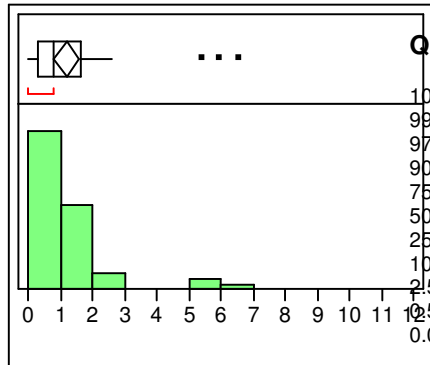


final thrombin model 3
 active-RMSD of ranked_all_090606_3D.prediction.RMSD

Distributions group 2 RMSD=1 (RMSD <=2 Å)
 abs (exper - LV4)

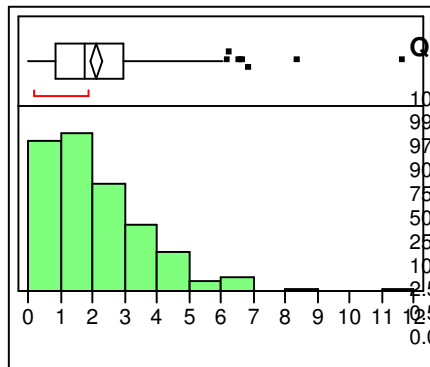


Quantiles	
100.0%	maximum
99.5%	
97.5%	
90.0%	
75.0%	quartile
50.0%	median
25.0%	quartile
10.0%	
2.5%	
0.5%	
0.0%	minimum

Moments

6,5189	Mean	1,2022143
6,5189	Std Dev	1,4032442
6,3702	Std Err Mean	0,2004635
2,1426	upper 95% Mean	1,6052731
1,6574	lower 95% Mean	0,7991555
0,7809	N	49

Distributions group 2 RMSD=2 (RMSD >2 Å)
 abs (exper - LV4)

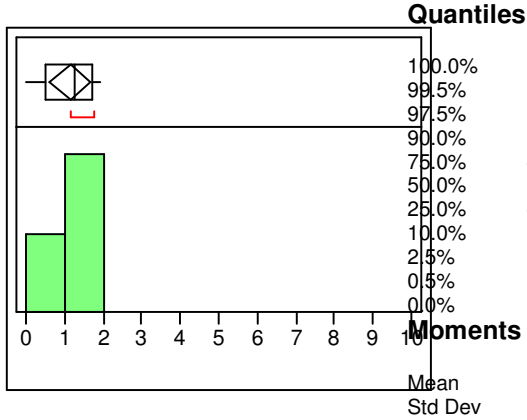


Quantiles	
100.0%	maximum
99.5%	
97.5%	
90.0%	
75.0%	quartile
50.0%	median
25.0%	quartile
10.0%	
2.5%	
0.5%	
0.0%	minimum

Moments

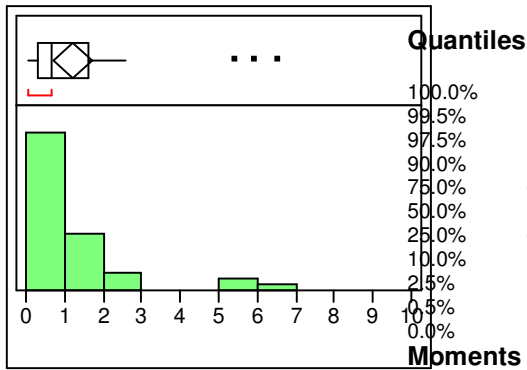
11,634	Mean	2,1348847
10,435	Std Dev	1,6491818
6,315	Std Err Mean	0,0999963
4,157	upper 95% Mean	2,3317531
2,977	lower 95% Mean	1,9380163
0,874	N	272

**Distributions group RMSD=1 (RMSD <=1 Å)
abs (exper - LV4)**



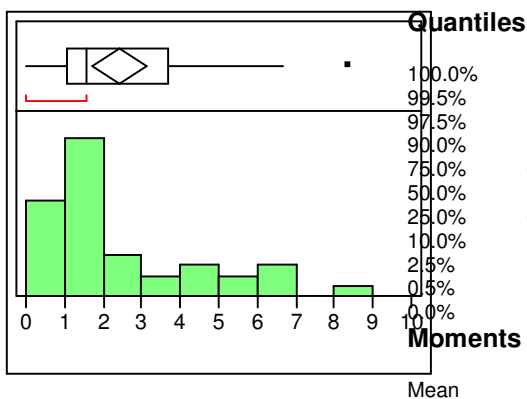
Std Err Mean	0,223043
upper 95% Mean	1,6532715
lower 95% Mean	0,6245952
N	9

**Distributions group RMSD=2 (1 > RMSD <=2 Å)
abs (exper - LV4)**



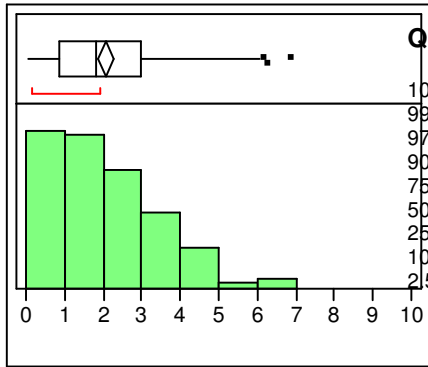
Std Err Mean	0,2413776
upper 95% Mean	1,7046848
lower 95% Mean	0,7282202
N	40

**Distributions group RMSD=3 (2 > RMSD <=5 Å)
abs (exper - LV4)**



Std Err Mean	0,3452503
upper 95% Mean	3,1086954
lower 95% Mean	1,7108502
N	39

**Distributions group RMSD=4 (RMSD >5 Å)
abs (exper - LV4)**



Quantiles

100.0%	maximum	11,634
99.5%		10,824
97.5%		5,750
90.0%		4,049
75.0%	quartile	2,964
50.0%	median	1,834
25.0%	quartile	0,854
10.0%		0,370
2.5%		0,082

0.5%		0,036
0.0%	minimum	0,035

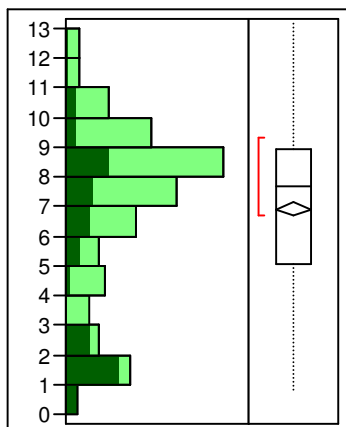
Moments

Mean	2,0888734
Std Dev	1,5494363
Std Err Mean	0,1015069
upper 95% Mean	2,2888666
lower 95% Mean	1,8888801
N	233

Distributions

RMSD of
ranked_all_090606_3D.prediction.RMSD

RMSD



52 ligands

Quantiles

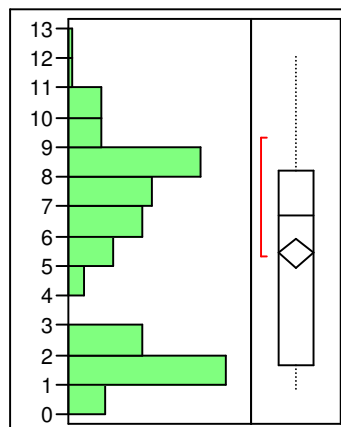
100.0%	maximum	13,215
99.5%		12,873
97.5%		11,831
90.0%		10,058
75.0%	quartile	8,904
50.0%	median	7,672
25.0%	quartile	5,030
10.0%		1,650
2.5%		1,111
0.5%		0,842
0.0%	minimum	0,809

Moments

Mean	6,9184638
Std Dev	2,9007775
Std Err Mean	0,1283228
upper 95% Mean	7,1705702
lower 95% Mean	6,6663574
N	511

sum elec < -10 of RMSD of
ranked_all_090606_3D.prediction.RMSD

RMSD



33 ligands

Quantiles

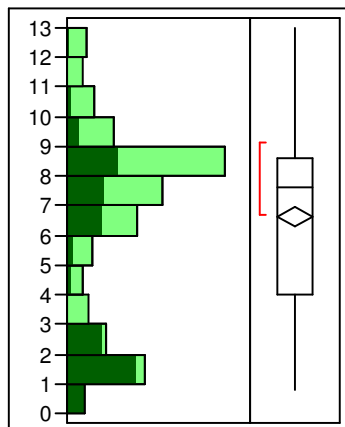
100.0%	maximum	12,077
99.5%		12,077
97.5%		10,871
90.0%		9,056
75.0%	quartile	8,206
50.0%	median	6,668
25.0%	quartile	1,629
10.0%		1,178
2.5%		0,898
0.5%		0,809
0.0%	minimum	0,809

Moments

Mean	5,4274286
Std Dev	3,2459012
Std Err Mean	0,2504267
upper 95% Mean	5,9218388
lower 95% Mean	4,9330184
N	168

active-RMSD of
ranked_all_090606_3D.prediction.RMSD

RMSD



33 ligands

Quantiles

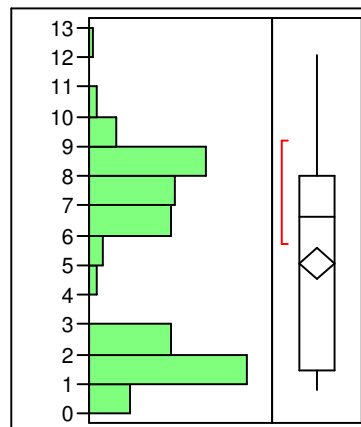
100.0%	maximum	12,982
99.5%		12,864
97.5%		12,092
90.0%		10,062
75.0%	quartile	8,625
50.0%	median	7,605
25.0%	quartile	4,020
10.0%		1,434
2.5%		0,961
0.5%		0,818
0.0%	minimum	0,809

Moments

Mean	6,6449907
Std Dev	3,100741
Std Err Mean	0,1730665
upper 95% Mean	6,9854825
lower 95% Mean	6,3044988
N	321

sum elec -10 of active-RMSD of
ranked_all_090606_3D.prediction.RMSD

RMSD



27 ligands

Quantiles

100.0%	maximum	12,077
99.5%		12,077
97.5%		9,716
90.0%		8,713
75.0%	quartile	8,016
50.0%	median	6,618
25.0%	quartile	1,469
10.0%		1,176
2.5%		0,877
0.5%		0,809
0.0%	minimum	0,809

Moments

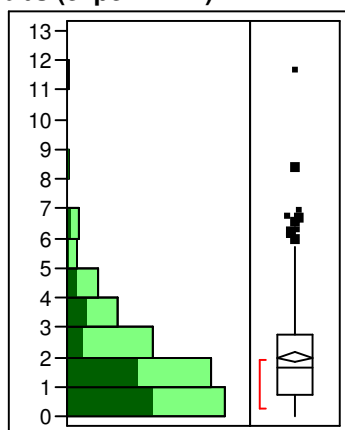
Mean	5,0562374
Std Dev	3,1791866
Std Err Mean	0,2696551
upper 95% Mean	5,5894274
lower 95% Mean	4,5230475
N	139

final thrombin model 3

active-RMSD of ranked_all_090606_3D.prediction.RMSD

active-RMSD of ranked_all_090606_3D.prediction.RMSD

abs (exper - LV4)



33 ligands

Quantiles

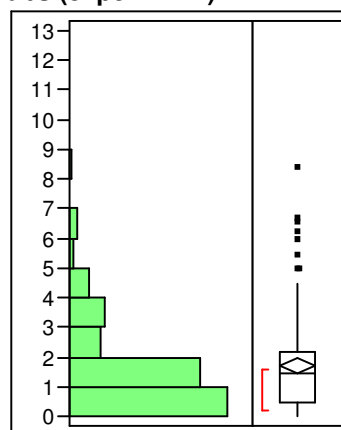
100.0%	maximum	11,634
99.5%		9,630
97.5%		6,259
90.0%		4,111
75.0%	quartile	2,762
50.0%	median	1,637
25.0%	quartile	0,699
10.0%		0,283
2.5%		0,060
0.5%		0,019
0.0%	minimum	0,014

Moments

Mean	1,9925145
Std Dev	1,6466822
Std Err Mean	0,0919088
upper 95% Mean	2,1733364
lower 95% Mean	1,8116926
N	321

sum elec < -10 of active-RMSD of ranked_all_090606_3D.prediction.RMSD

abs (exper - LV4)



27 ligands

Quantiles

100.0%	maximum	8,3492
99.5%		8,3492
97.5%		6,3442
90.0%		3,9312
75.0%	quartile	2,1557
50.0%	median	1,4468
25.0%	quartile	0,4570
10.0%		0,2265
2.5%		0,0368
0.5%		0,0136
0.0%	minimum	0,0136

Moments

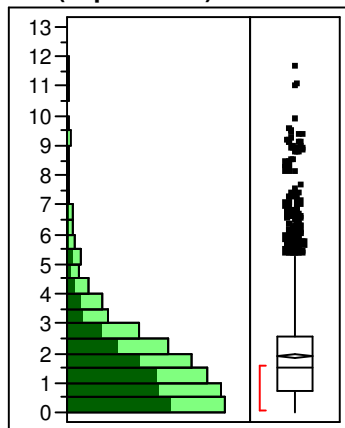
Mean	1,713725
Std Dev	1,5904222
Std Err Mean	0,1348978
upper 95% Mean	1,980459
lower 95% Mean	1,446991
N	139

Distributions

active of

ranked_all_090606_3D.prediction.RMSD

abs (exper - LV4)



254 ligands

Quantiles

100.0%	maximum	11,634
99.5%		9,088
97.5%		6,485
90.0%		3,937
75.0%	quartile	2,544
50.0%	median	1,512
25.0%	quartile	0,707
10.0%		0,277
2.5%		0,076
0.5%		0,018
0.0%	minimum	0,00238

Moments

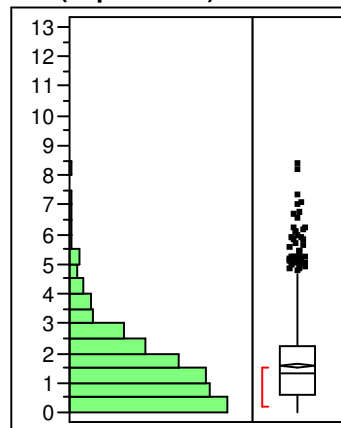
Mean	1,9046469
Std Dev	1,652452
Std Err Mean	0,0327878
upper 95% Mean	1,9689404
lower 95% Mean	1,8403534
N	2540

Distributions

sum elec -10 of active of

ranked_all_090606_3D.prediction.RMSD

abs (exper - LV4)



233 ligands

Quantiles

100.0%	maximum	8,3492
99.5%		6,5987
97.5%		5,0676
90.0%		3,2893
75.0%	quartile	2,2188
50.0%	median	1,3205
25.0%	quartile	0,5895
10.0%		0,2470
2.5%		0,0627
0.5%		0,0180
0.0%	minimum	0,0024

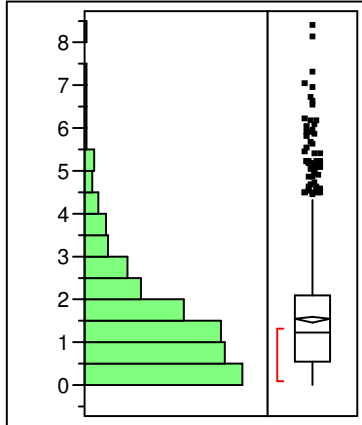
Moments

Mean	1,5815798
Std Dev	1,2810327
Std Err Mean	0,0341882
upper 95% Mean	1,6486454
lower 95% Mean	1,5145142
N	1404

Distributions

gold > 0, sum elec -10 of active of ranked_all_090606_3D.prediction.RMSD

abs (exper - LV4)



217 ligands

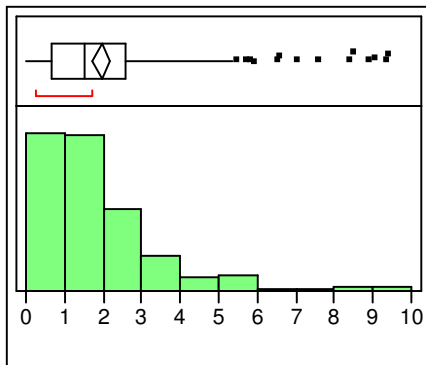
Quantiles

100.0%	maximum	8,3492
99.5%		6,6345
97.5%		5,1182
90.0%		3,3705
75.0%	quartile	2,0855
50.0%	median	1,2459
25.0%	quartile	0,5680
10.0%		0,2332
2.5%		0,0602
0.5%		0,0160
0.0%	minimum	0,0024

Moments

Mean	1,5390618
Std Dev	1,3045724
Std Err Mean	0,0360028
upper 95% Mean	1,6096911
lower 95% Mean	1,4684325
N	1313

best ranked docking
abs (exper - LV4)



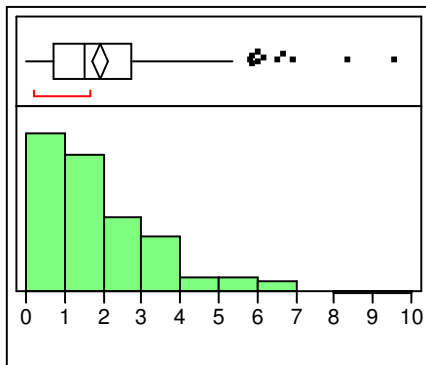
Quantiles

100.0%	maximum	9,3865
99.5%		9,3758
97.5%		8,1050
90.0%		4,0937
75.0%	quartile	2,5712
50.0%	median	1,5190
25.0%	quartile	0,6748
10.0%		0,2785
2.5%		0,1026
0.5%		0,0223
0.0%	minimum	0,0084

Moments

Mean	1,9650912
Std Dev	1,8059513
Std Err Mean	0,1133155
upper 95% Mean	2,1882529
lower 95% Mean	1,7419294
N	254

lowest sum_elec
Distributions sort sum elec=1
abs (exper - LV4)



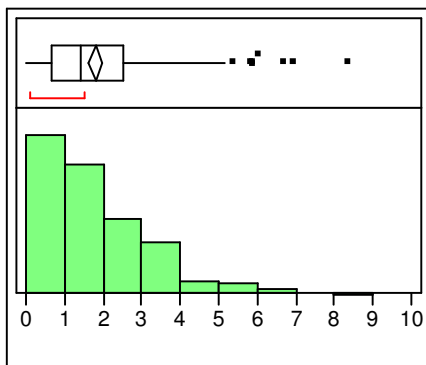
Quantiles

100.0%	maximum	9,5515
99.5%		9,2208
97.5%		6,0959
90.0%		3,9413
75.0%	quartile	2,7034
50.0%	median	1,5009
25.0%	quartile	0,6860
10.0%		0,2368
2.5%		0,0577
0.5%		0,0030
0.0%	minimum	0,0024

Moments

Mean	1,9178945
Std Dev	1,629856
Std Err Mean	0,1022663
upper 95% Mean	2,1192961
lower 95% Mean	1,7164929
N	254

lowest sum_elec and sum_elec < -10
Distributions
abs (exper - LV4)



Quantiles

100.0%	maximum	8,3492
99.5%		8,1076
97.5%		5,8632
90.0%		3,7944
75.0%	quartile	2,5162
50.0%	median	1,4238
25.0%	quartile	0,6536
10.0%		0,2359
2.5%		0,0655
0.5%		0,0028
0.0%	minimum	0,0024

Moments

Mean	1,7970455
Std Dev	1,4807424
Std Err Mean	0,0970067
upper 95% Mean	1,9881721
lower 95% Mean	1,6059189
N	233

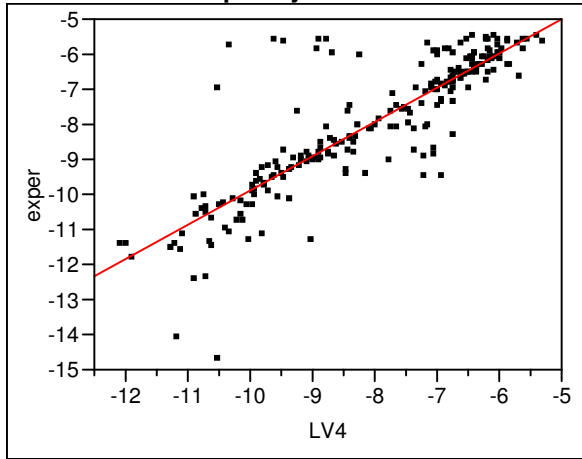
exper < -5.5 and min abs(exper-LV4)
 active of
 ranked_all_090606_3D.prediction.RMSD

— Linear Fit

Linear Fit

exper = -0,137426 + 0,9778154 LV4

Bivariate Fit of exper By LV4



Summary of Fit

RSquare	0,736107
RSquare Adj	0,734913
Root Mean Square Error	0,978118
Mean of Response	-7,99183
Observations (or Sum Wgts)	223

Analysis of Variance

Source	DF	Sum of Squares	Mean Square
Model	1	589,77865	589,779
Error	221	211,43406	0,957
C. Total	222	801,21271	

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob> t
Intercept	-0,137426	0,323054	-0,43	0,6710
LV4	0,9778154	0,039383	24,83	<,0001

This best correlation which is possible with the data, but cannot be retrieved without knowing the experimental ΔG .