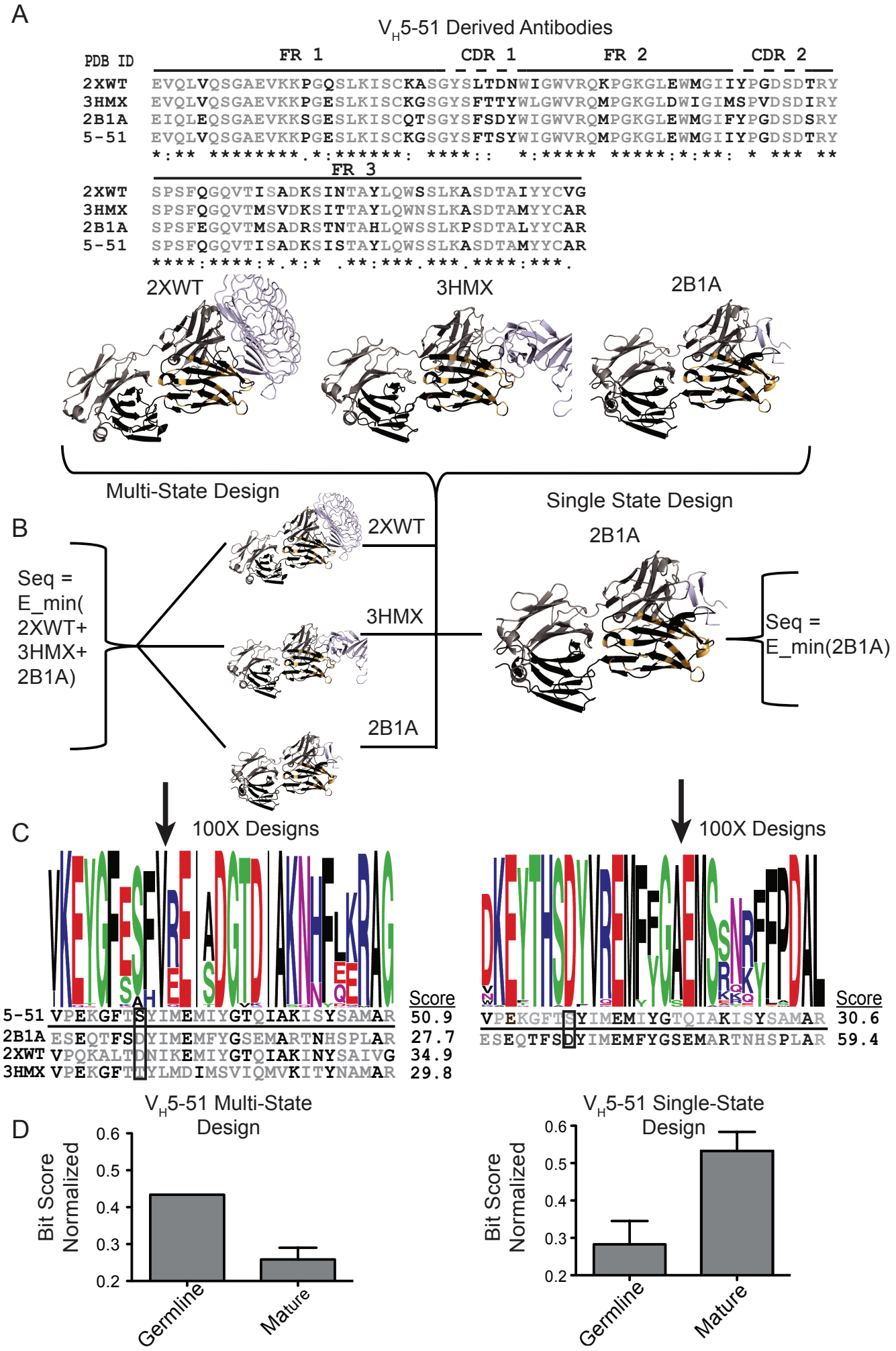
A
V_H5-51 Derived Antibodies
PDB ID
FR 1
CDR 1
FR 2
CDR 2
2XWT EVQLVQSGAEVKKPGQSLKISCKASGYSLTDNWIGWVRQKPGKGLEWMGIIYPGDSDTRY
3HMX EVQLVQSGAEVKKPGESLKISCKGSGYSFTTYWLGWVRQMPGKGLDWIGIMSPVDSDIRY
2B1A EIQLEQSGAEVKKSGESLKISCQTSGYSFSDYWIGWVRQMPGKGLEWMGIFYPGDSDSRY
5-51 EVQLVQSGAEVKKPGESLKISCKGSGYSFTSYWIGWVRQMPGKGLEWMGIIYPGDSDTRY
FR 3
2XWT SPSFQGQVTISADKSINTAYLQWSSLKASDTAIYYCVG
3HMX SPSFQGQVTMSVDKSITTAYLQWNSLKASDTAMYYCAR
2B1A SPSFEGQVTMSADRSTNTAHLQWSSLKPSDTALYYCAR
5-51 SPSFQGQVTISADKSISTAYLQWSSLKASDTAMYYCAR
2XWT
3HMX
2B1A
Multi-State Design
Single State Design
B
Seq = E_min(2XWT+ 3HMX+ 2B1A)
2XWT
3HMX
2B1A
Seq = E_min(2B1A)
C
100X Designs
100X Designs
Score
5-51 VPEKGFTSYIMEMIYGTQIAKISYSAMAR 50.9
2B1A ESEQTFSDYIMEMFYGSEMARTNHSPLAR 27.7
2XWT VPQKALTDNIKEMIYGTQIAKINYSAIVG 34.9
3HMX VPEKGFTLYLMDIMSVIQMVKITYNAMAR 29.8
Score
VPEKGFTSYIMEMIYGTQIAKISYSAMAR 30.6
ESEQTFSDYIMEMFYGSEMARTNHSPLAR 59.4
D
V_H5-51 Multi-State Design
Bit Score Normalized
0.6
0.5
0.4
0.3
0.2
Germline
Mature
V_H5-51 Single-State Design
Bit Score Normalized
0.6
0.5
0.4
0.3
0.2
Germline
Mature