The new fragment picker

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Summary

1. Why fragmentpicker?
2. Fragmentpicking overview
3. Fragmentpicking quick examples
   - NNmake - style protocol
   - CS-Rosetta type protocol
4. Fragmentpicking details
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5. Fragmentpicker: under the hood
6. The end
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   - Acknowledgements

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- core/fragment/picking/* by Andrew Ban
  (→ core/fragment/picking_old/)

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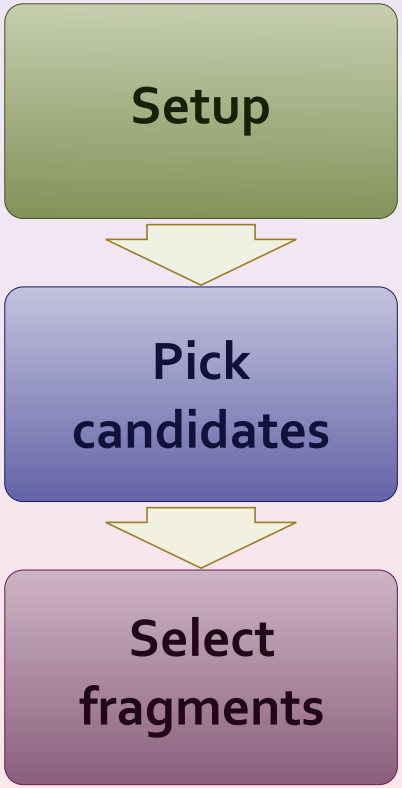
Overview & input files



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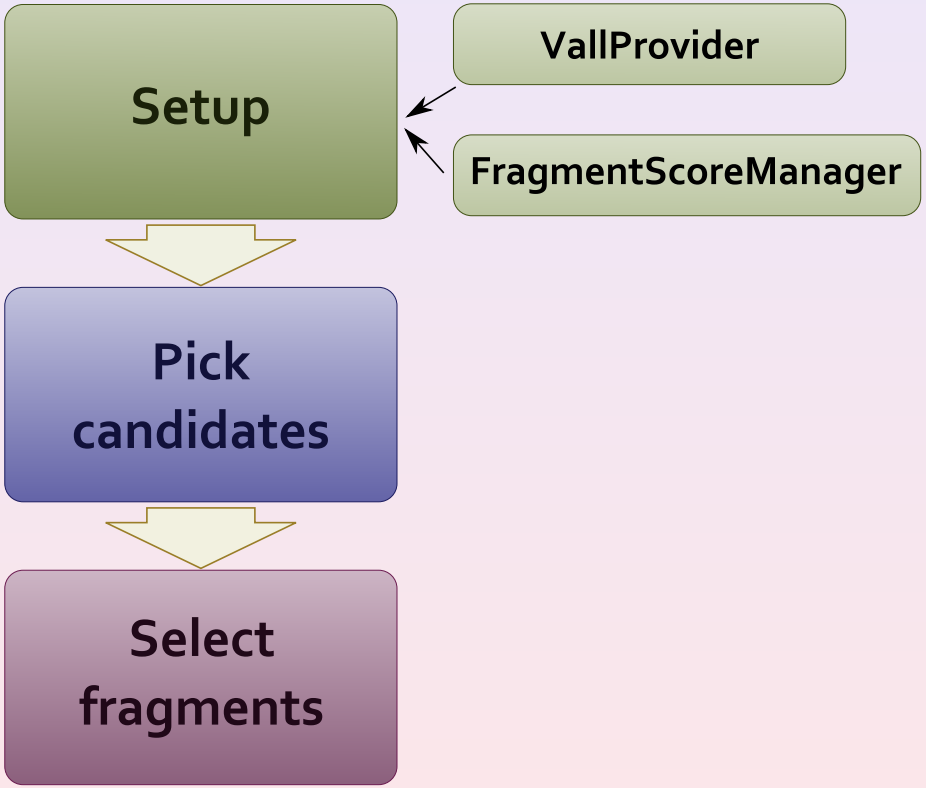

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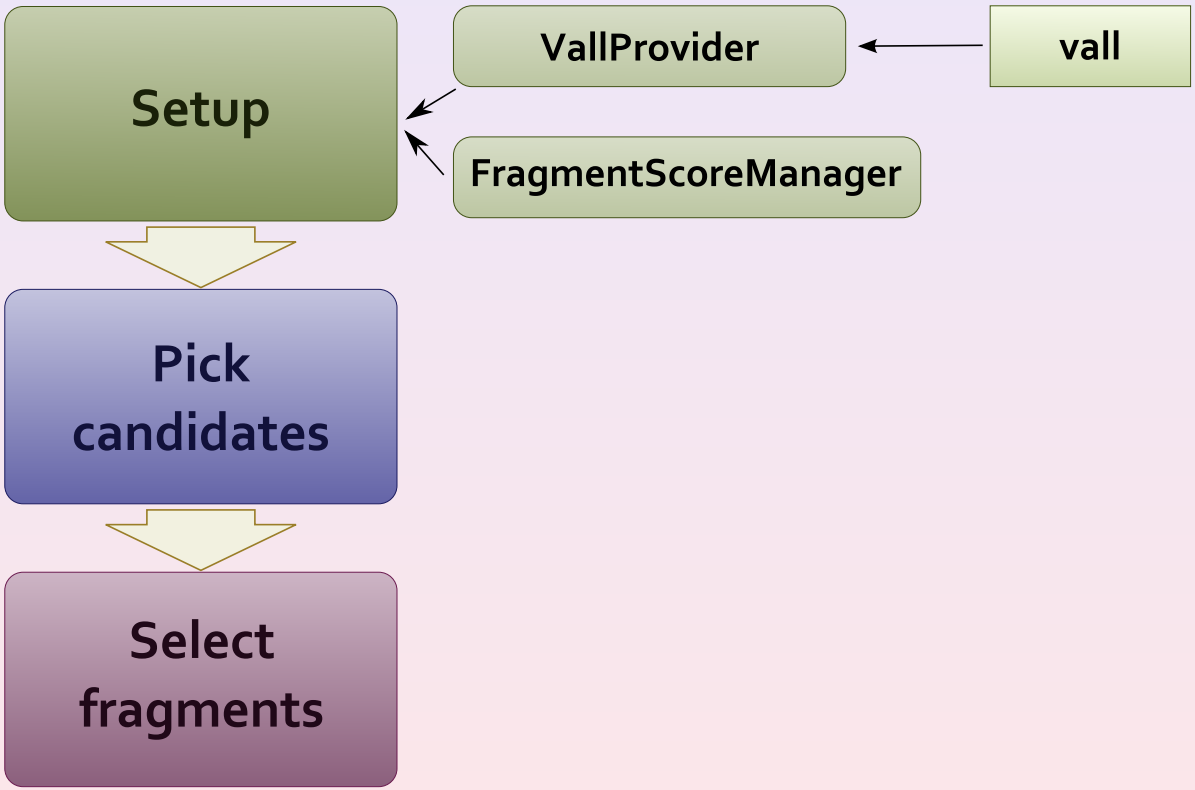

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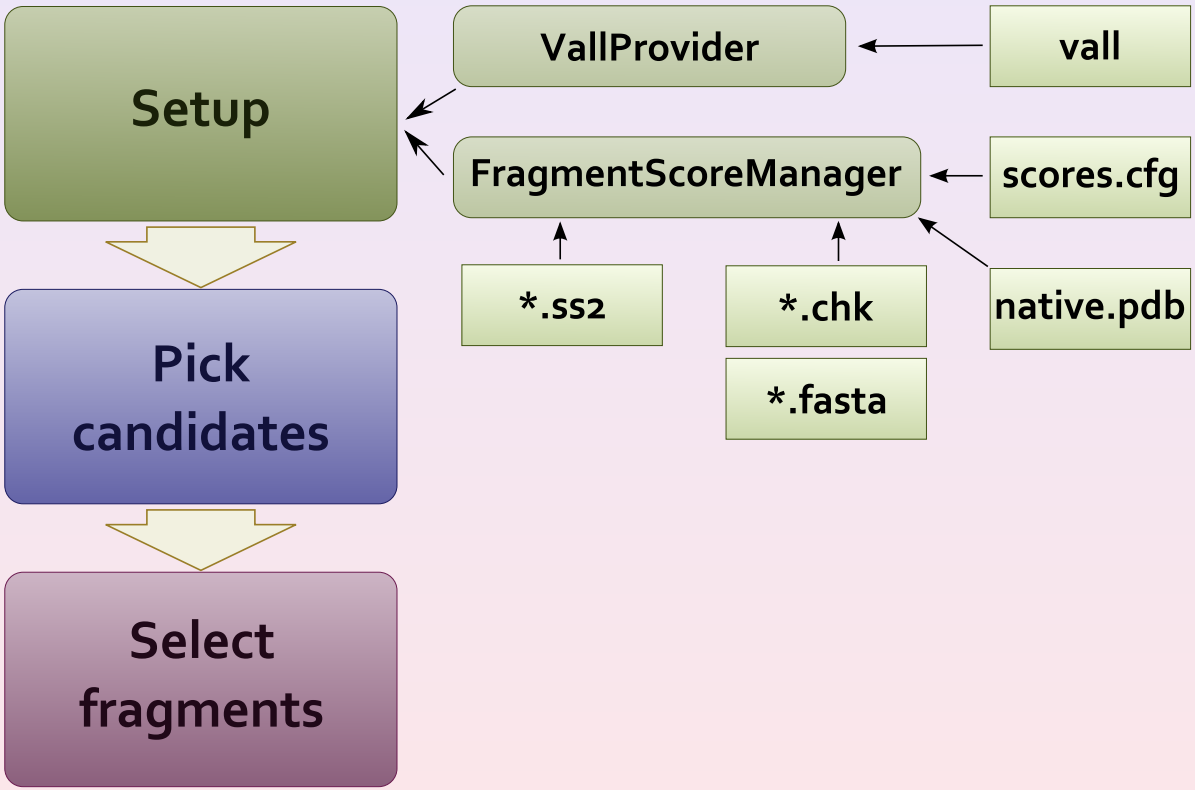

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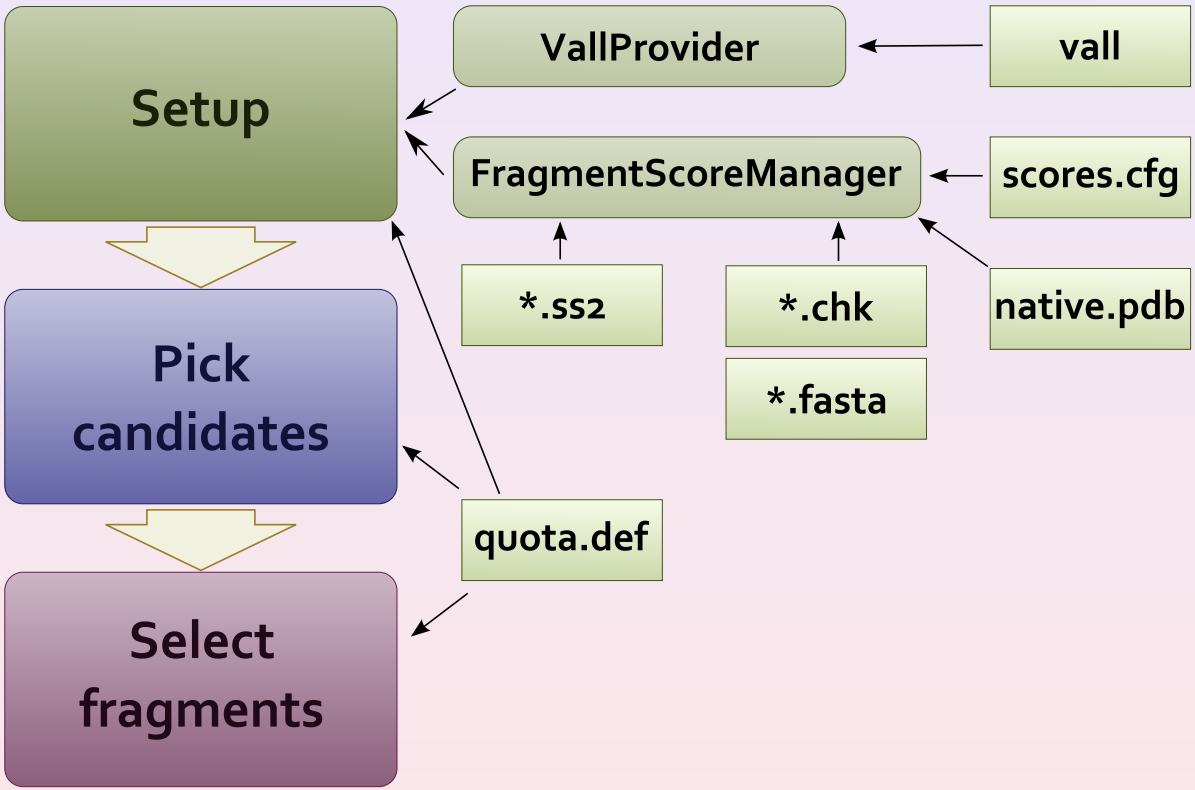

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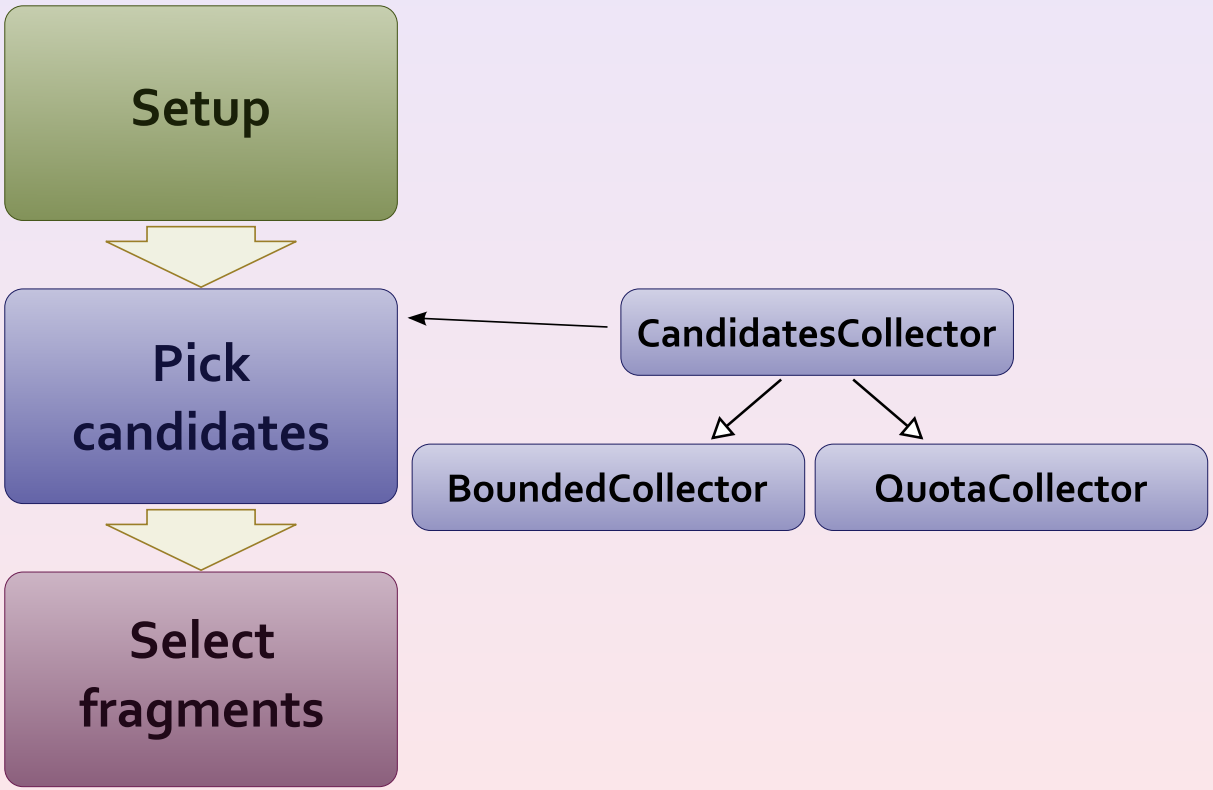

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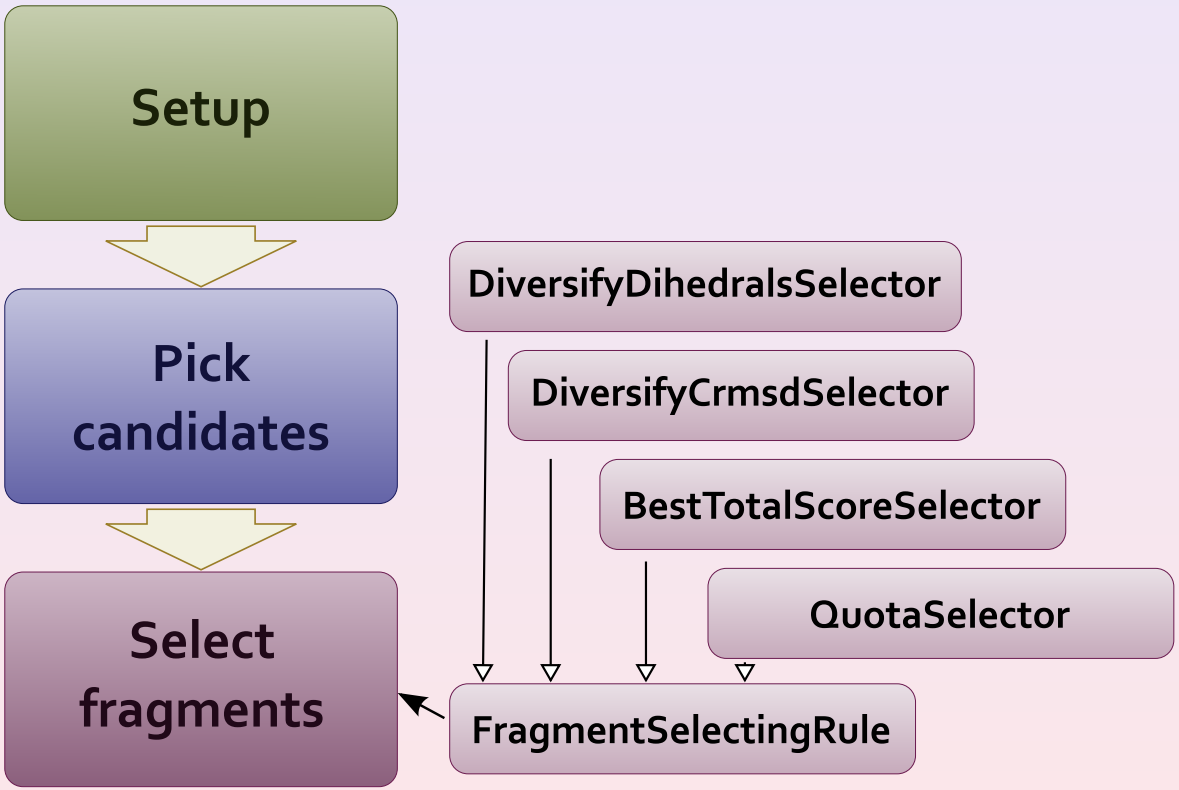

NNmake - style protocol

See `Psi-Jufo-Sam-L1-Quota` demo

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- scoring:(file: `psi_sam_jufo_L1-Q.cfg`)

```
# score name        priority wght cutoff extras
SecondarySimilarity   350 1.0 - psipred
SecondarySimilarity   300 1.0 - sam
SecondarySimilarity   250 1.0 - jufo
RamaScore             150 50.0 -
ProfileScoreL1        200 1.0   -
PhiPsiSquareWell      100 0.0 -
FragmentCrmsd         30  0.0  -
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```

- quota setup (file: `Quota.def`):

```
#pool_id pool_name fraction
1  psipred  0.6
2  jufo     0.2
3  sam     0.2
```

CS-Rosetta protocol

See `CS-Talos-L1-Rama` demo

- collector: BoundedCollector

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```
# score name  priority  wght cutoff  extras
CSScore              375   3.0    -
RamaScore            400   50.0   -    talos
SecondarySimilarity  350   3.0    -    talos
ProfileScoreL1       200   1.0    -
PhiPsiSquareWell     100   0.0    -
FragmentCrmsd        30    0.0    -
GunnCostScore        20    0.0    -
```

Picking results

- fragment files

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How quota works

Vall fragment

12asA	F	E	167	163	...
12asA	V	E	168	162	...
12asA	H	E	169	161	...
12asA	S	H	170	160	...
12asA	Q	H	171	159	...
12asA	E	H	172	158	...
12asA	L	H	173	157	...
12asA	L	H	174	156	...
12asA	S	H	175	155	...

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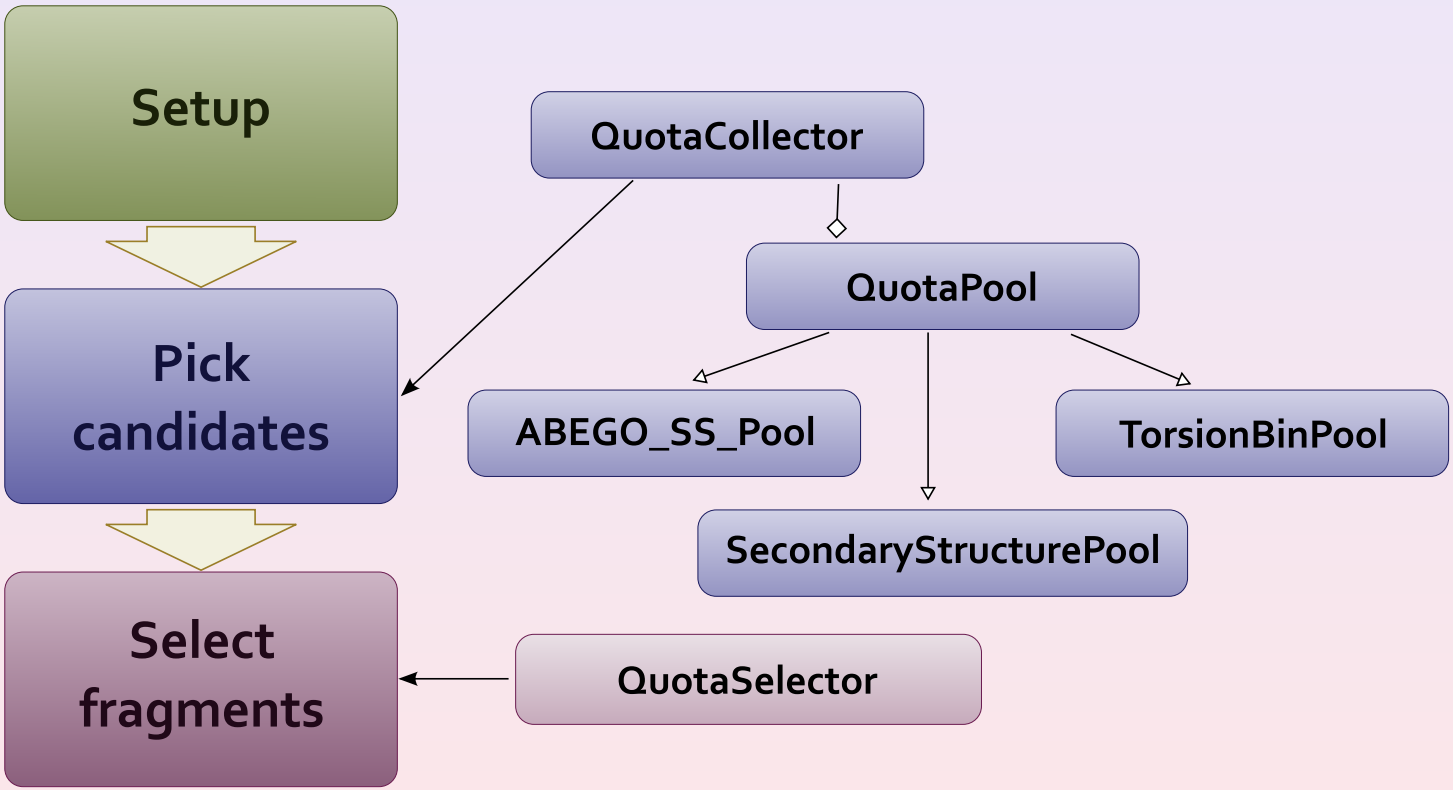
PsiPred prediction

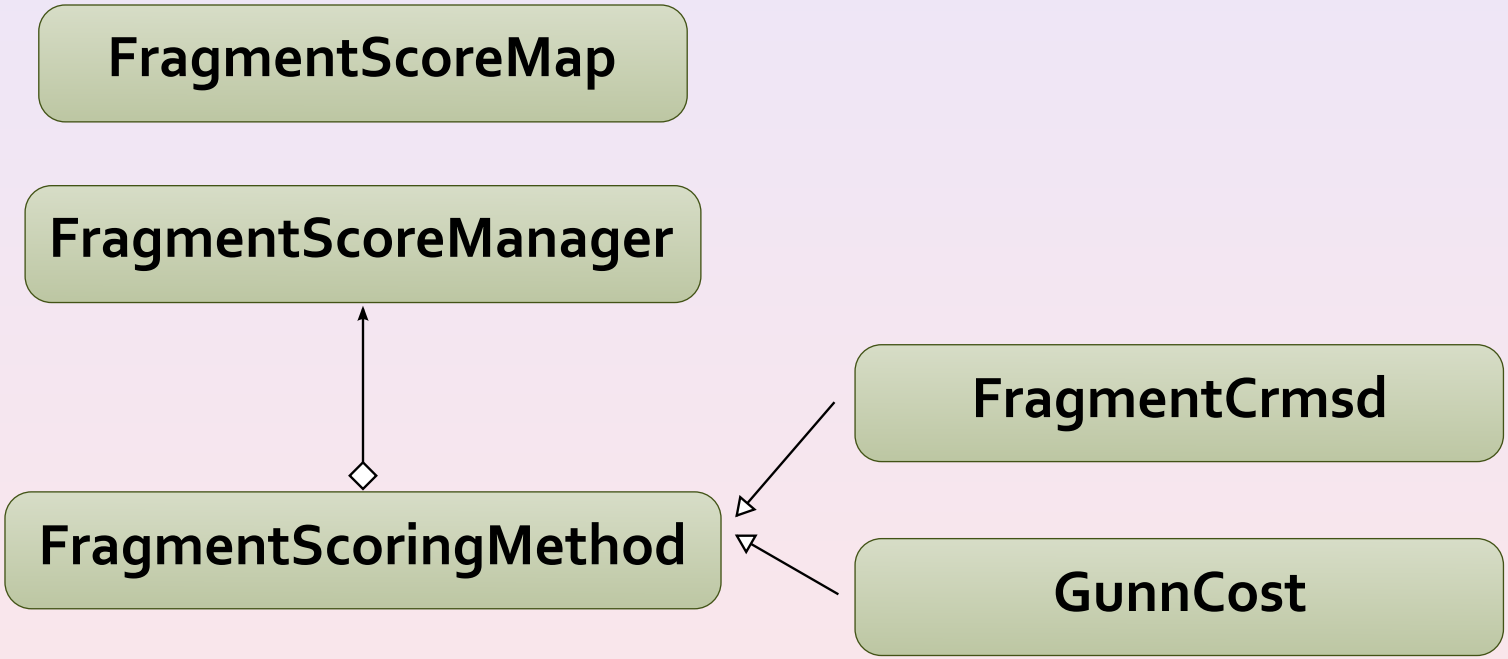
16	T	E	0.030	0.016	0.924
17	T	E	0.065	0.207	0.636
18	T	E	0.101	0.258	0.569
19	E	H	0.114	0.586	0.348
20	A	H	0.083	0.335	0.582
21	V	H	0.125	0.521	0.354
22	D	H	0.545	0.177	0.215
23	A	H	0.079	0.916	0.011
24	A	H	0.052	0.933	0.003

psipred-C : $0.125 \times 200 \times 0.6 = 15$
psipred-H : $0.521 \times 200 \times 0.6 = 63$
psipred-E : $0.354 \times 200 \times 0.6 = 42$

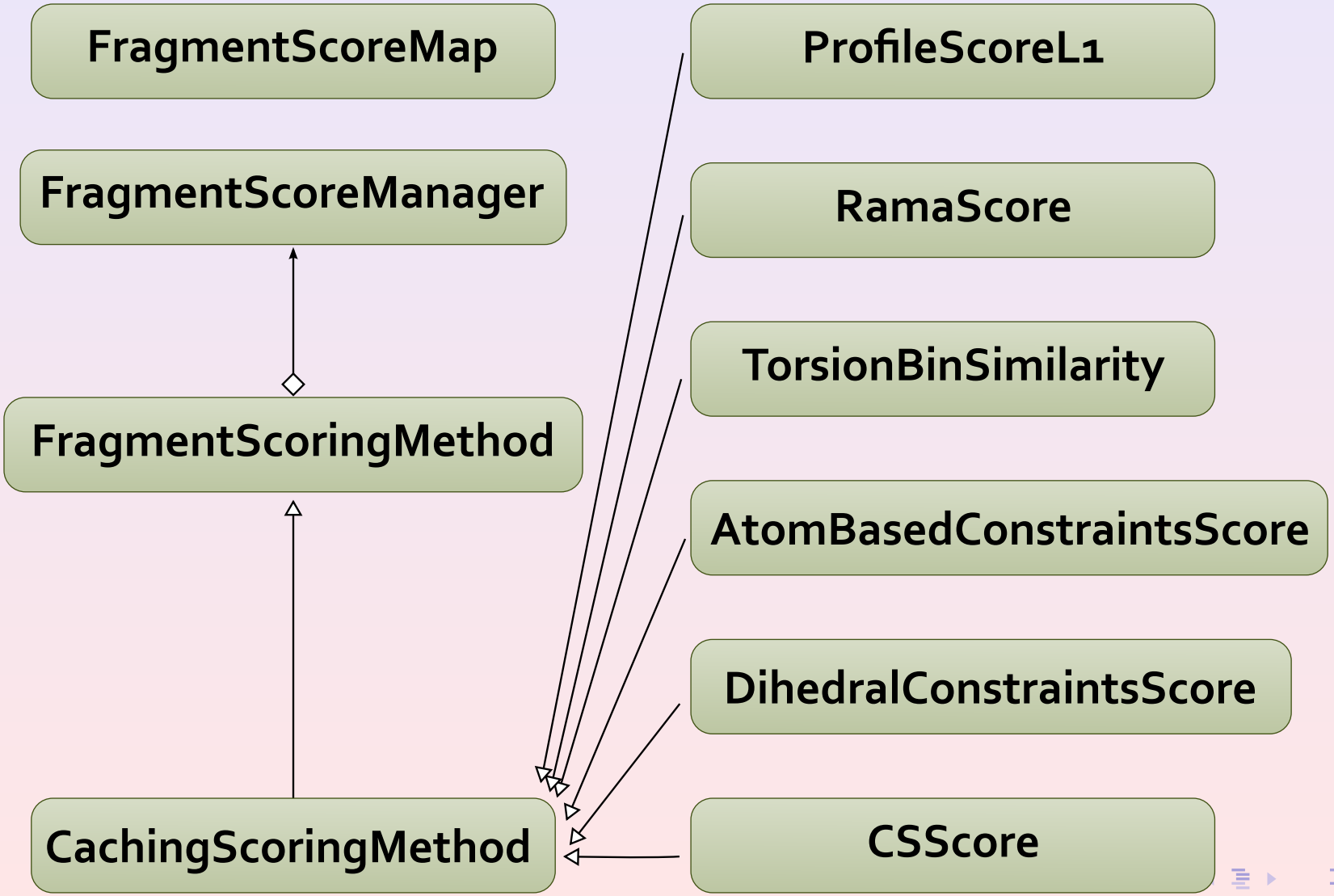
Quota-related parts



Scoring-related classes



Scoring-related classes (2)



fragmentpicker_integration_demo.cc

see
mini/src/apps/pilot/dgront/fragmentpicker/fragmentpicker_integration_demo.c

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- drink Porter, no more Jufo

Future plans

- more scores

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- SQL database instead of vall

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