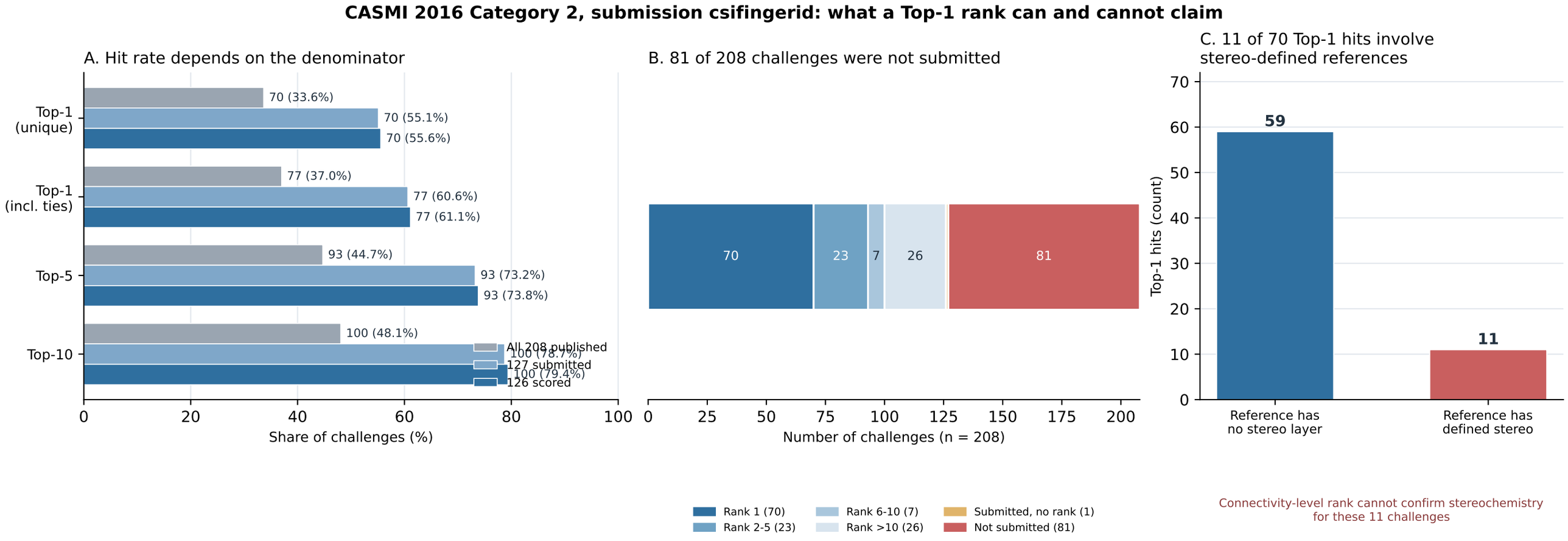
CASMI 2016 Category 2, submission csifingerid: what a Top-1 rank can and cannot claim
A. Hit rate depends on the denominator
Top-1 (unique)
Top-1 (incl. ties)
Top-5
Top-10
70 (33.6%)
70 (55.1%)
70 (55.6%)
77 (37.0%)
77 (60.6%)
77 (61.1%)
93 (44.7%)
93 (73.2%)
93 (73.8%)
100 (48.1%)
100 (78.7%)
100 (79.4%)
All 208 published
127 submitted
126 scored
0
20
40
60
80
100
Share of challenges (%)
B. 81 of 208 challenges were not submitted
70
23
7
26
81
0
25
50
75
100
125
150
175
200
Number of challenges (n = 208)
Rank 1 (70)
Rank 2-5 (23)
Rank 6-10 (7)
Rank >10 (26)
Submitted, no rank (1)
Not submitted (81)
C. 11 of 70 Top-1 hits involve stereo-defined references
Top-1 hits (count)
0
10
20
30
40
50
60
70
59
11
Reference has no stereo layer
Reference has defined stereo
Connectivity-level rank cannot confirm stereochemistry for these 11 challenges