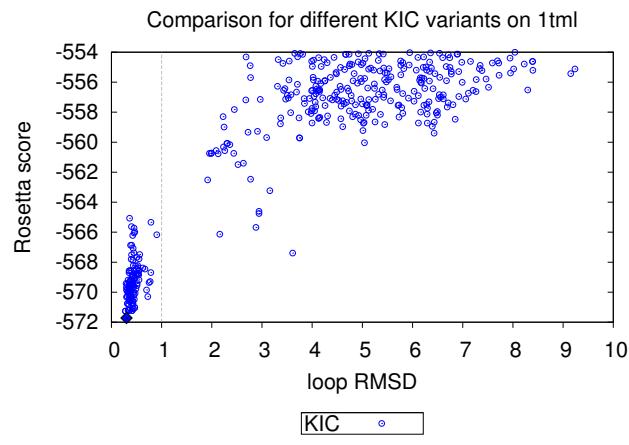




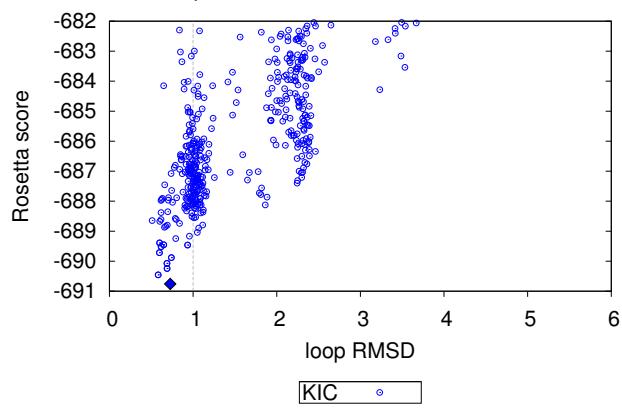




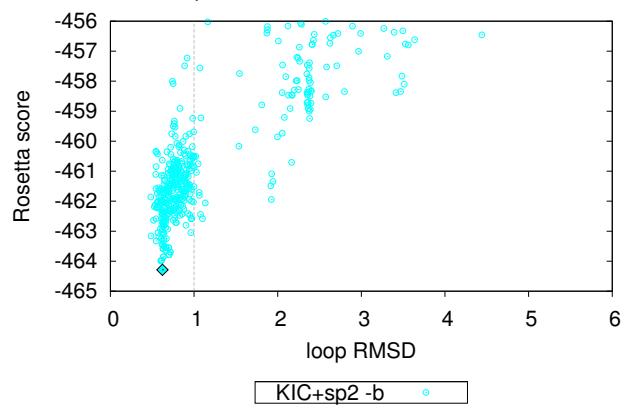




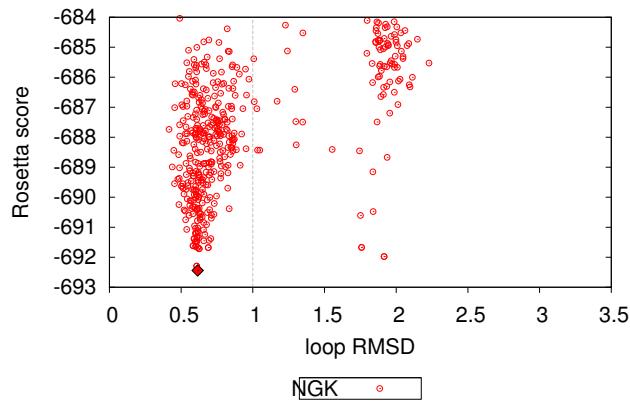
Comparison for different KIC variants on 1xif



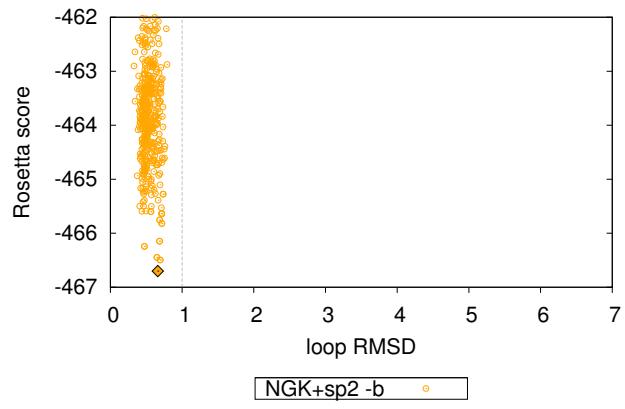
Comparison for different KIC variants on 1xif

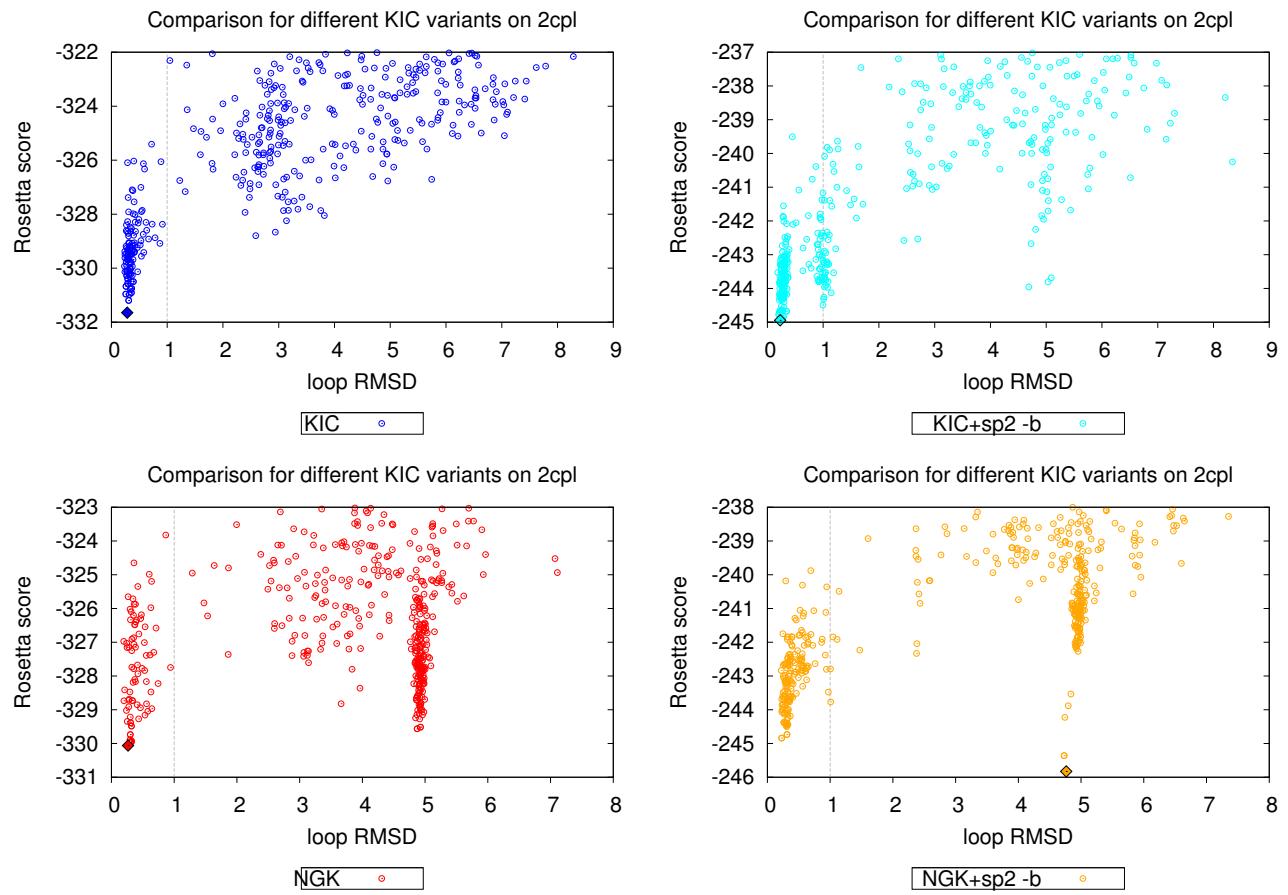


Comparison for different KIC variants on 1xif

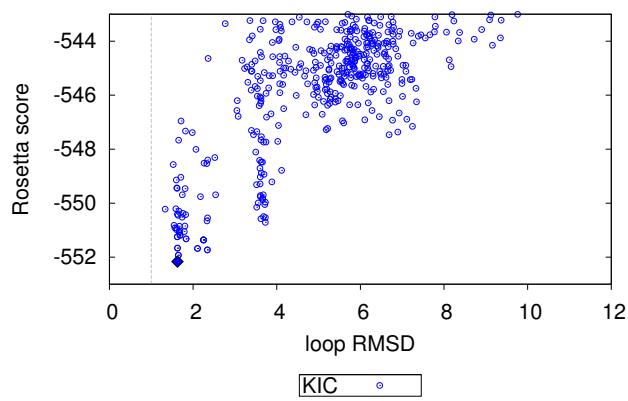


Comparison for different KIC variants on 1xif

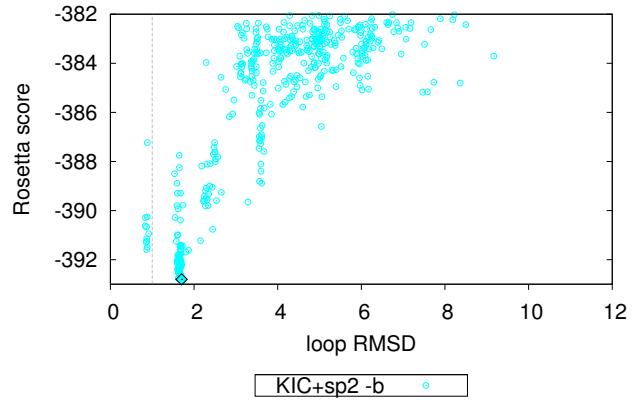




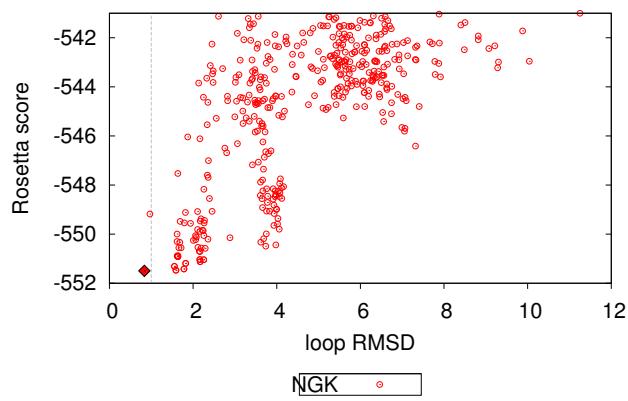
Comparison for different KIC variants on 2ebn



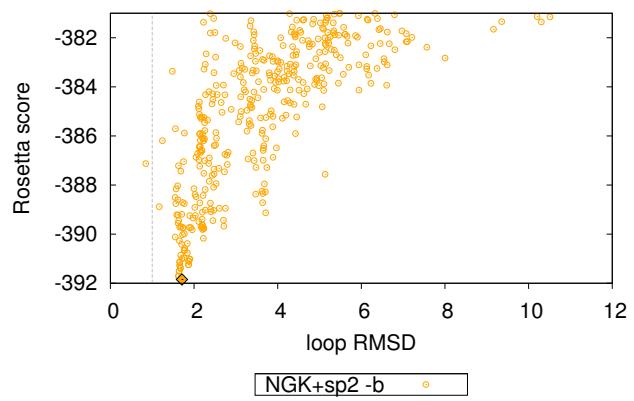
Comparison for different KIC variants on 2ebn



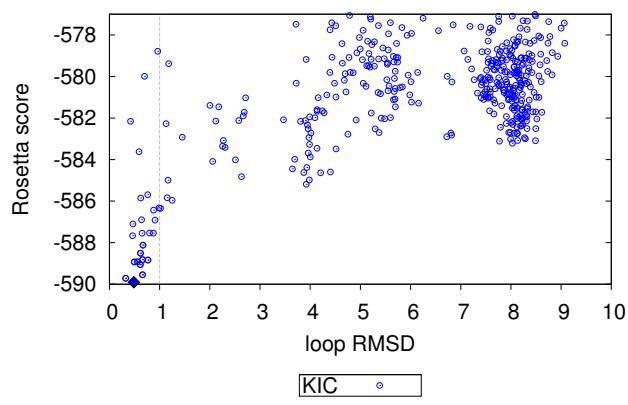
Comparison for different KIC variants on 2ebn



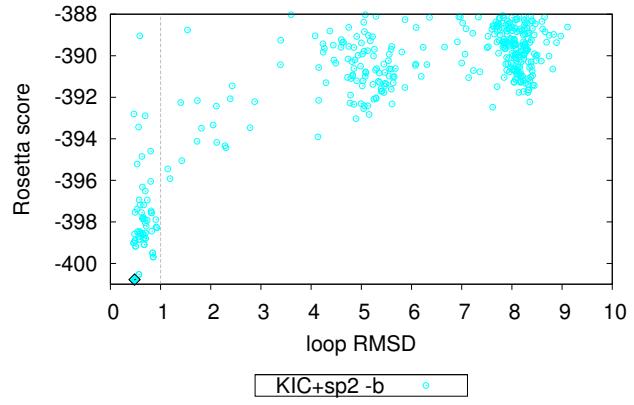
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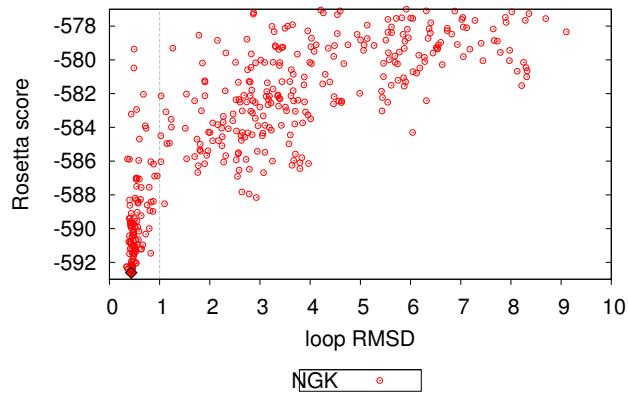
Comparison for different KIC variants on 2exo



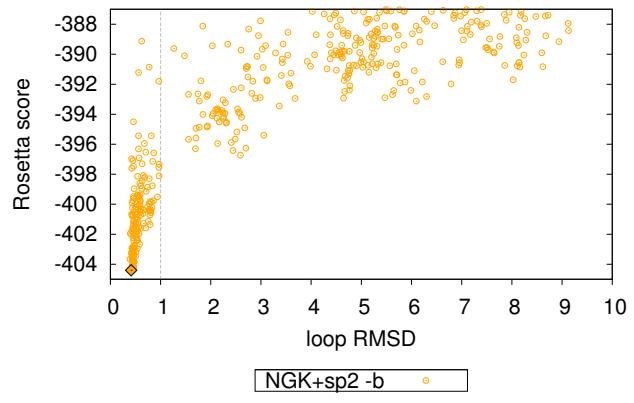
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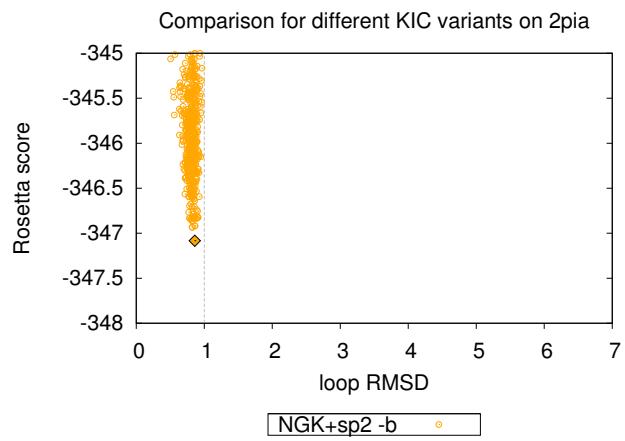
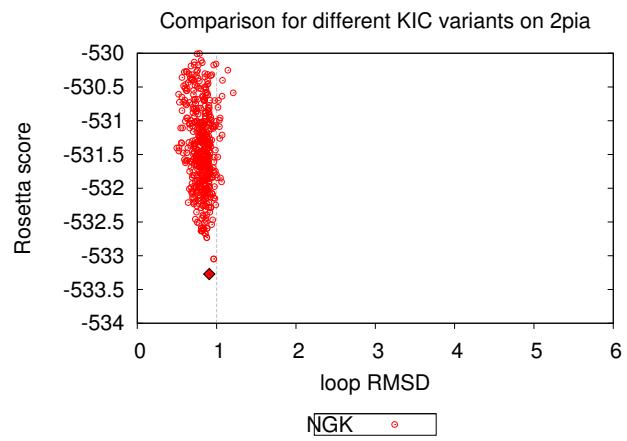
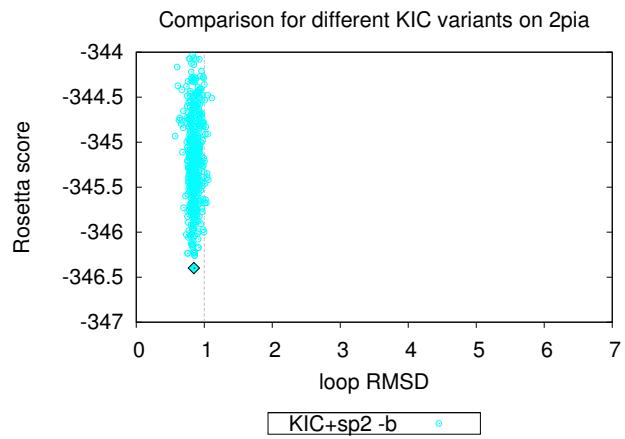
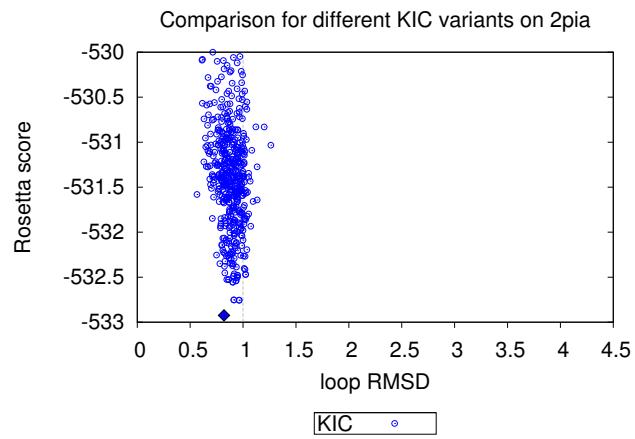


Comparison for different KIC variants on 2exo

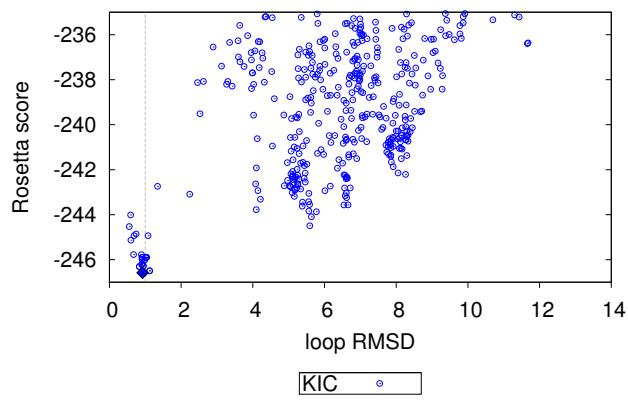


Comparison for different KIC variants on 2exo

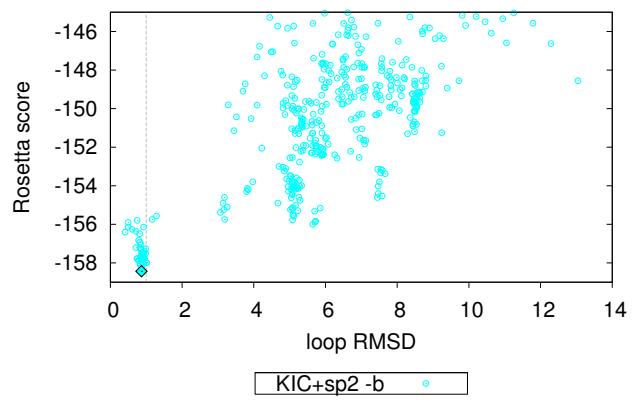




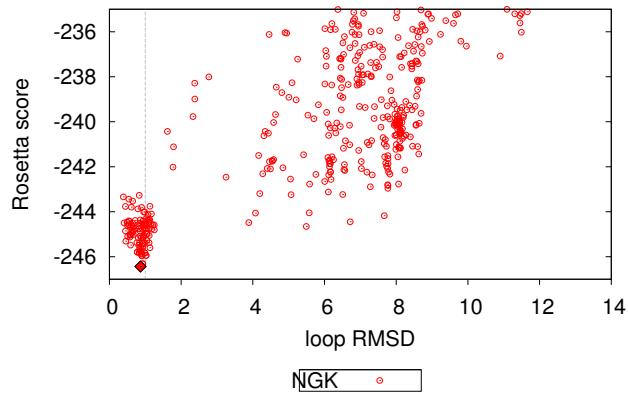
Comparison for different KIC variants on 2rn2



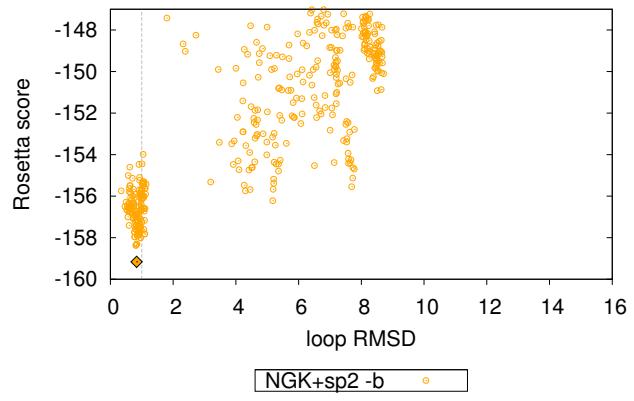
Comparison for different KIC variants on 2rn2



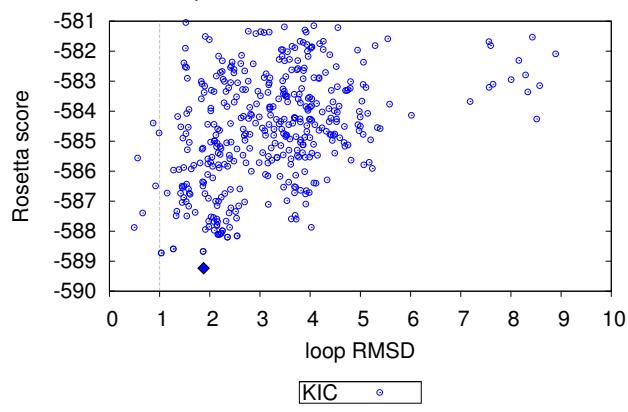
Comparison for different KIC variants on 2rn2



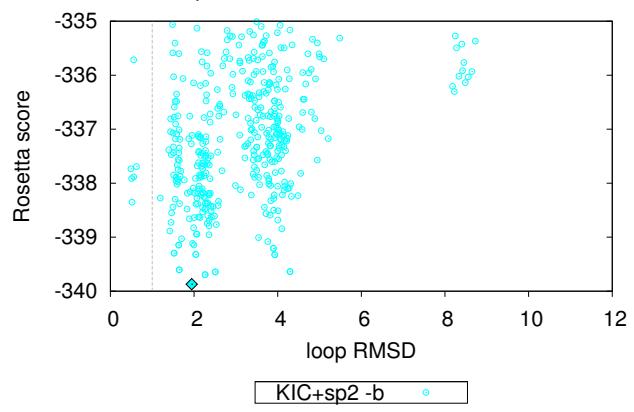
Comparison for different KIC variants on 2rn2



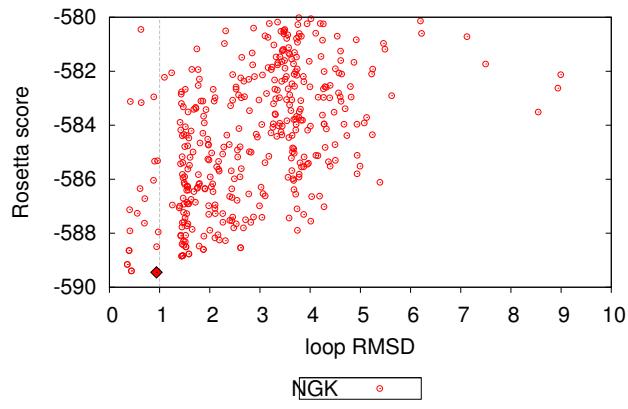
Comparison for different KIC variants on 2sil



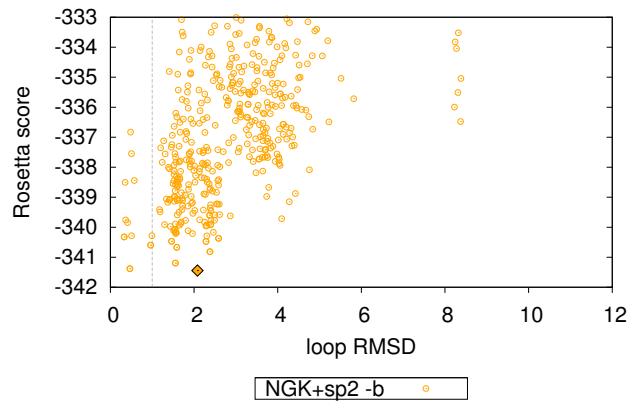
Comparison for different KIC variants on 2sil

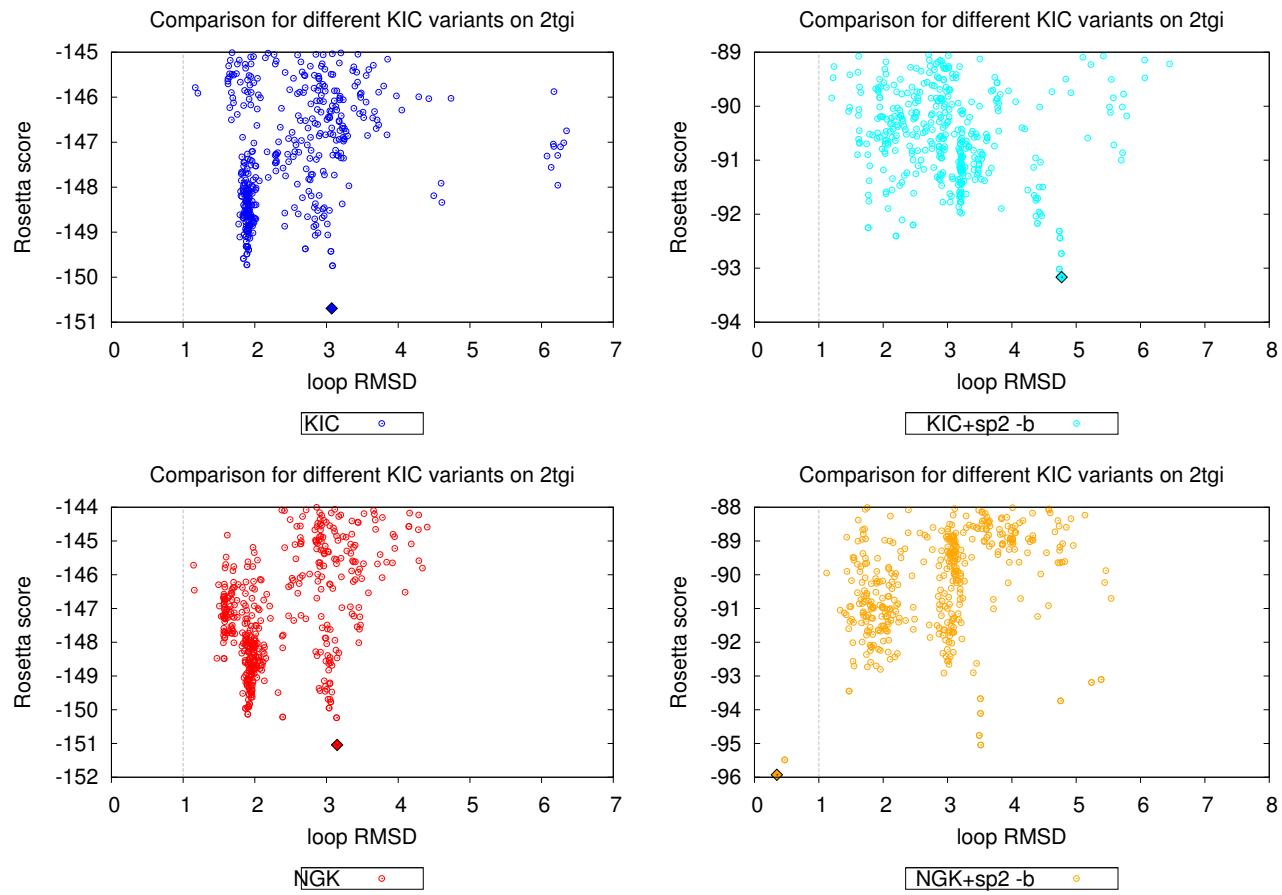


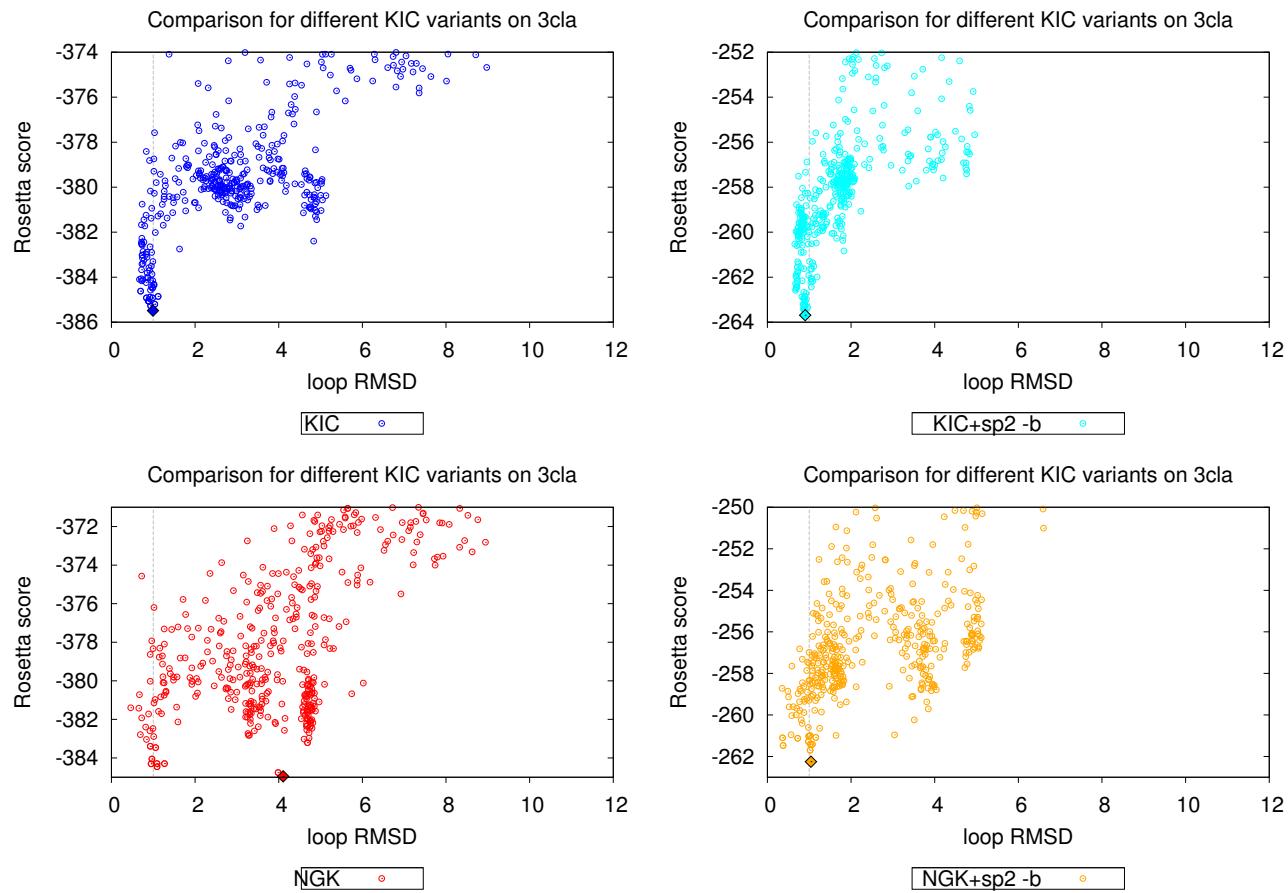
Comparison for different KIC variants on 2sil



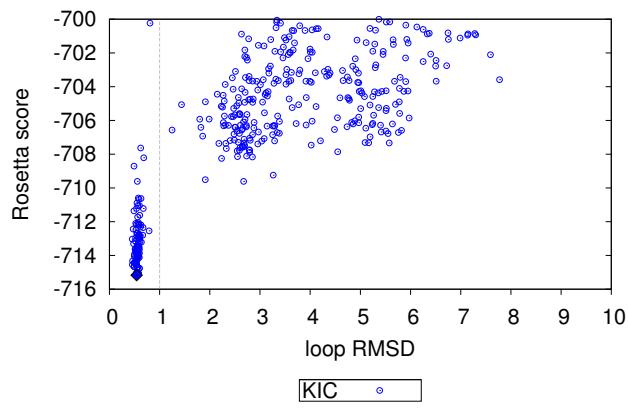
Comparison for different KIC variants on 2sil



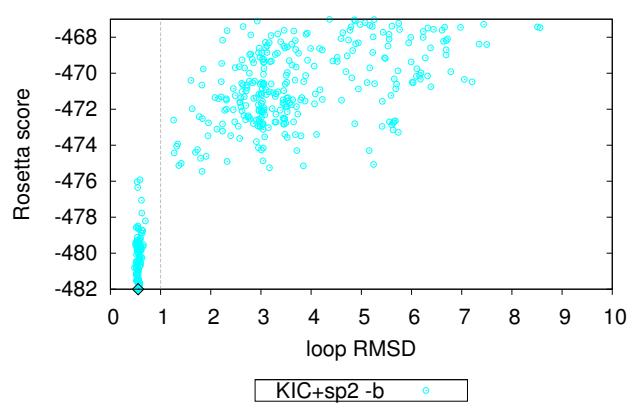




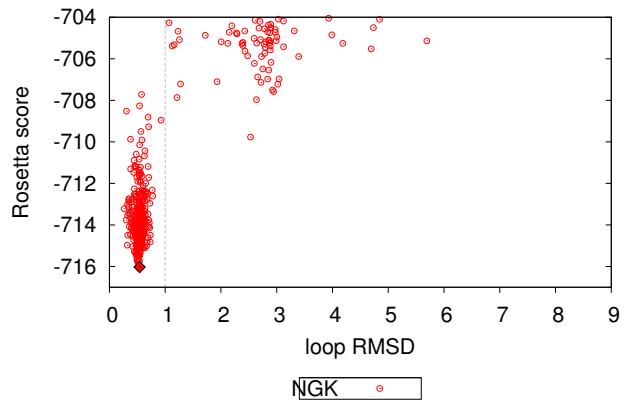
Comparison for different KIC variants on 3hsc



Comparison for different KIC variants on 3hsc



Comparison for different KIC variants on 3hsc



Comparison for different KIC variants on 3hsc

