

Integrative Structure Validation Report ?

February 18, 2025 - 08:34 AM PST

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PyMOL Version 2.5.0

PDB ID	9A2F
PDB-Dev ID	PDBDEV_00000164
Structure Title	Structures of the PSG Supramodule of PSD-95 Resolved by Screening of FRET-derived Distance Restraints against Simulated Structures
Structure Authors	Hamilton, G.; Saikia, N.; Basak, S.; Welcome, F. S.; Wu, F.; Kubiak, J.; Zhang, C.; Hao, Y.; Seidel, C. A. M.; Ding, F.; Sanabria, H.; Bowen, M. E.
Deposited on	2022-09-14

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

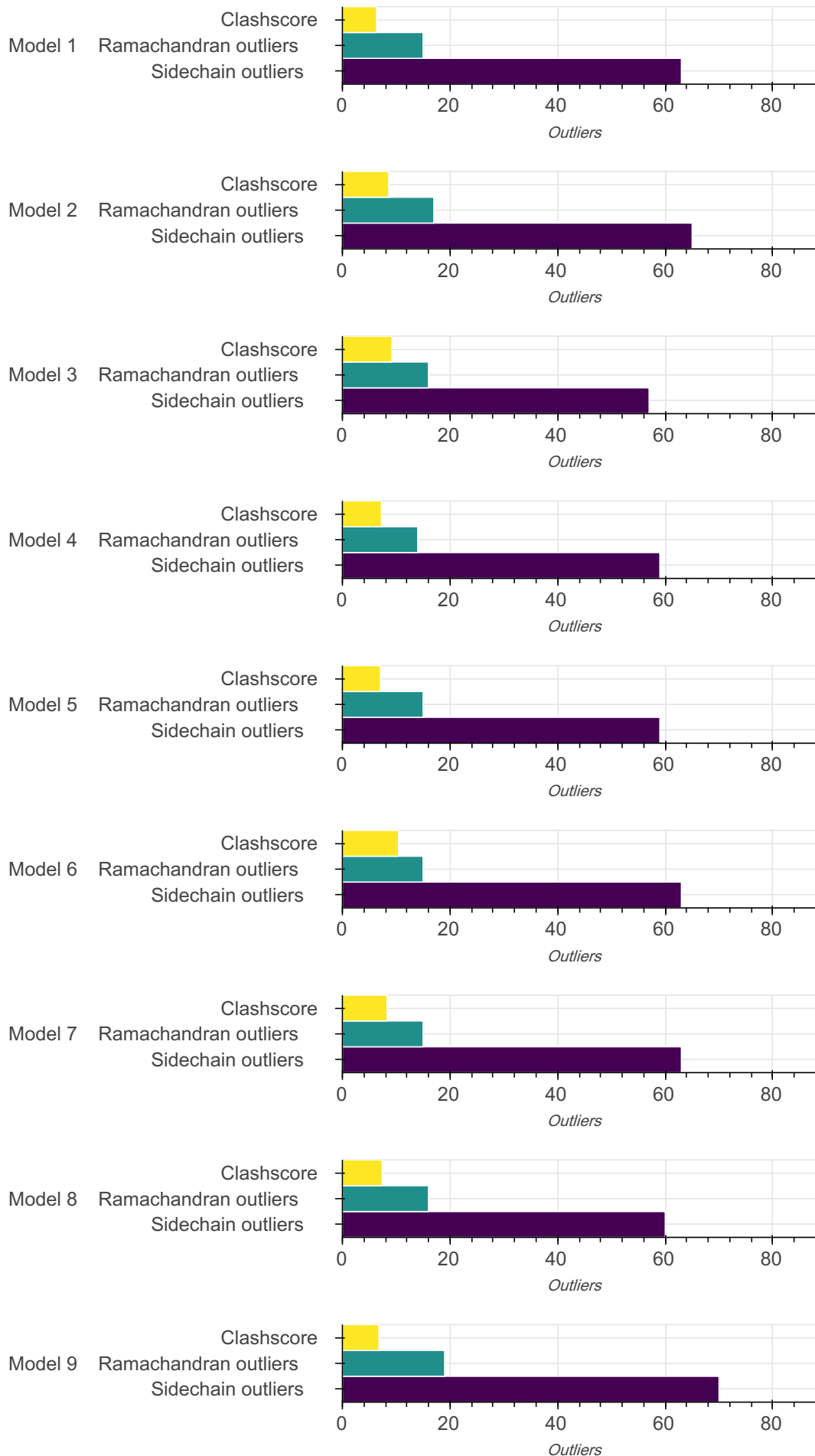
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

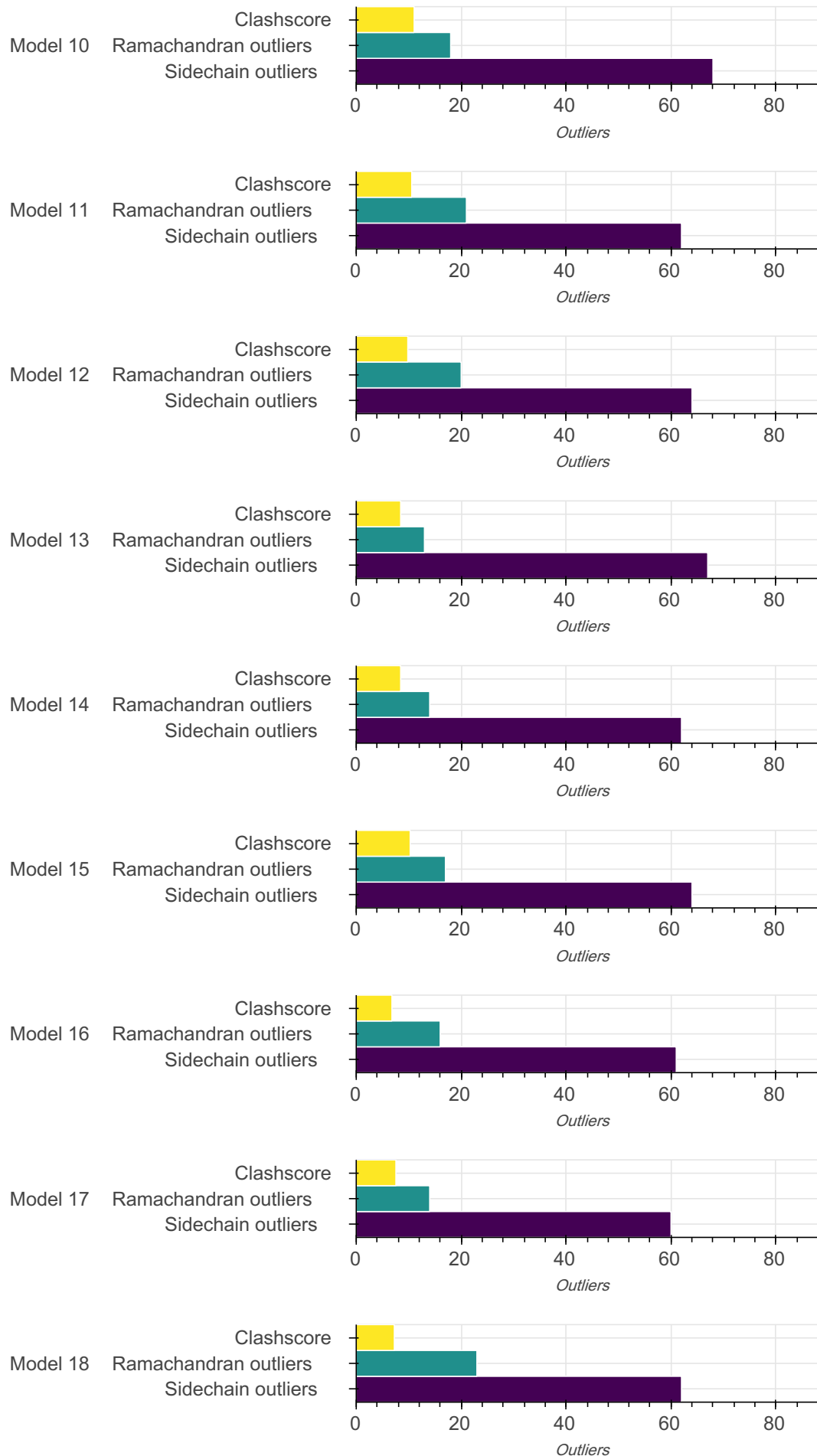
List of references used to build this report is available [here](#).

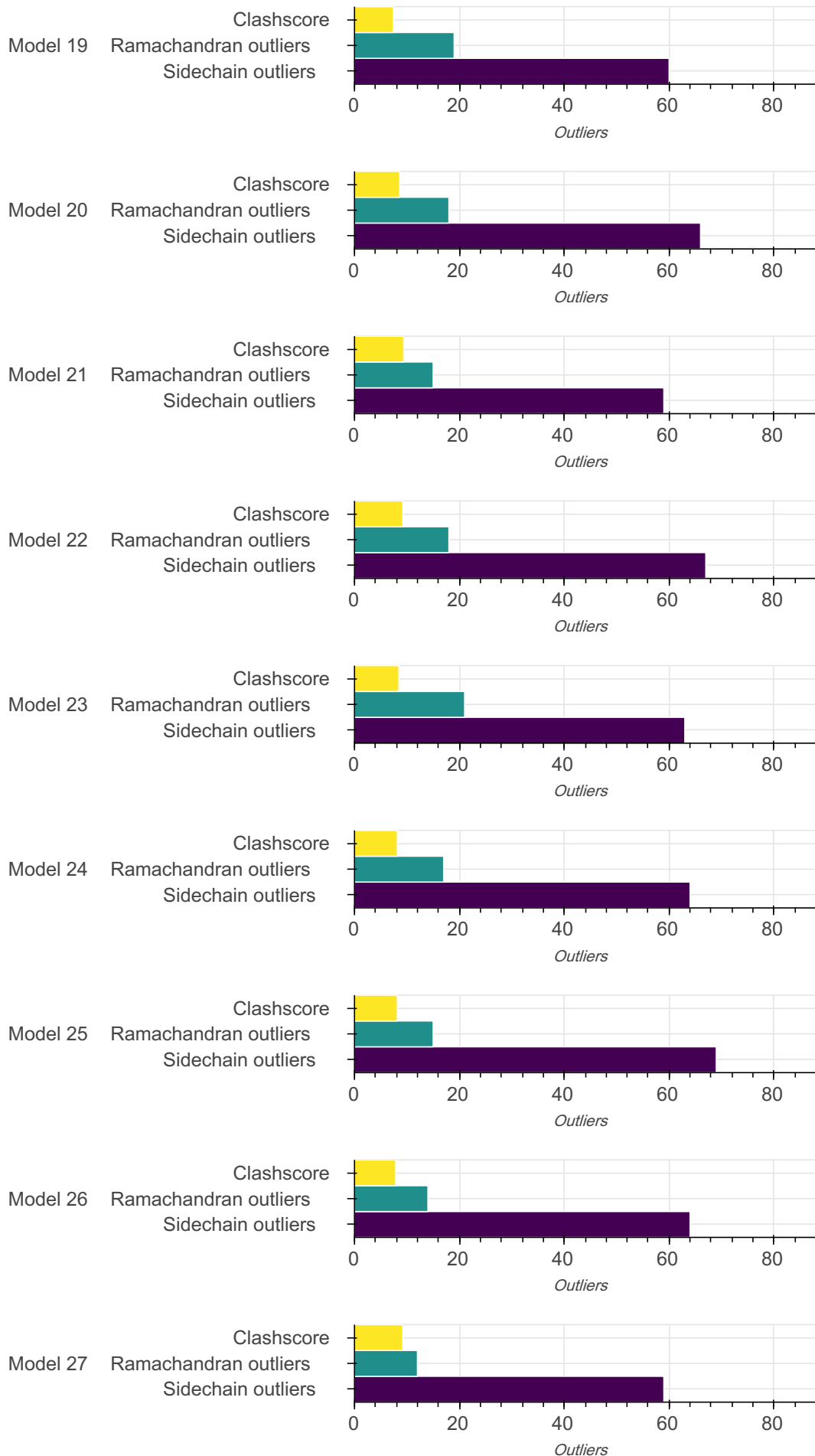
Overall quality ?

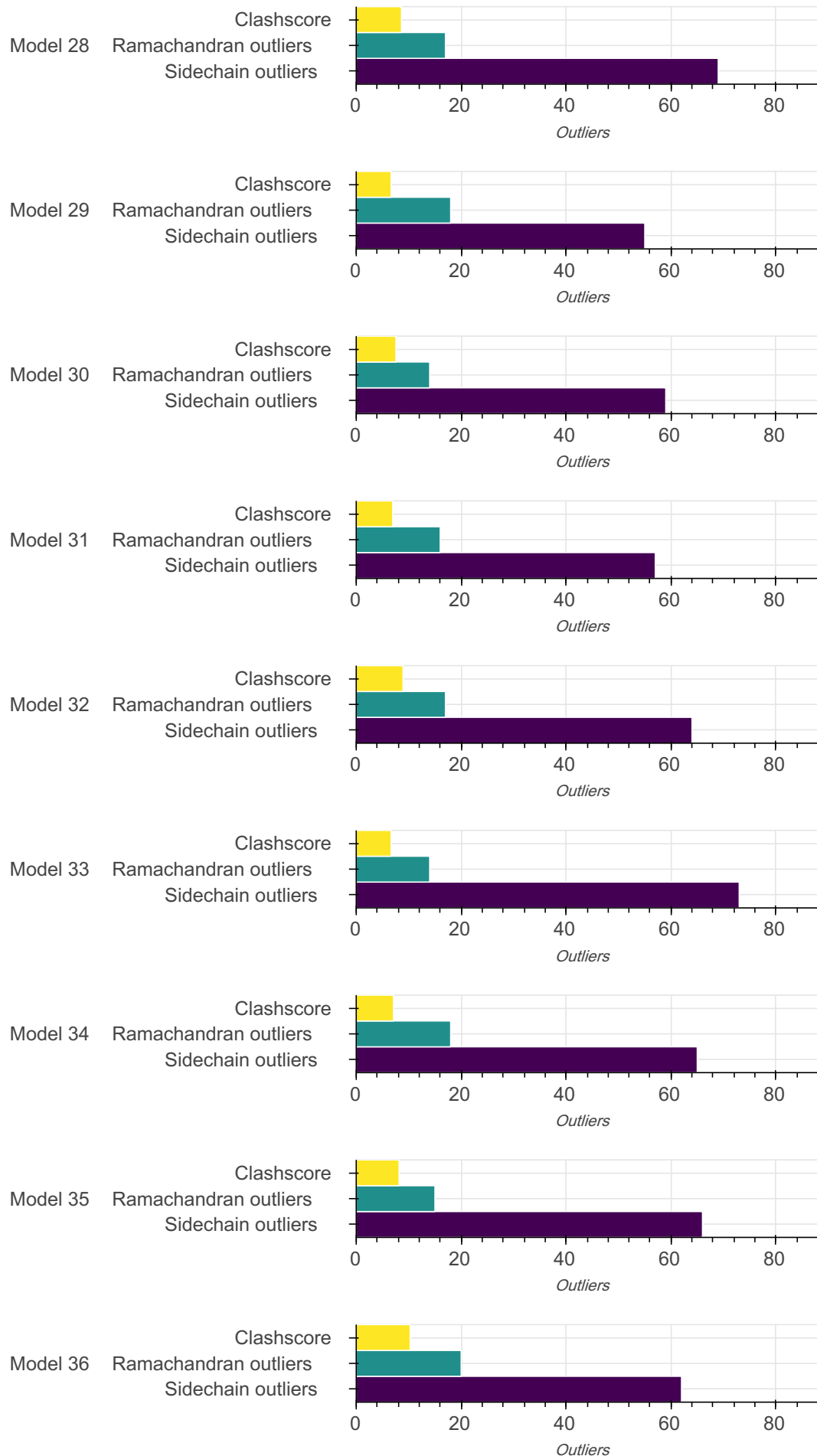
This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

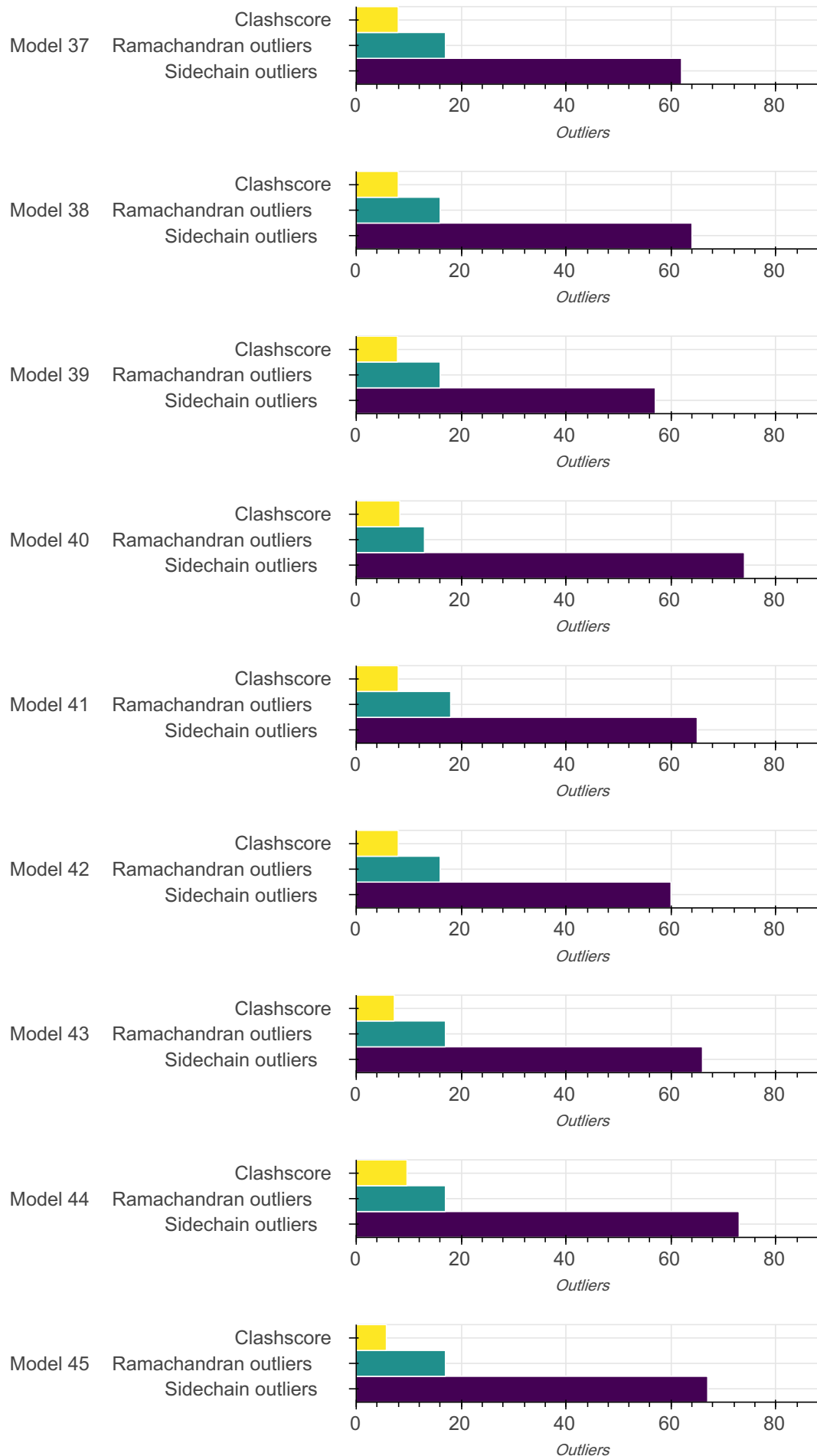
Model Quality: MolProbity Analysis

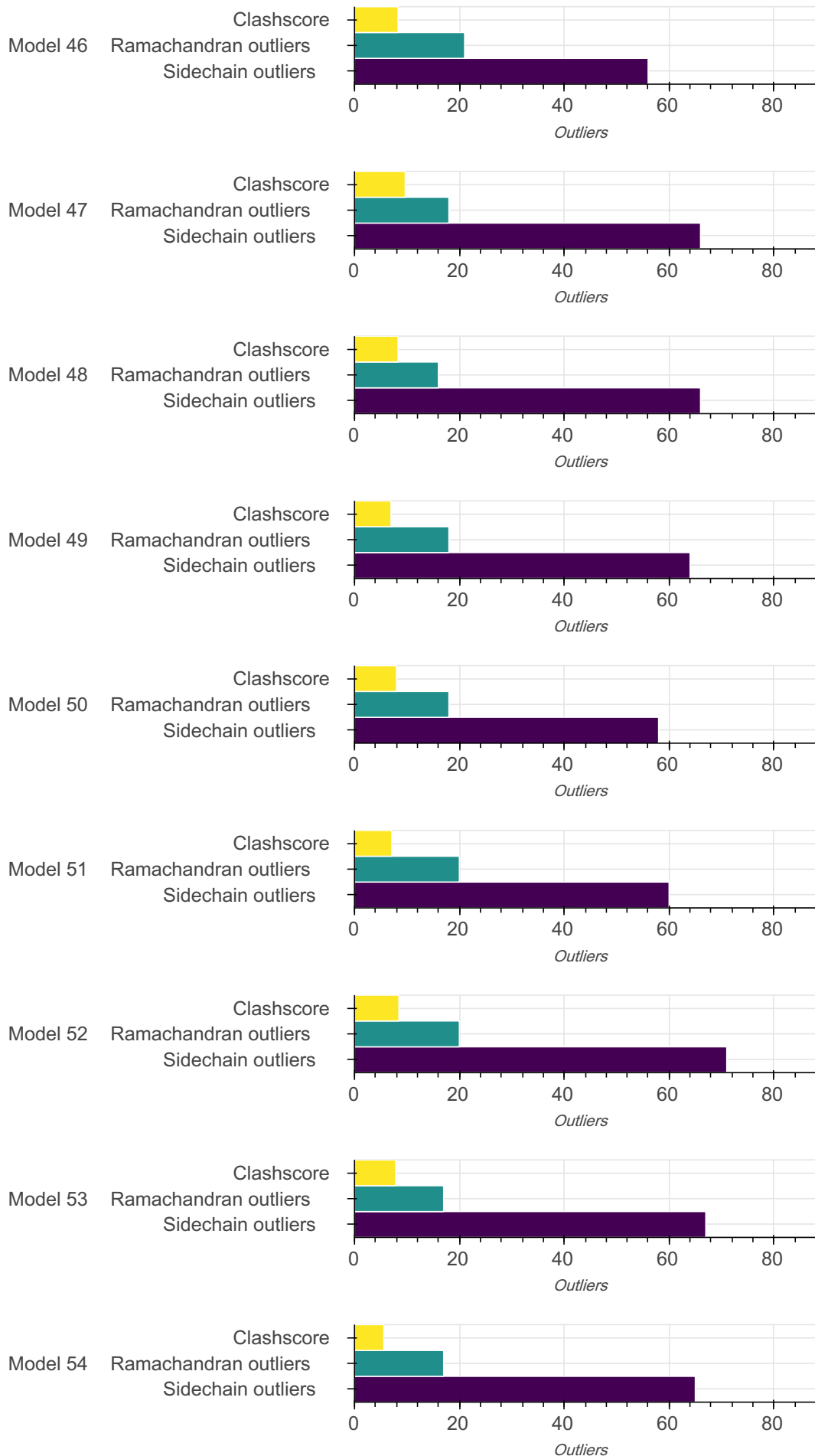


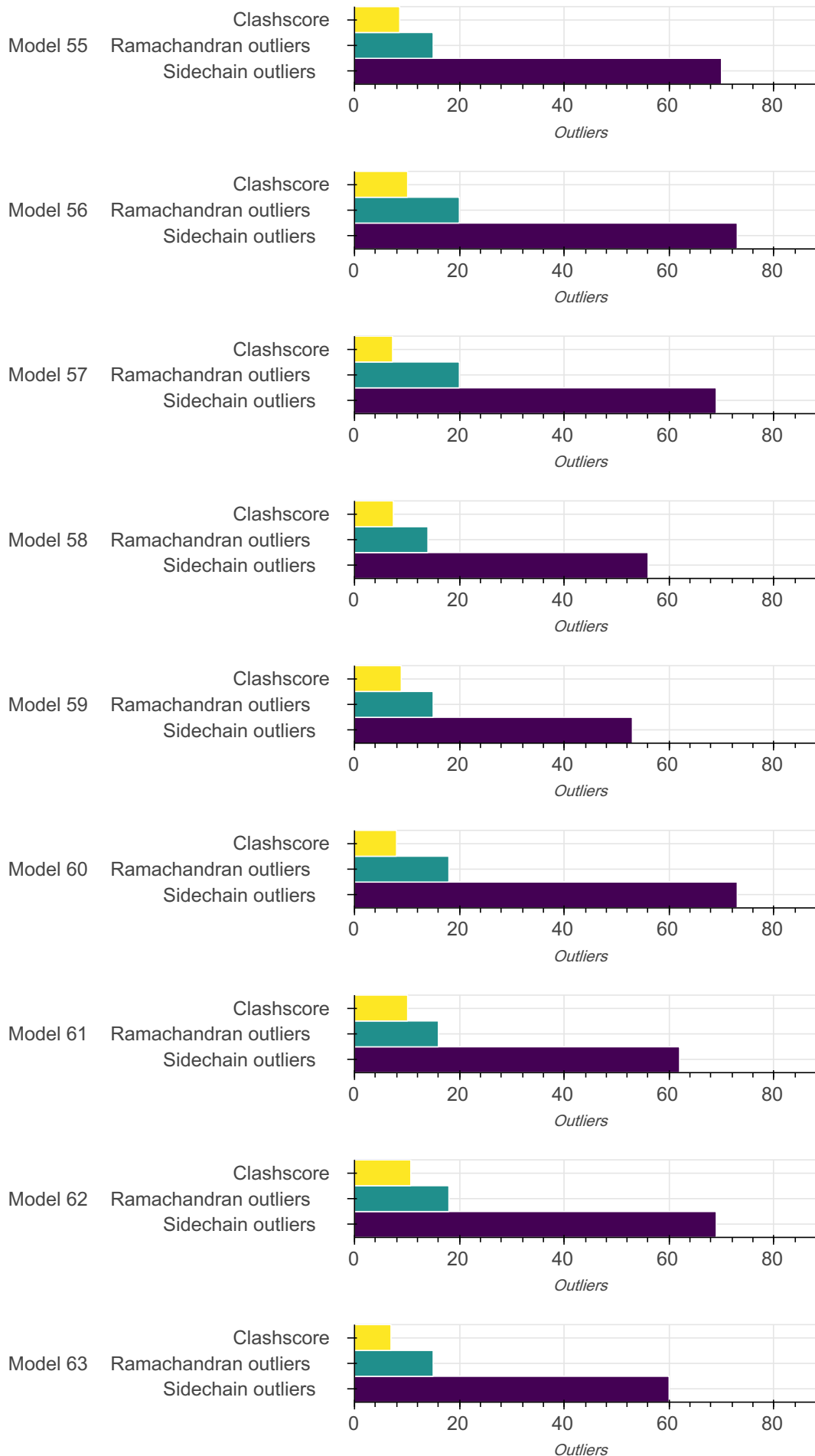


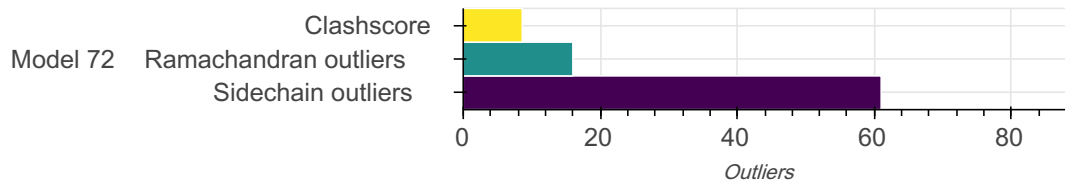
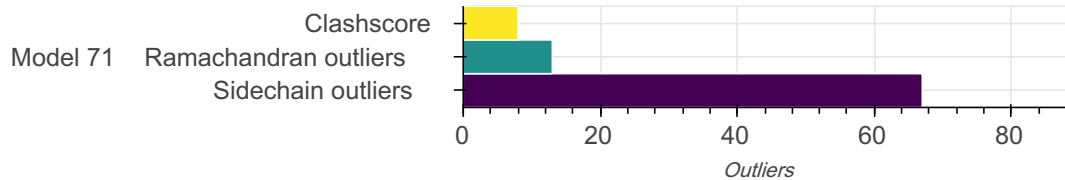
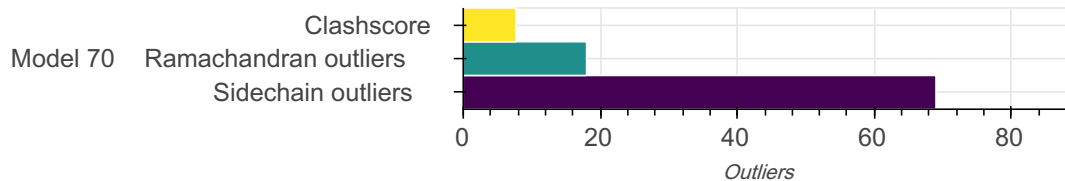
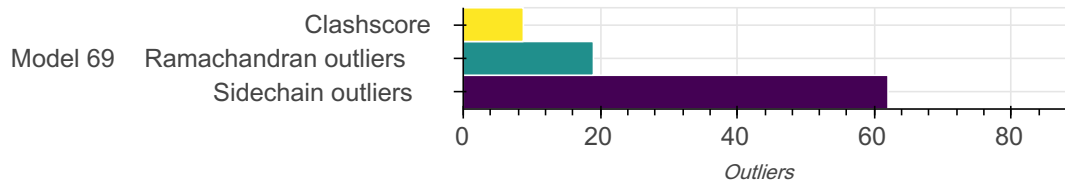
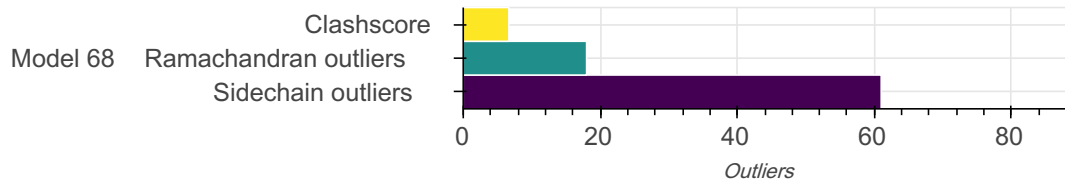
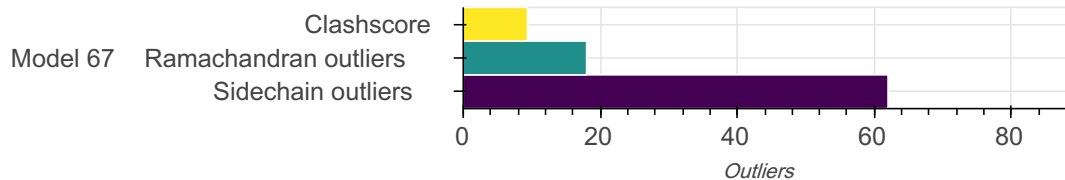
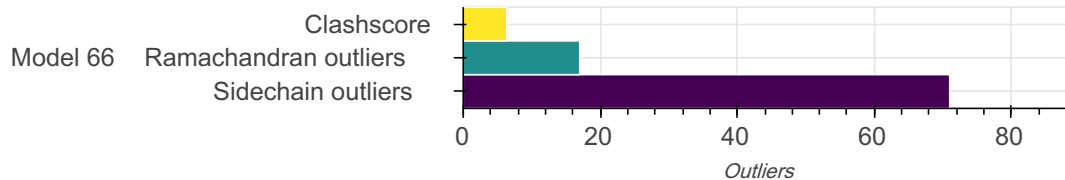
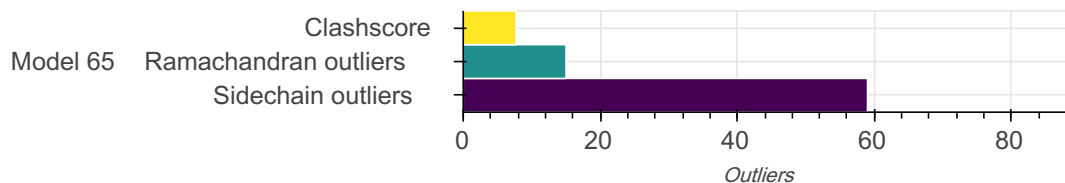
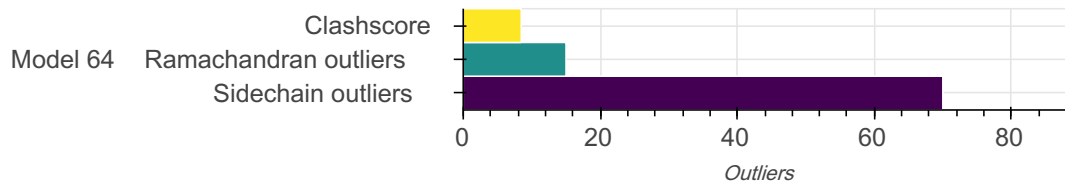


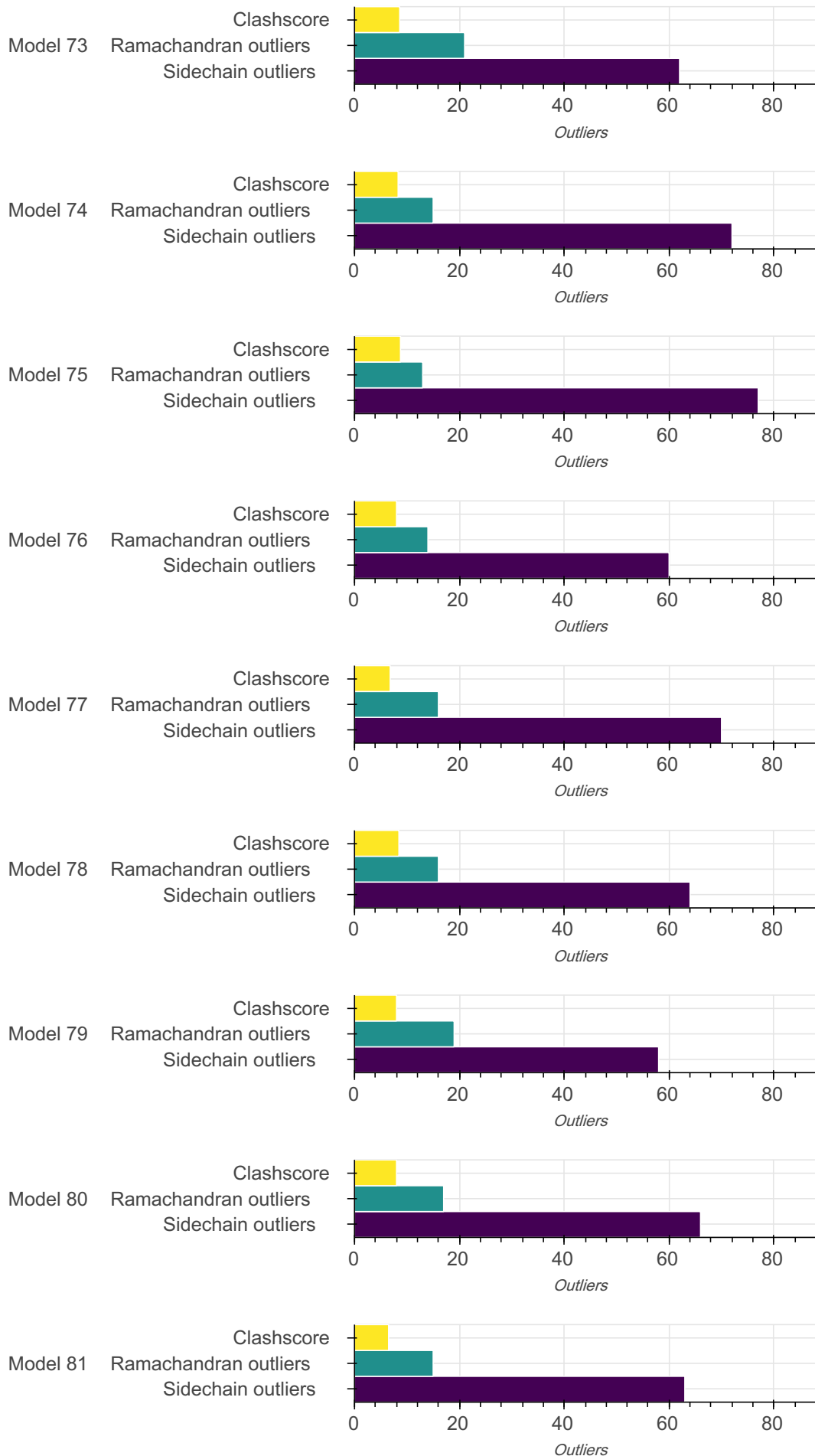


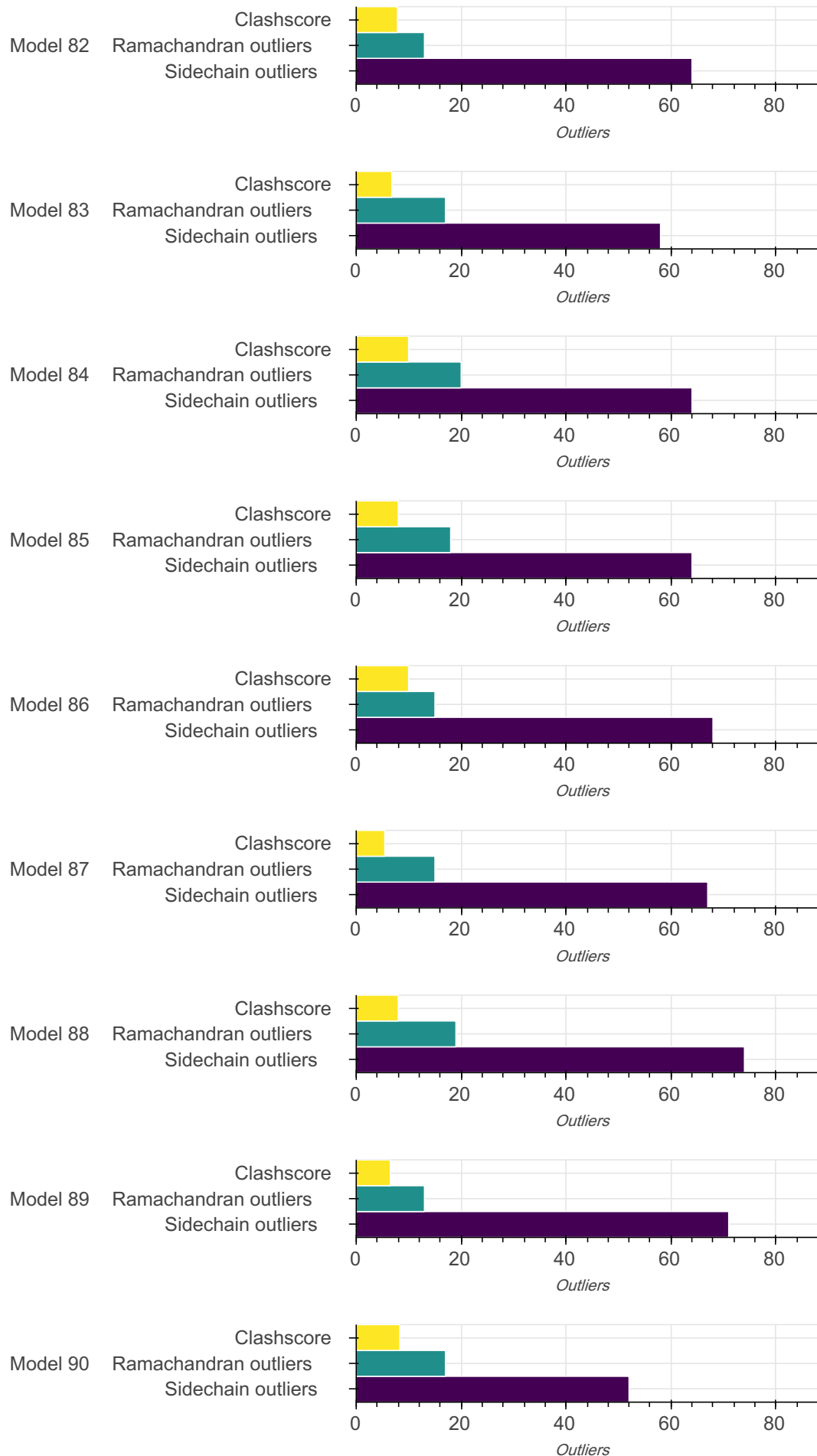


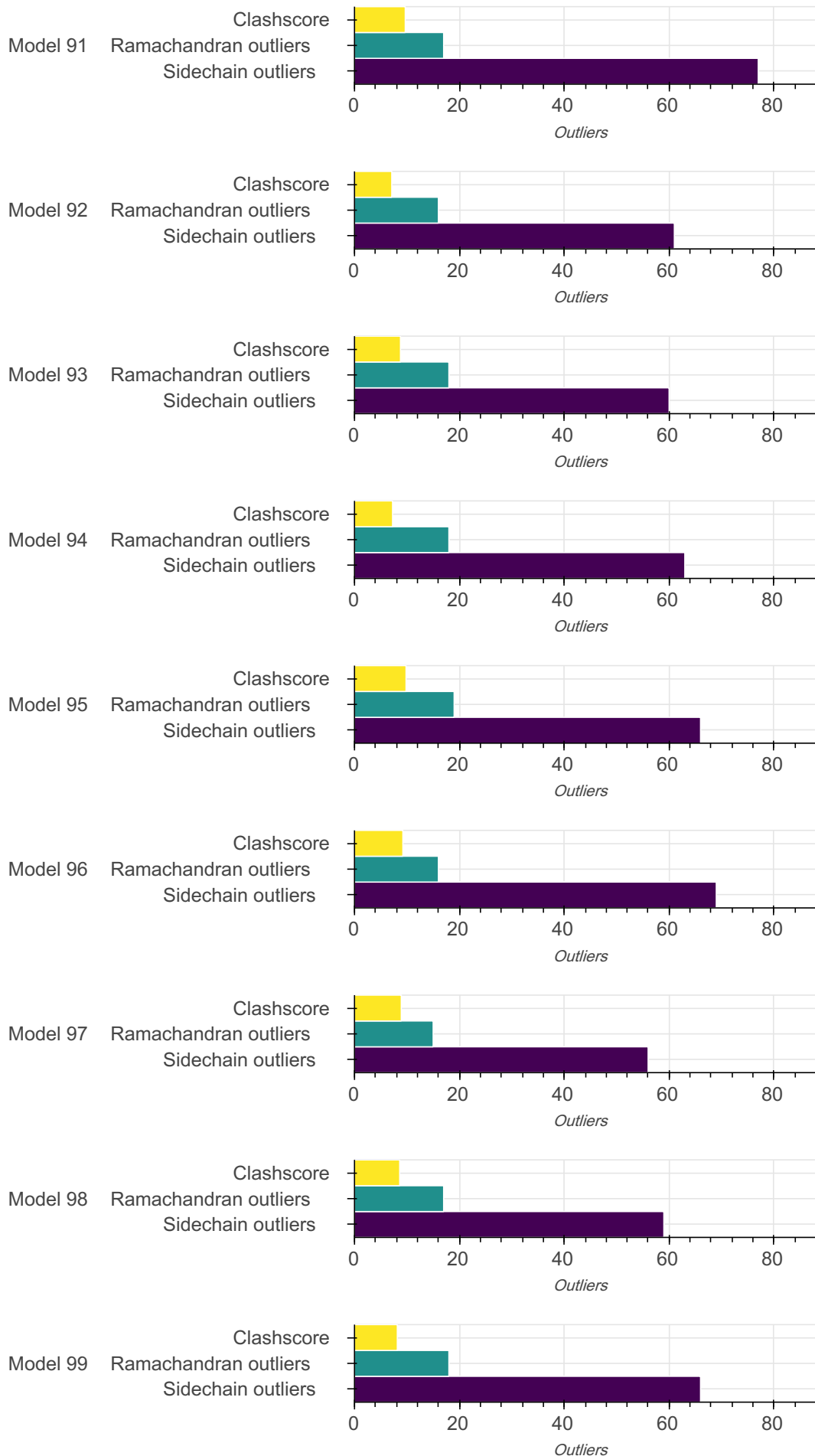


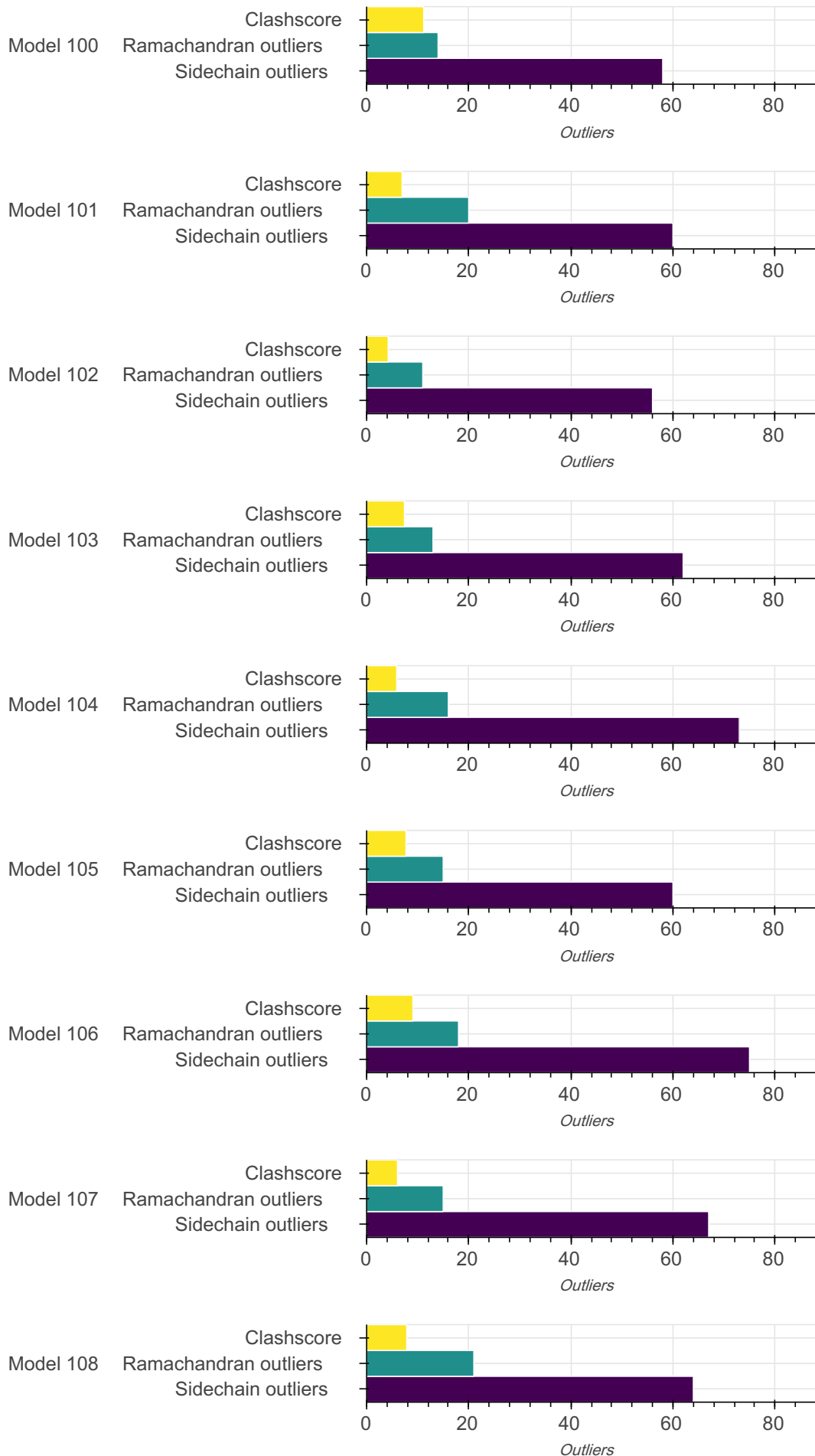


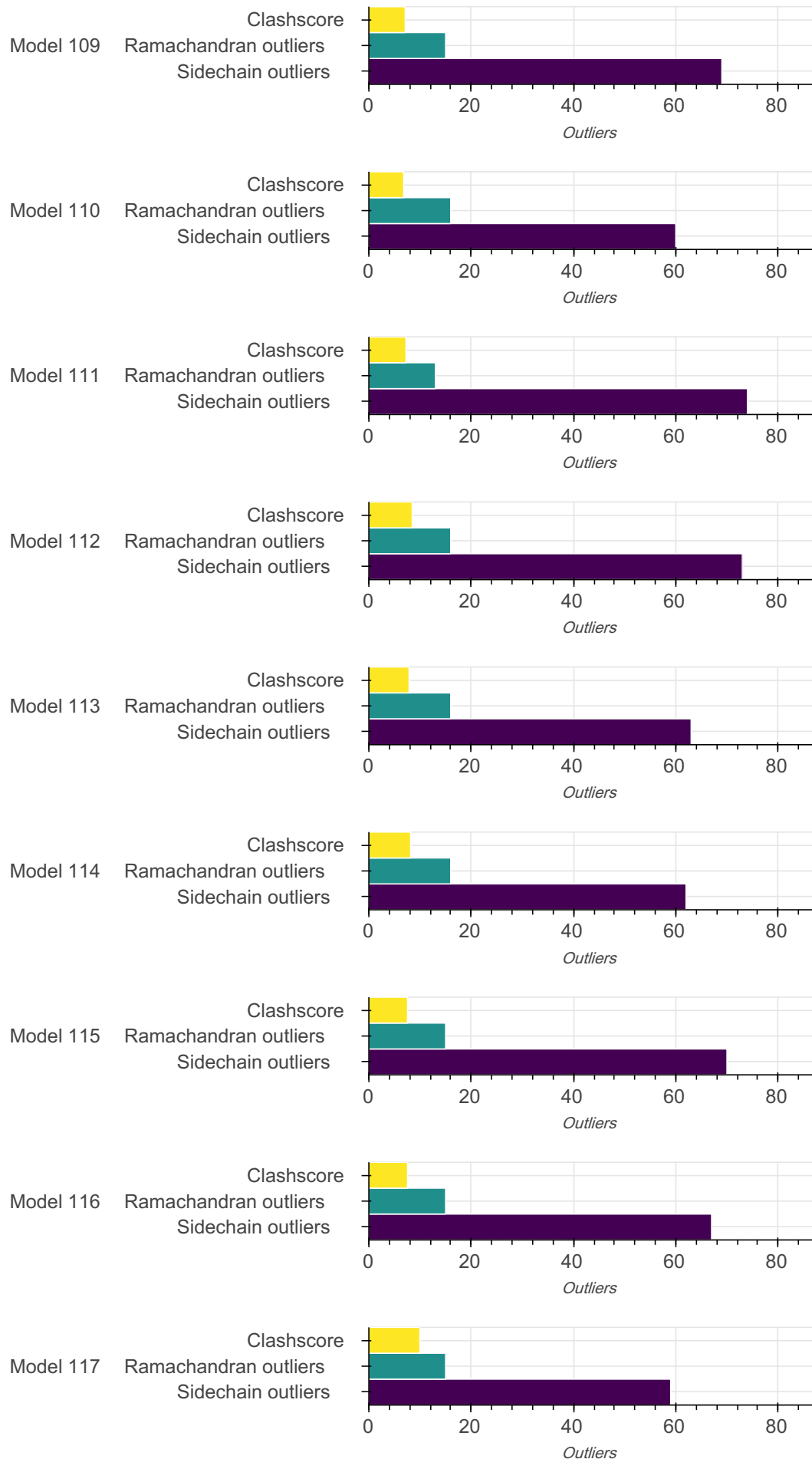


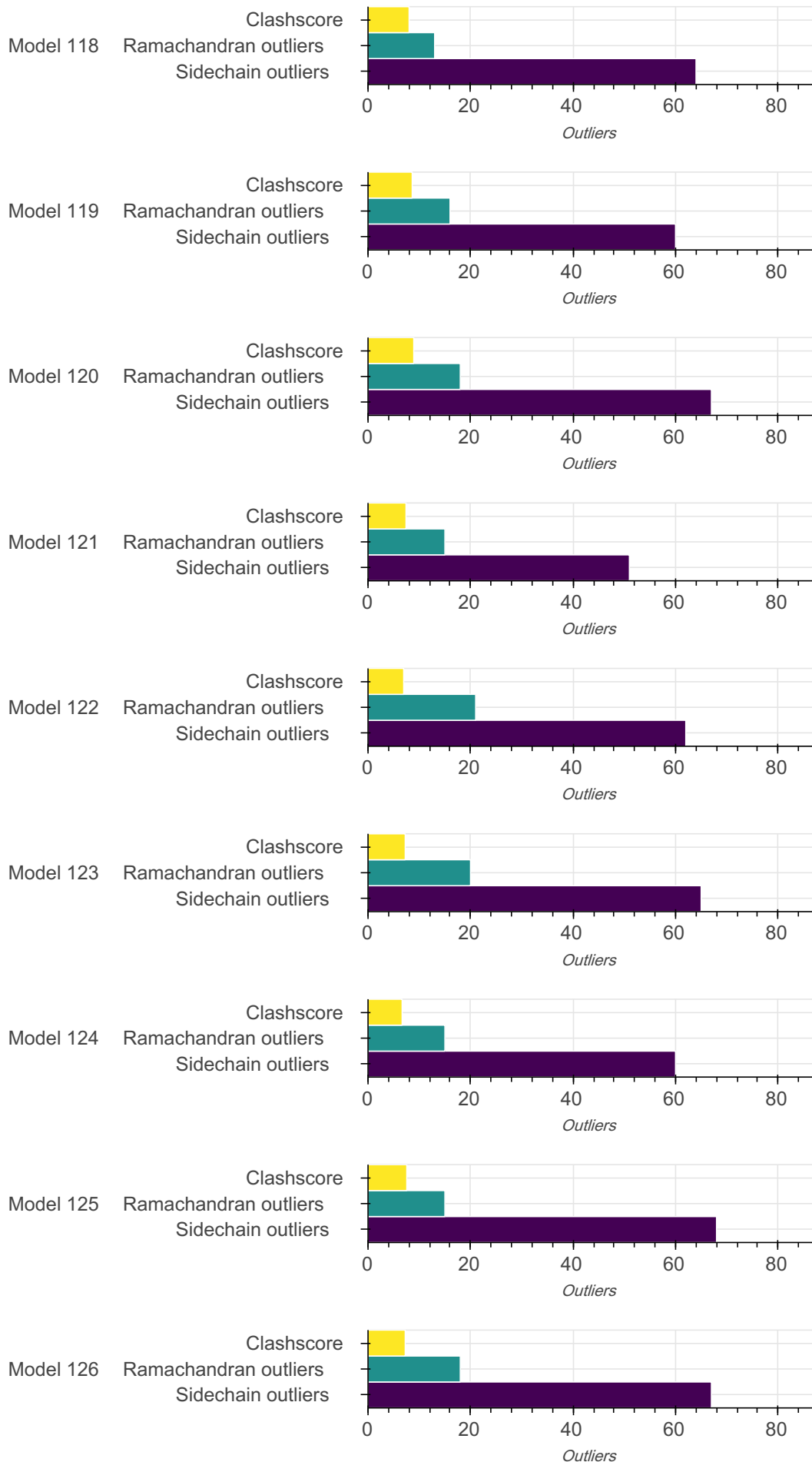


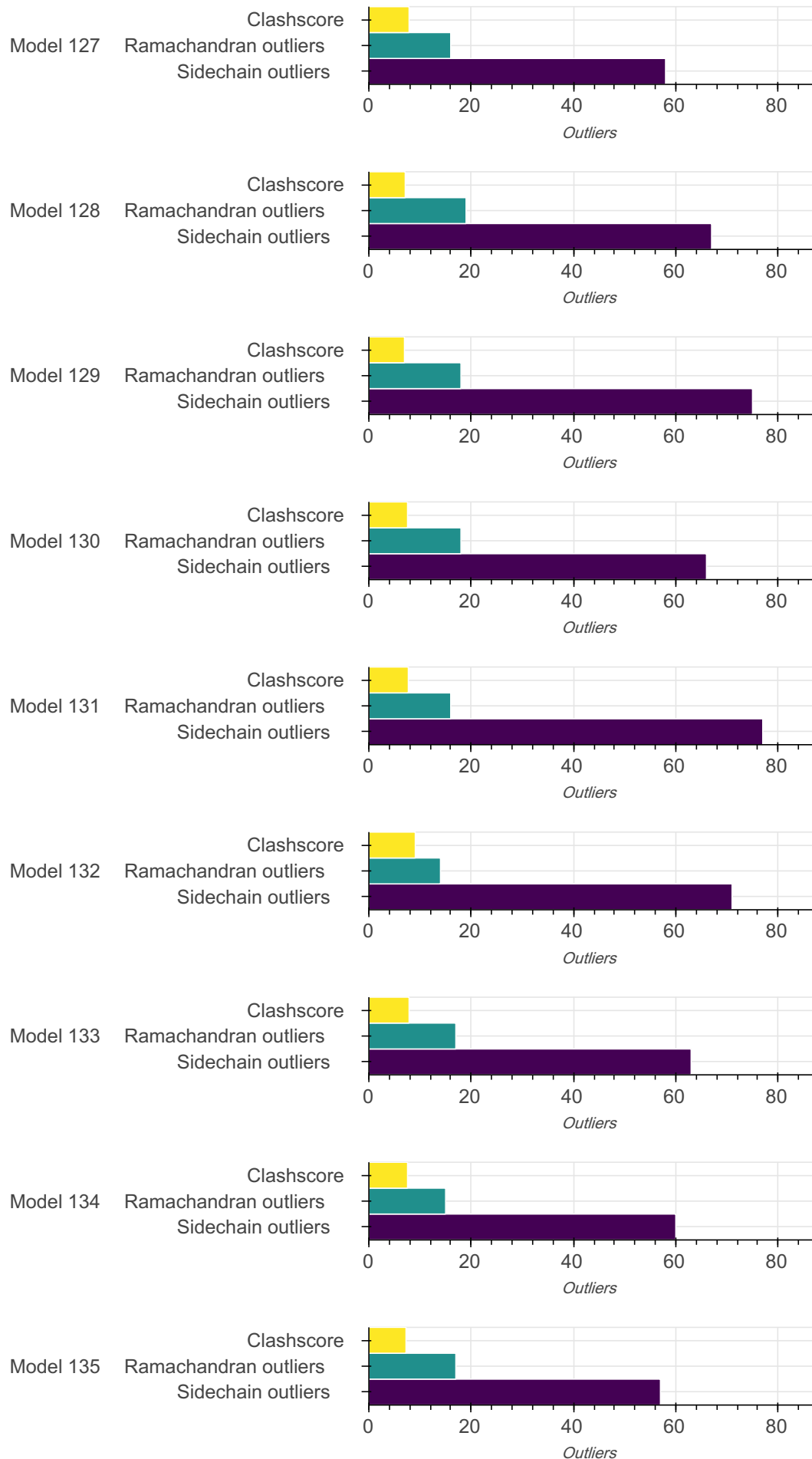


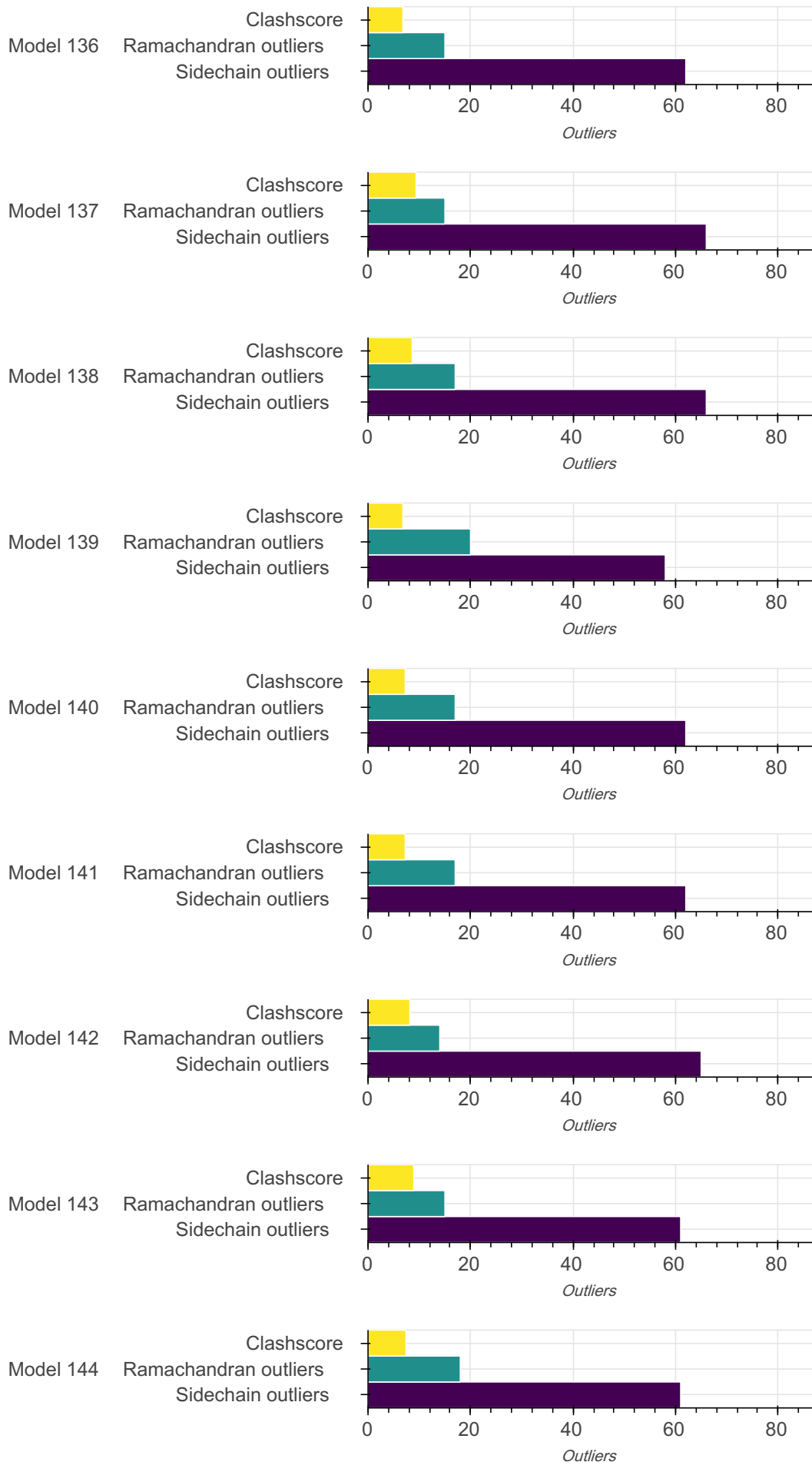


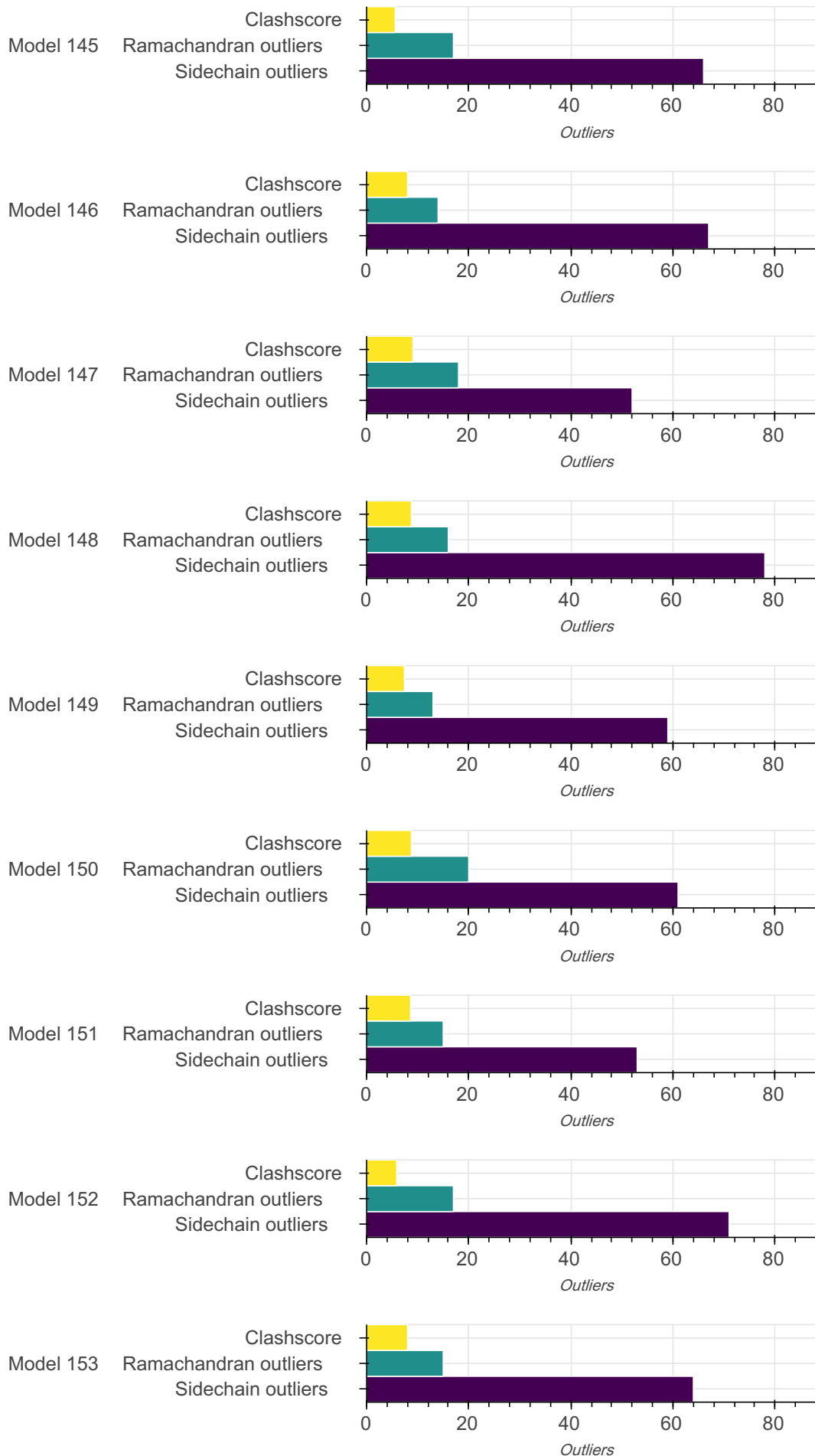


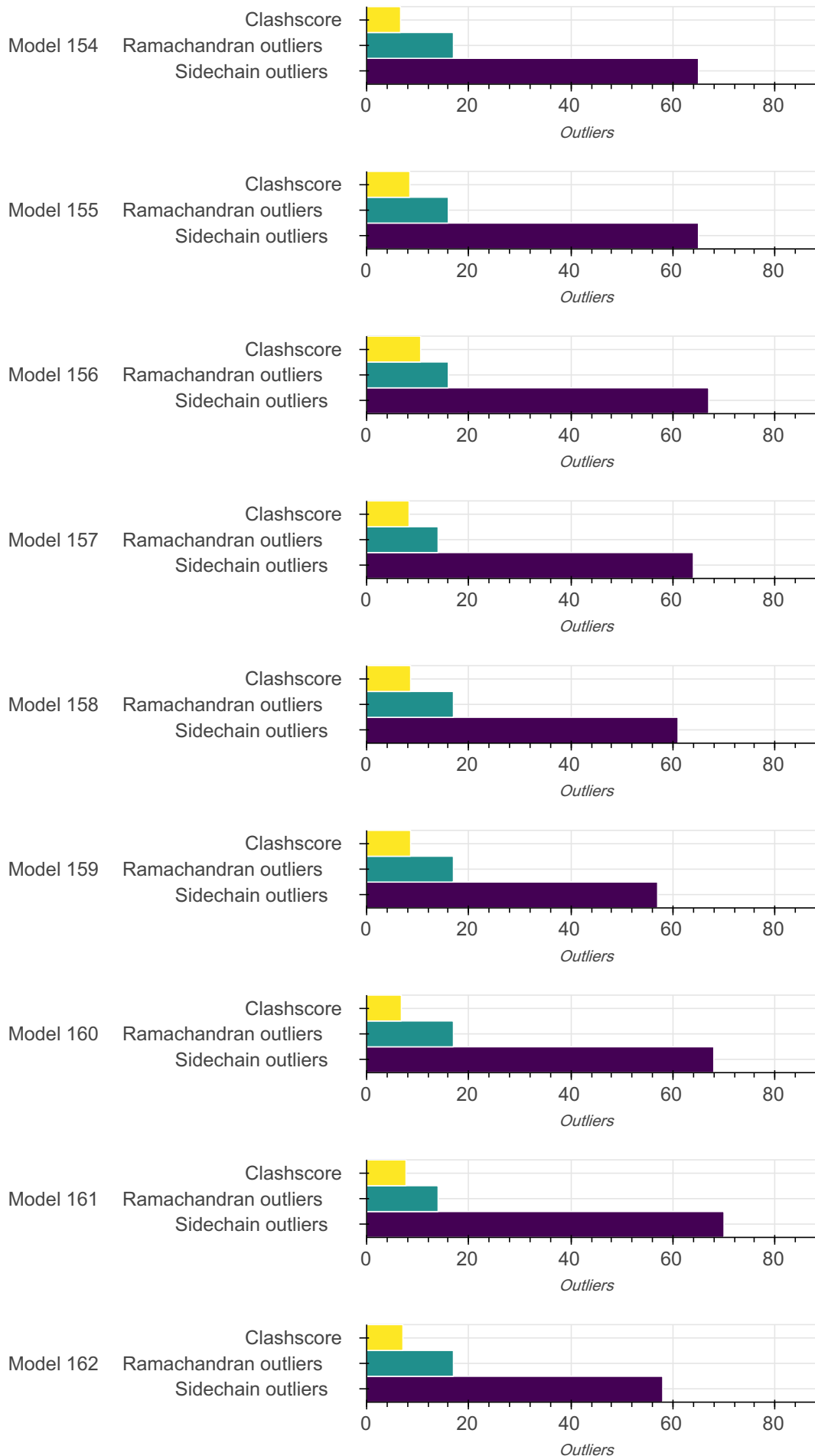


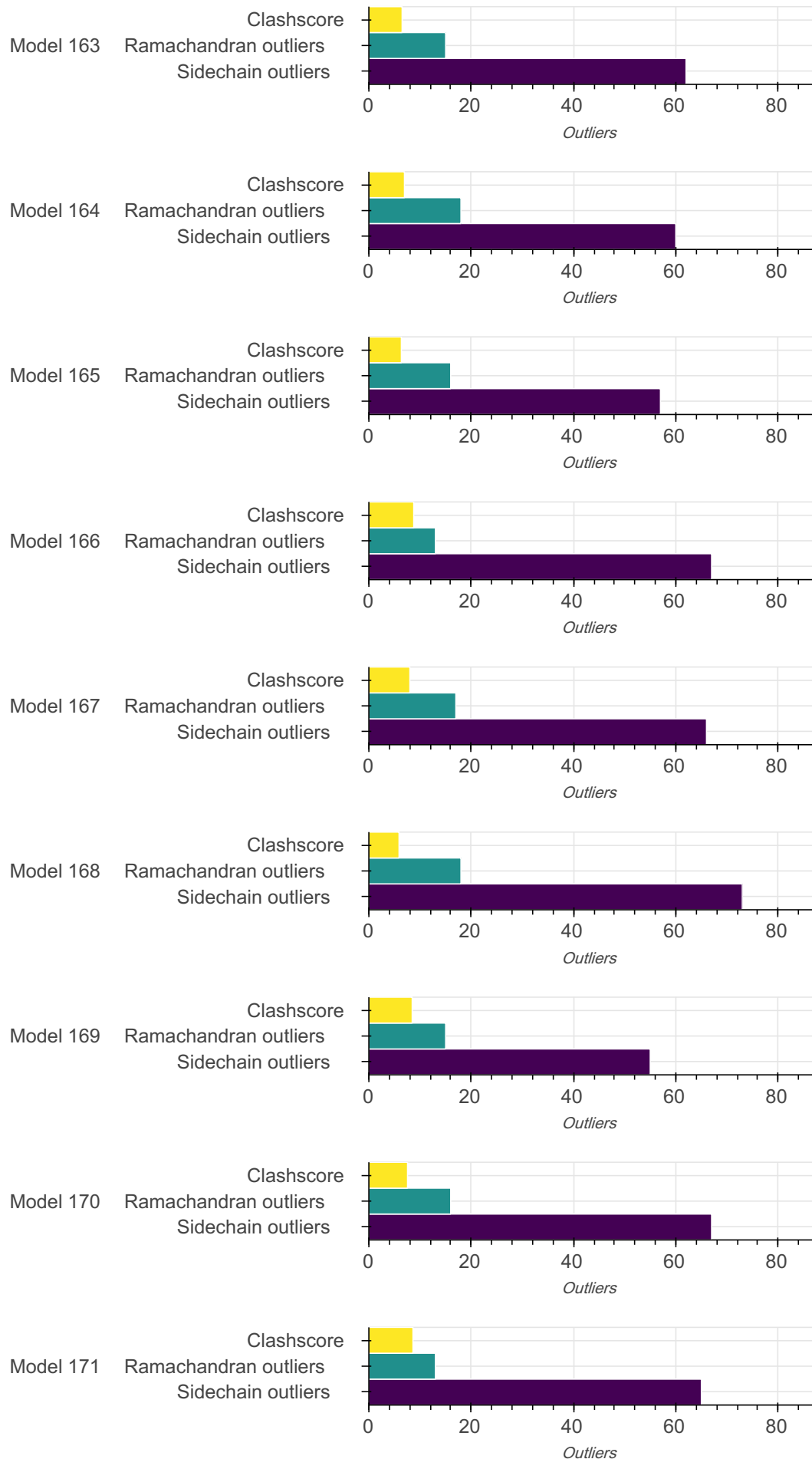


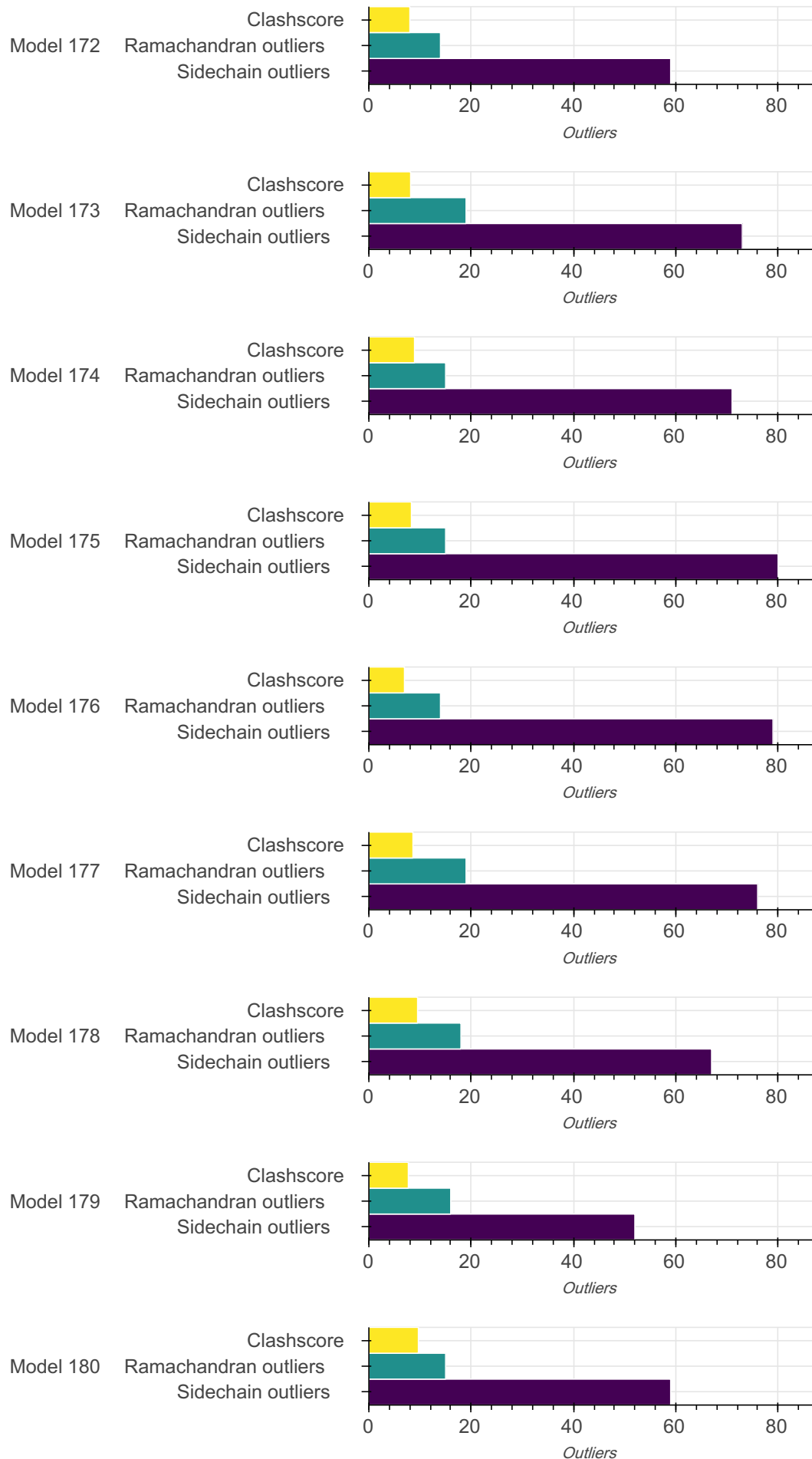


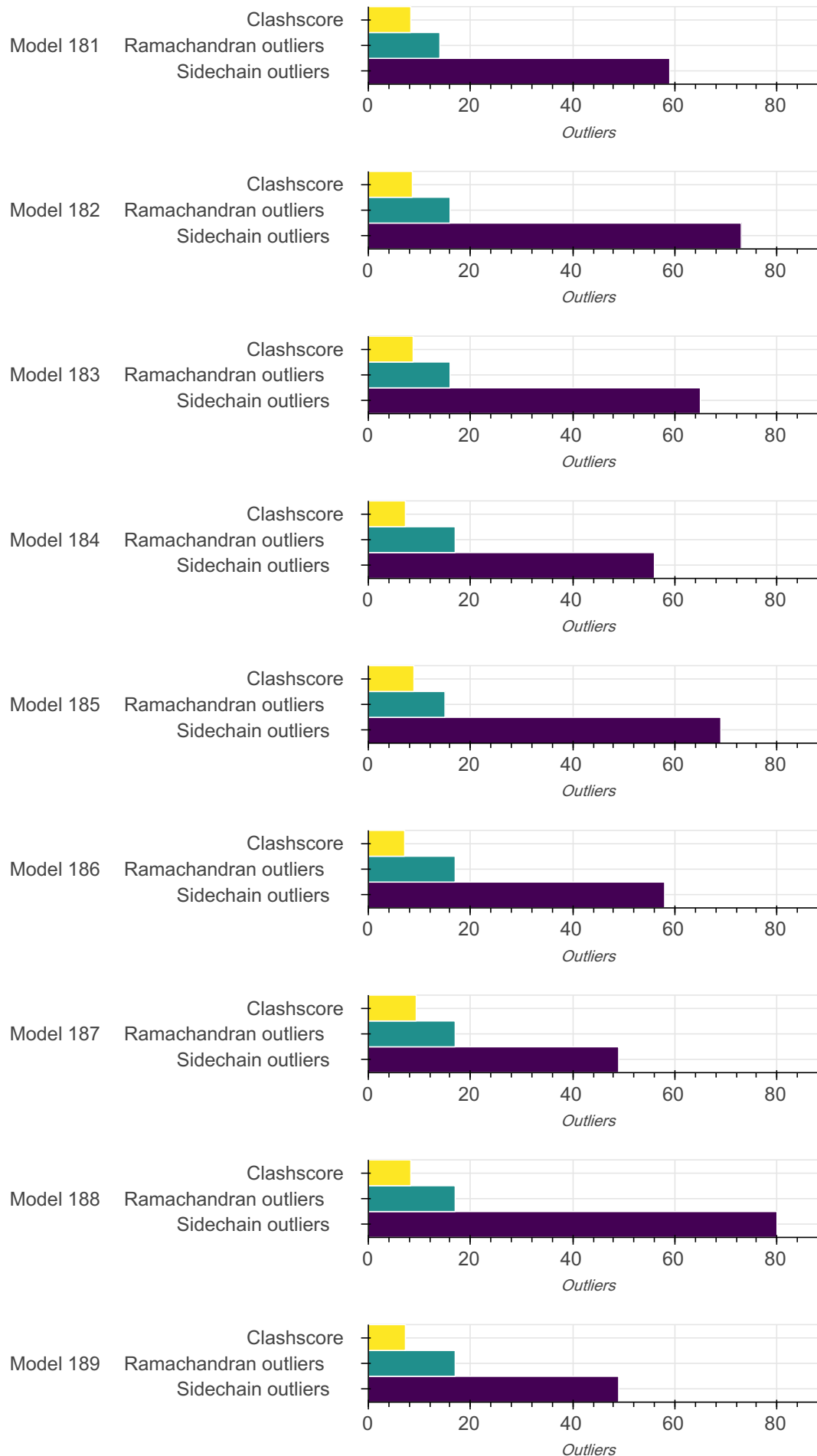


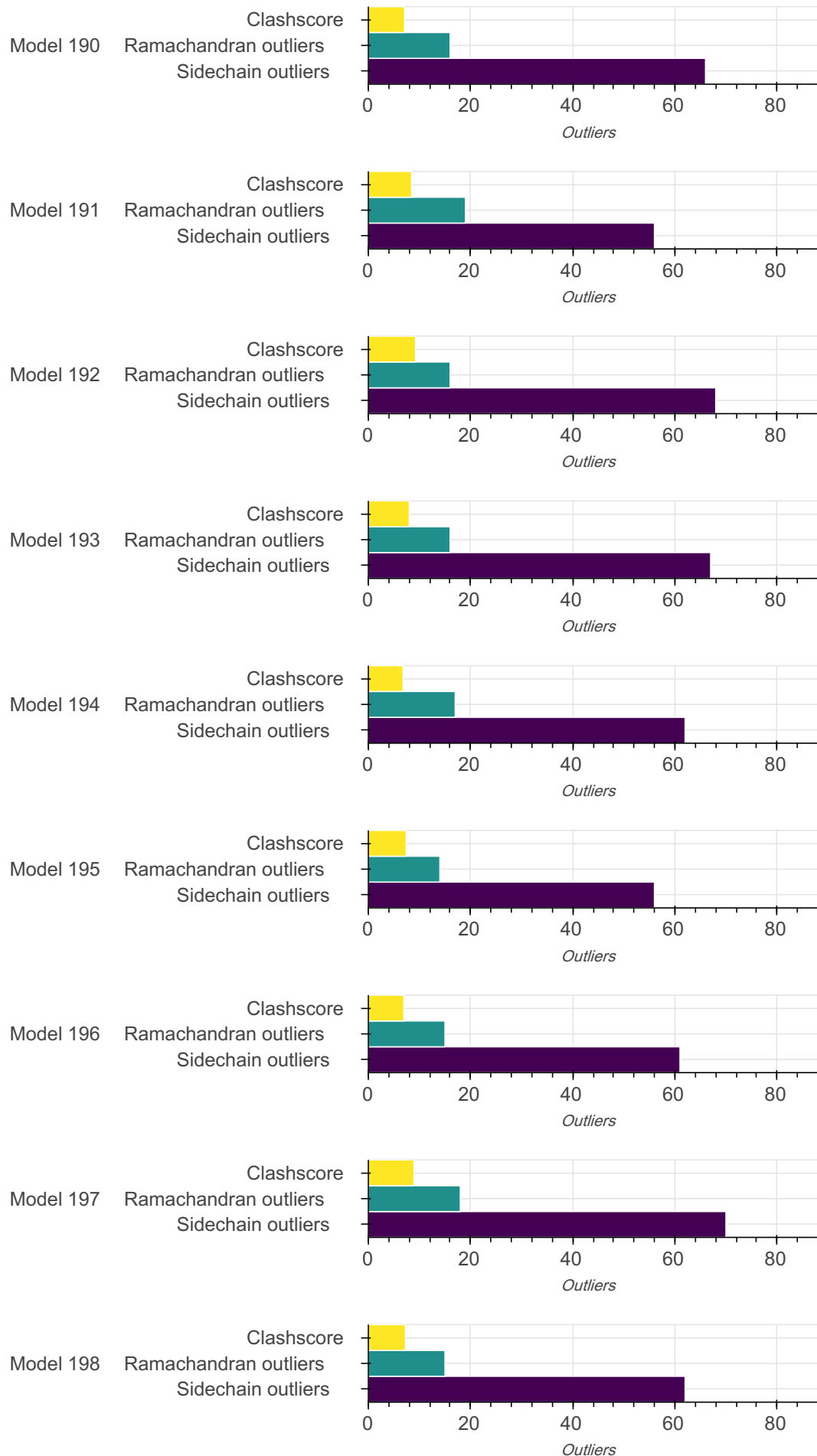


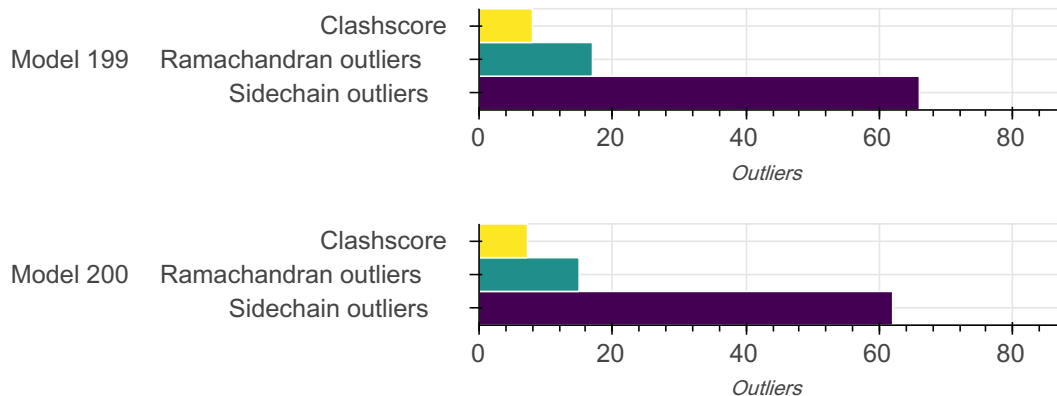












Ensemble information ?

This entry consists of 2 distinct ensemble(s).

Summary ?

This entry consists of 200 model(s). A total of 34 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-200	1	Postsynaptic density protein 95 (PSD95) PDZ3-SH3-GuK Module	A	417	-	1-417	100.00 / 100.00	Atomic

Datasets used for modeling ?

There are 34 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Other	Zenodo	10.5281/zenodo.7125978
2	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978

ID	Dataset type	Database name	Data access code
3	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
4	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
5	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
6	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
7	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
8	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
9	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
10	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
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12	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
13	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
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19	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
20	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
21	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
22	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
23	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
24	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
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28	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
29	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
30	Single molecule FRET data	Zenodo	10.5281/zenodo.7125978
31	Integrative model	Zenodo	10.5281/zenodo.7125978
32	Comparative model	Zenodo	10.5281/zenodo.7125978
33	Experimental model	Zenodo	10.5281/zenodo.7125978
34	Experimental model	Zenodo	10.5281/zenodo.7125978

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Unbiased DMD Simulations	DMD simulations	None	20871	True	False
2	1	FRET-guided screening of structures from molecular dynamics simulations	None	None	4439	True	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AvTraj	0.0.9	Model Building	github.com/Fluorescence-Tools/avtraj
2	pDMD	1.10	Molecular Dynamics Simulations	moleculesinaction.com/pdmd.html

Data quality ?

Single molecule FRET

Validation for this section is under development.

Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers ?

There are no bond length outliers.

Standard geometry: angle outliers ?

There are 6117 bond angle outliers in this entry (0.67% of 919000 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	274	HIS	CB-CG-CD2	7.68	121.22	131.20	88	200
A	243	ASP	CA-CB-CG	6.79	119.39	112.60	78	200
A	357	ARG	CD-NE-CZ	6.68	133.75	124.40	56	200
A	232	ILE	C-N-CA	6.62	133.62	121.70	74	200
A	279	ARG	CD-NE-CZ	5.95	132.73	124.40	70	200
A	274	HIS	CA-CB-CG	5.73	108.07	113.80	12	200
A	258	HIS	C-CA-CB	5.46	120.47	110.10	36	200

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	258	HIS	C-N-CA	5.42	131.46	121.70	78	200
A	258	HIS	CB-CG-CD2	5.39	124.20	131.20	31	200
A	232	ILE	C-CA-CB	5.23	122.05	111.60	126	200
A	395	HIS	CB-CG-CD2	5.22	124.41	131.20	104	200
A	2	ARG	NE-CZ-NH1	5.21	116.29	121.50	18	2
A	59	ASP	CA-CB-CG	5.13	117.73	112.60	178	6
A	177	ASP	CA-CB-CG	5.09	117.69	112.60	149	11
A	172	ASP	CA-CB-CG	5.07	117.67	112.60	164	9
A	50	ASP	CA-CB-CG	5.04	117.64	112.60	81	6
A	160	ASP	CA-CB-CG	5.00	117.60	112.60	159	6
A	258	HIS	CA-CB-CG	5.00	108.80	113.80	158	200
A	101	ARG	NE-CZ-NH1	4.99	116.51	121.50	187	4
A	298	ASN	C-N-CA	4.96	130.63	121.70	85	200
A	157	ASP	CA-CB-CG	4.92	117.52	112.60	116	10
A	56	ASN	CA-CB-CG	4.92	117.52	112.60	185	11
A	99	ASP	CA-CB-CG	4.91	117.51	112.60	61	5
A	131	ASP	CA-CB-CG	4.89	117.49	112.60	134	10
A	119	ASN	CA-CB-CG	4.86	117.46	112.60	79	13
A	25	ASP	CA-CB-CG	4.84	117.44	112.60	107	4
A	289	HIS	CB-CG-CD2	4.81	124.95	131.20	66	200
A	106	ASN	CA-CB-CG	4.79	117.39	112.60	177	8
A	62	ASN	CA-CB-CG	4.77	117.37	112.60	7	8
A	74	ASN	CA-CB-CG	4.76	117.36	112.60	36	10
A	133	ASP	CA-CB-CG	4.70	117.30	112.60	31	9
A	189	ARG	NE-CZ-NH1	4.70	116.80	121.50	132	5
A	211	ASP	CA-CB-CG	4.69	117.29	112.60	133	5
A	19	ASN	CA-CB-CG	4.65	117.25	112.60	22	5
A	186	ARG	NE-CZ-NH1	4.62	116.88	121.50	104	2
A	41	ASP	CA-CB-CG	4.60	117.20	112.60	29	7
A	357	ARG	NE-CZ-NH1	4.58	126.08	121.50	10	200
A	53	LEU	CD1-CG-CD2	4.57	100.75	110.80	143	22
A	109	LEU	CD1-CG-CD2	4.57	100.75	110.80	165	22
A	129	LEU	CD1-CG-CD2	4.56	100.76	110.80	176	28
A	141	LEU	CD1-CG-CD2	4.55	100.79	110.80	126	26
A	362	GLN	OE1-CD-NE2	4.54	118.06	122.60	74	200

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	104	LEU	CD1-CG-CD2	4.52	100.85	110.80	147	28
A	42	LEU	CD1-CG-CD2	4.52	100.85	110.80	107	22
A	409	ILE	CA-CB-CG1	4.52	118.08	110.40	11	3
A	122	ARG	NE-CZ-NH1	4.50	117.00	121.50	192	3
A	153	LEU	CD1-CG-CD2	4.50	100.90	110.80	147	19
A	92	ARG	NE-CZ-NH1	4.50	117.00	121.50	13	3
A	9	ILE	CA-CB-CG1	4.50	118.04	110.40	59	3
A	16	LEU	CD1-CG-CD2	4.49	100.92	110.80	146	20
A	151	ASP	CA-CB-CG	4.49	117.09	112.60	25	5
A	116	LEU	CD1-CG-CD2	4.48	100.94	110.80	86	27
A	100	LEU	CD1-CG-CD2	4.48	100.95	110.80	23	24
A	417	LEU	CA-C-O	4.47	128.40	120.80	78	1
A	5	ARG	NE-CZ-NH1	4.45	117.05	121.50	13	2
A	199	ASP	CA-CB-CG	4.45	117.05	112.60	128	3
A	47	ARG	NE-CZ-NH1	4.44	117.06	121.50	78	1
A	35	LEU	CD1-CG-CD2	4.43	101.05	110.80	6	20
A	74	ASN	OD1-CG-ND2	4.43	118.17	122.60	114	1
A	72	LEU	CD1-CG-CD2	4.43	101.06	110.80	70	24
A	145	LEU	CD1-CG-CD2	4.42	101.07	110.80	192	18
A	46	LEU	CD1-CG-CD2	4.41	101.10	110.80	195	17
A	152	VAL	CA-CB-CG1	4.40	117.88	110.40	198	7
A	61	ARG	NE-CZ-NH1	4.40	117.10	121.50	162	6
A	87	PRO	N-CA-CB	4.40	107.84	103.00	49	1
A	224	VAL	CA-CB-CG1	4.40	117.87	110.40	63	6
A	181	ILE	CA-CB-CG1	4.39	117.87	110.40	177	3
A	119	ASN	OD1-CG-ND2	4.39	118.21	122.60	173	1
A	52	ILE	CA-CB-CG1	4.38	117.85	110.40	10	1
A	286	ILE	CA-CB-CG1	4.38	117.84	110.40	78	200
A	417	LEU	CD1-CG-CD2	4.35	101.23	110.80	1	27
A	335	HIS	CB-CG-CD2	4.33	125.56	131.20	21	200
A	195	LEU	CD1-CG-CD2	4.33	101.26	110.80	13	22
A	214	LEU	CD1-CG-CD2	4.33	101.28	110.80	144	26
A	67	GLN	OE1-CD-NE2	4.32	118.28	122.60	19	2
A	8	VAL	CA-CB-CG1	4.32	117.74	110.40	68	2
A	19	ASN	OD1-CG-ND2	4.31	118.29	122.60	106	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	164	TRP	CG-CD1-NE1	4.30	104.61	110.20	136	1
A	126	ILE	CA-CB-CG1	4.30	117.71	110.40	73	3
A	81	ILE	CA-CB-CG1	4.30	117.71	110.40	75	3
A	176	ASP	CA-CB-CG	4.29	116.89	112.60	155	5
A	200	TRP	CA-C-O	4.29	113.51	120.80	37	1
A	185	ARG	NE-CZ-NH2	4.29	123.06	119.20	131	1
A	103	GLN	OE1-CD-NE2	4.29	118.31	122.60	123	1
A	6	ARG	NE-CZ-NH1	4.28	117.22	121.50	98	2
A	381	PHE	CA-CB-CG	4.28	118.08	113.80	177	200
A	56	ASN	OD1-CG-ND2	4.28	118.32	122.60	185	3
A	58	VAL	CA-CB-CG1	4.26	117.63	110.40	76	1
A	60	LEU	CD1-CG-CD2	4.25	101.44	110.80	21	24
A	241	ASN	OD1-CG-ND2	4.25	118.35	122.60	13	200
A	194	ARG	NE-CZ-NH1	4.24	117.26	121.50	91	1
A	209	ARG	NE-CZ-NH1	4.24	117.26	121.50	137	1
A	167	ARG	NE-CZ-NH1	4.23	117.27	121.50	74	1
A	25	ASP	CA-C-O	4.22	113.62	120.80	83	1
A	156	ILE	CA-CB-CG1	4.22	117.57	110.40	170	1
A	51	GLN	OE1-CD-NE2	4.22	118.38	122.60	103	2
A	4	PRO	N-CA-CB	4.22	107.64	103.00	131	1
A	108	SER	CA-C-O	4.22	113.63	120.80	160	1
A	96	LYS	CA-C-O	4.20	113.65	120.80	94	1
A	34	ILE	CA-CB-CG1	4.20	117.55	110.40	79	2

Too-close contacts ?

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all atomic models in this entry.

Model ID	Clash score	Number of clashes
1	6.35	42
2	8.62	57
3	9.22	61
4	7.26	48
5	7.11	47
6	10.43	69
7	8.32	55

Model ID	Clash score	Number of clashes
8	7.41	49
9	6.80	45
10	11.04	73
11	10.58	70
12	9.83	65
13	8.47	56
14	8.47	56
15	10.28	68
16	6.80	45
17	7.56	50
18	7.26	48
19	7.41	49
20	8.62	57
21	9.37	62
22	9.22	61
23	8.47	56
24	8.16	54
25	8.16	54
26	7.86	52
27	9.22	61
28	8.62	57
29	6.65	44
30	7.56	50
31	6.95	46
32	8.92	59
33	6.65	44
34	7.11	47
35	8.16	54
36	10.28	68
37	8.01	53
38	8.01	53
39	7.86	52
40	8.32	55
41	8.01	53
42	8.01	53

Model ID	Clash score	Number of clashes
43	7.26	48
44	9.68	64
45	5.75	38
46	8.32	55
47	9.68	64
48	8.32	55
49	6.95	46
50	8.01	53
51	7.11	47
52	8.47	56
53	7.86	52
54	5.59	37
55	8.62	57
56	10.13	67
57	7.26	48
58	7.41	49
59	8.92	59
60	8.01	53
61	10.13	67
62	10.73	71
63	6.95	46
64	8.47	56
65	7.71	51
66	6.35	42
67	9.37	62
68	6.65	44
69	8.77	58
70	7.71	51
71	8.01	53
72	8.62	57
73	8.62	57
74	8.32	55
75	8.77	58
76	8.01	53
77	6.80	45

Model ID	Clash score	Number of clashes
78	8.47	56
79	8.01	53
80	8.01	53
81	6.50	43
82	7.86	52
83	6.80	45
84	9.98	66
85	8.01	53
86	9.98	66
87	5.44	36
88	8.01	53
89	6.50	43
90	8.32	55
91	9.68	64
92	7.11	47
93	8.77	58
94	7.26	48
95	9.83	65
96	9.22	61
97	8.92	59
98	8.62	57
99	8.16	54
100	11.19	74
101	6.95	46
102	4.23	28
103	7.41	49
104	5.90	39
105	7.71	51
106	9.07	60
107	6.05	40
108	7.86	52
109	7.11	47
110	6.80	45
111	7.26	48
112	8.47	56

Model ID	Clash score	Number of clashes
113	7.86	52
114	8.16	54
115	7.56	50
116	7.56	50
117	9.98	66
118	8.01	53
119	8.62	57
120	8.92	59
121	7.41	49
122	6.95	46
123	7.26	48
124	6.65	44
125	7.56	50
126	7.26	48
127	7.86	52
128	7.11	47
129	6.95	46
130	7.56	50
131	7.71	51
132	9.07	60
133	7.86	52
134	7.56	50
135	7.26	48
136	6.80	45
137	9.37	62
138	8.62	57
139	6.80	45
140	7.26	48
141	7.26	48
142	8.16	54
143	8.92	59
144	7.41	49
145	5.59	37
146	8.01	53
147	9.07	60

Model ID	Clash score	Number of clashes
148	8.77	58
149	7.41	49
150	8.77	58
151	8.62	57
152	5.90	39
153	8.01	53
154	6.65	44
155	8.47	56
156	10.58	70
157	8.32	55
158	8.62	57
159	8.62	57
160	6.80	45
161	7.71	51
162	7.11	47
163	6.50	43
164	6.95	46
165	6.35	42
166	8.77	58
167	8.01	53
168	5.90	39
169	8.47	56
170	7.56	50
171	8.62	57
172	8.01	53
173	8.16	54
174	8.92	59
175	8.32	55
176	6.95	46
177	8.62	57
178	9.53	63
179	7.71	51
180	9.68	64
181	8.32	55
182	8.62	57

Model ID	Clash score	Number of clashes
183	8.77	58
184	7.26	48
185	8.92	59
186	7.11	47
187	9.37	62
188	8.32	55
189	7.26	48
190	7.11	47
191	8.47	56
192	9.22	61
193	8.01	53
194	6.80	45
195	7.41	49
196	6.95	46
197	8.92	59
198	7.26	48
199	8.01	53
200	7.26	48

There are 10589 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:40:ALA:HB1	A:46:LEU:HB3	1.18	75	5
A:219:VAL:HB	A:410:TRP:HB3	1.18	194	96
A:23:GLY:HA3	A:27:GLU:HB3	1.17	62	21
A:156:ILE:HB	A:165:GLN:HB3	1.16	13	12
A:23:GLY:HA3	A:27:GLU:HB2	1.14	192	30
A:2:ARG:HB2	A:85:TYR:HB2	1.14	136	5
A:24:GLU:HB3	A:27:GLU:HB3	1.14	173	3
A:145:LEU:HB2	A:179:GLY:HA3	1.13	199	45
A:17:GLY:HA2	A:35:LEU:HD12	1.13	39	8
A:2:ARG:HB3	A:85:TYR:HB3	1.09	19	11
A:169:VAL:HG22	A:174:GLU:HG2	1.07	12	24
A:121:LYS:HB2	A:158:ALA:HB3	1.06	175	10
A:134:LYS:HD2	A:141:LEU:HA	1.06	52	1
A:53:LEU:HD11	A:84:GLN:HG3	1.05	11	5

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:134:LYS:HB3	A:146:SER:HB2	1.05	162	2
A:22:GLY:HA3	A:65:HIS:HB2	1.05	18	3
A:55:VAL:HG22	A:81:ILE:HG12	1.05	24	28
A:133:ASP:HB3	A:136:LYS:HB3	1.04	103	4
A:17:GLY:HA3	A:38:GLY:HA3	1.04	167	10
A:219:VAL:HB	A:410:TRP:HB2	1.04	19	5
A:145:LEU:HB3	A:181:ILE:HG23	1.04	138	18
A:19:ASN:HB3	A:33:PHE:HB3	1.03	57	10
A:186:ARG:HD2	A:189:ARG:HD3	1.03	104	2
A:60:LEU:HB3	A:63:ALA:HB2	1.03	120	5
A:7:ILE:HD11	A:45:GLU:HB2	1.03	169	2
A:128:ALA:HA	A:216:TYR:HB3	1.02	191	2
A:2:ARG:HB2	A:85:TYR:HB3	1.02	84	19
A:33:PHE:HZ	A:157:ASP:HA	1.02	93	1
A:16:LEU:HD21	A:79:VAL:HG21	1.02	43	30
A:29:ILE:HD13	A:68:ALA:HB2	1.02	15	21
A:172:ASP:HA	A:410:TRP:HZ3	1.02	177	4
A:87:PRO:HB2	A:90:TYR:HB2	1.01	34	5
A:58:VAL:HB	A:71:ALA:HB2	1.01	100	1
A:24:GLU:HB3	A:27:GLU:HB2	1.01	81	5
A:219:VAL:HG12	A:412:PRO:HD3	1.00	104	38
A:140:PHE:HD1	A:141:LEU:HG	1.00	149	1
A:134:LYS:HG3	A:140:PHE:HB2	1.00	20	1
A:16:LEU:HD11	A:79:VAL:HG21	1.00	155	21
A:30:PHE:HB3	A:51:GLN:HG2	1.00	103	5
A:134:LYS:HB3	A:137:ASP:HB2	1.00	149	1
A:1:PRO:HD2	A:86:LYS:HA	0.99	4	3
A:153:LEU:HB3	A:166:ALA:HB1	0.99	96	3
A:135:THR:HB	A:140:PHE:HB2	0.99	152	2
A:16:LEU:HD22	A:141:LEU:HD13	0.99	27	1
A:132:TYR:HE1	A:134:LYS:HG2	0.99	42	1
A:220:THR:HG21	A:414:ARG:HB3	0.99	135	7
A:97:ILE:HD11	A:417:LEU:HD12	0.99	130	1
A:30:PHE:HZ	A:86:LYS:HD3	0.98	120	1
A:128:ALA:HA	A:216:TYR:HD1	0.98	56	16

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:67:GLN:HA	A:70:ILE:HD12	0.98	147	14
A:166:ALA:HB2	A:181:ILE:HD13	0.98	133	20
A:21:VAL:HG22	A:100:LEU:HB2	0.98	87	1
A:1:PRO:HG3	A:91:SER:HB3	0.98	91	1
A:196:LYS:HD2	A:200:TRP:HB2	0.98	112	1
A:30:PHE:HB3	A:51:GLN:HG3	0.98	174	7
A:163:TRP:HB3	A:180:PHE:HB3	0.98	8	16
A:97:ILE:HG13	A:101:ARG:HG3	0.98	16	1
A:166:ALA:HB2	A:181:ILE:HB	0.98	178	31
A:214:LEU:HD13	A:378:THR:HG21	0.97	26	1
A:129:LEU:HG	A:149:PHE:CE1	0.97	199	7
A:136:LYS:HA	A:140:PHE:HB2	0.97	143	1
A:406:GLY:HA2	A:409:ILE:HG12	0.97	114	12
A:97:ILE:HG12	A:101:ARG:HD3	0.97	98	1
A:155:VAL:HG11	A:417:LEU:HD21	0.97	180	1
A:122:ARG:HB2	A:157:ASP:HB3	0.97	156	2
A:126:ILE:HD11	A:417:LEU:HD13	0.97	118	5
A:102:GLU:HA	A:105:MET:HB2	0.97	30	1
A:200:TRP:HB3	A:203:SER:HB3	0.97	66	1
A:21:VAL:HB	A:32:SER:HB2	0.96	65	16
A:54:SER:HB3	A:82:ILE:HB	0.96	129	11
A:51:GLN:HB2	A:86:LYS:HB2	0.96	116	2
A:54:SER:HB3	A:82:ILE:HG13	0.96	200	15
A:16:LEU:HD21	A:79:VAL:HG11	0.96	181	6
A:32:SER:HA	A:90:TYR:HE1	0.96	25	6
A:1:PRO:HG2	A:97:ILE:HB	0.96	96	1
A:7:ILE:HG21	A:46:LEU:HB2	0.96	148	2
A:121:LYS:HB2	A:157:ASP:HB3	0.96	21	2
A:127:ARG:HG3	A:152:VAL:HG13	0.95	26	2
A:34:ILE:HD11	A:48:LYS:HG2	0.95	129	3
A:16:LEU:HG	A:18:PHE:CZ	0.95	75	2
A:188:GLU:HG3	A:213:VAL:HG13	0.95	18	2
A:9:ILE:HG22	A:79:VAL:HB	0.95	118	3
A:55:VAL:HB	A:60:LEU:HD12	0.95	128	2
A:31:ILE:HD13	A:34:ILE:HD11	0.95	188	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:413:ALA:HB3	A:416:ARG:HB2	0.95	153	2
A:152:VAL:HB	A:169:VAL:HB	0.95	91	81
A:171:SER:HB2	A:403:ASP:HB3	0.95	187	2
A:24:GLU:HG2	A:27:GLU:HB2	0.95	188	1
A:188:GLU:HA	A:213:VAL:HG21	0.95	60	14
A:135:THR:HB	A:139:GLY:HA2	0.95	59	2
A:166:ALA:HB2	A:181:ILE:HG12	0.94	139	17
A:120:PRO:HD3	A:417:LEU:HG	0.94	60	1
A:224:VAL:HB	A:226:TYR:CE2	0.94	192	11
A:64:SER:HB3	A:67:GLN:HB2	0.94	27	1
A:50:ASP:HB3	A:83:ALA:HB1	0.94	122	12
A:126:ILE:HG12	A:218:THR:HG22	0.94	192	10
A:48:LYS:HG2	A:98:HIS:HB2	0.93	31	1
A:49:GLY:HA2	A:97:ILE:HG21	0.93	147	1
A:53:LEU:HD11	A:84:GLN:HB2	0.93	7	17
A:134:LYS:HD3	A:144:ALA:HB3	0.93	47	5

Torsion angles: Protein backbone ?

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	415	366	34	15
2	415	361	37	17
3	415	362	37	16
4	415	360	41	14
5	415	364	36	15
6	415	362	38	15
7	415	357	43	15
8	415	355	44	16
9	415	363	33	19
10	415	356	41	18
11	415	348	46	21
12	415	352	43	20
13	415	356	46	13
14	415	358	43	14
15	415	356	42	17

Model ID	Analysed	Favored	Allowed	Outliers
16	415	355	44	16
17	415	361	40	14
18	415	351	41	23
19	415	357	39	19
20	415	364	33	18
21	415	363	37	15
22	415	356	41	18
23	415	361	33	21
24	415	354	44	17
25	415	361	39	15
26	415	355	46	14
27	415	365	38	12
28	415	365	33	17
29	415	354	43	18
30	415	357	44	14
31	415	351	48	16
32	415	347	51	17
33	415	366	35	14
34	415	346	51	18
35	415	356	44	15
36	415	354	41	20
37	415	357	41	17
38	415	355	44	16
39	415	354	45	16
40	415	360	42	13
41	415	351	46	18
42	415	355	44	16
43	415	354	44	17
44	415	362	36	17
45	415	363	35	17
46	415	348	46	21
47	415	358	39	18
48	415	352	47	16
49	415	360	37	18
50	415	355	42	18

Model ID	Analysed	Favored	Allowed	Outliers
51	415	355	40	20
52	415	351	44	20
53	415	369	29	17
54	415	359	39	17
55	415	359	41	15
56	415	353	42	20
57	415	358	37	20
58	415	360	41	14
59	415	361	39	15
60	415	361	36	18
61	415	361	38	16
62	415	354	43	18
63	415	355	45	15
64	415	365	35	15
65	415	361	39	15
66	415	354	44	17
67	415	359	38	18
68	415	357	40	18
69	415	351	45	19
70	415	362	35	18
71	415	353	49	13
72	415	360	39	16
73	415	355	39	21
74	415	358	42	15
75	415	362	40	13
76	415	360	41	14
77	415	362	37	16
78	415	361	38	16
79	415	346	50	19
80	415	359	39	17
81	415	360	40	15
82	415	365	37	13
83	415	359	39	17
84	415	354	41	20
85	415	353	44	18

Model ID	Analysed	Favored	Allowed	Outliers
86	415	356	44	15
87	415	360	40	15
88	415	354	42	19
89	415	365	37	13
90	415	358	40	17
91	415	360	38	17
92	415	362	37	16
93	415	365	32	18
94	415	360	37	18
95	415	356	40	19
96	415	361	38	16
97	415	356	44	15
98	415	364	34	17
99	415	360	37	18
100	415	357	44	14
101	415	355	40	20
102	415	362	42	11
103	415	356	46	13
104	415	361	38	16
105	415	359	41	15
106	415	360	37	18
107	415	368	32	15
108	415	361	33	21
109	415	362	38	15
110	415	353	46	16
111	415	366	36	13
112	415	356	43	16
113	415	355	44	16
114	415	356	43	16
115	415	360	40	15
116	415	353	47	15
117	415	364	36	15
118	415	364	38	13
119	415	362	37	16
120	415	361	36	18

Model ID	Analysed	Favored	Allowed	Outliers
121	415	366	34	15
122	415	356	38	21
123	415	351	44	20
124	415	367	33	15
125	415	363	37	15
126	415	356	41	18
127	415	354	45	16
128	415	352	44	19
129	415	357	40	18
130	415	353	44	18
131	415	358	41	16
132	415	364	37	14
133	415	365	33	17
134	415	360	40	15
135	415	349	49	17
136	415	360	40	15
137	415	356	44	15
138	415	358	40	17
139	415	360	35	20
140	415	355	43	17
141	415	356	42	17
142	415	360	41	14
143	415	350	50	15
144	415	356	41	18
145	415	356	42	17
146	415	369	32	14
147	415	356	41	18
148	415	349	50	16
149	415	357	45	13
150	415	353	42	20
151	415	359	41	15
152	415	356	42	17
153	415	359	41	15
154	415	359	39	17
155	415	354	45	16

Model ID	Analysed	Favored	Allowed	Outliers
156	415	355	44	16
157	415	355	46	14
158	415	365	33	17
159	415	365	33	17
160	415	364	34	17
161	415	352	49	14
162	415	353	45	17
163	415	360	40	15
164	415	363	34	18
165	415	365	34	16
166	415	372	30	13
167	415	361	37	17
168	415	362	35	18
169	415	364	36	15
170	415	363	36	16
171	415	358	44	13
172	415	366	35	14
173	415	358	38	19
174	415	359	41	15
175	415	358	42	15
176	415	350	51	14
177	415	357	39	19
178	415	361	36	18
179	415	355	44	16
180	415	359	41	15
181	415	363	38	14
182	415	358	41	16
183	415	365	34	16
184	415	358	40	17
185	415	356	44	15
186	415	357	41	17
187	415	351	47	17
188	415	356	42	17
189	415	352	46	17
190	415	367	32	16

Model ID	Analysed	Favored	Allowed	Outliers
191	415	360	36	19
192	415	363	36	16
193	415	360	39	16
194	415	359	39	17
195	415	365	36	14
196	415	345	55	15
197	415	357	40	18
198	415	358	42	15
199	415	359	39	17
200	415	358	42	15

There are 128 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	232	ILE	200
A	233	LEU	200
A	258	HIS	200
A	259	THR	200
A	356	LYS	200
A	412	PRO	200
A	161	GLU	169
A	135	THR	162
A	106	ASN	158
A	94	GLU	157
A	157	ASP	152
A	176	ASP	152
A	92	ARG	146
A	207	GLN	142
A	109	LEU	130
A	89	GLU	76
A	171	SER	66
A	87	PRO	25
A	110	GLY	25
A	120	PRO	23
A	407	PRO	23
A	26	GLY	22

Chain	Res	Type	Models (Total)
A	12	GLY	20
A	56	ASN	18
A	76	GLY	18
A	183	SER	18
A	123	GLY	13
A	139	GLY	13
A	149	PHE	13
A	201	GLY	12
A	36	ALA	11
A	208	GLY	11
A	4	PRO	10
A	23	GLY	10
A	15	GLY	9
A	48	LYS	9
A	88	GLU	9
A	112	GLY	9
A	205	GLY	9
A	206	SER	9
A	2	ARG	7
A	25	ASP	7
A	134	LYS	7
A	143	GLN	7
A	186	ARG	7
A	11	ARG	6
A	191	GLU	6
A	209	ARG	6
A	215	SER	6
A	28	GLY	5
A	75	ALA	5
A	138	CYS	5
A	182	PRO	5
A	22	GLY	4
A	77	GLN	4
A	91	SER	4
A	95	ALA	4

Chain	Res	Type	Models (Total)
A	97	ILE	4
A	108	SER	4
A	202	SER	4
A	204	SER	4
A	13	SER	3
A	27	GLU	3
A	85	TYR	3
A	107	SER	3
A	116	LEU	3
A	121	LYS	3
A	122	ARG	3
A	140	PHE	3
A	177	ASP	3
A	203	SER	3
A	210	GLU	3
A	211	ASP	3
A	410	TRP	3
A	416	ARG	3
A	24	GLU	2
A	31	ILE	2
A	32	SER	2
A	37	GLY	2
A	39	PRO	2
A	43	SER	2
A	45	GLU	2
A	46	LEU	2
A	61	ARG	2
A	64	SER	2
A	84	GLN	2
A	93	PHE	2
A	115	SER	2
A	118	SER	2
A	128	ALA	2
A	131	ASP	2
A	136	LYS	2

Chain	Res	Type	Models (Total)
A	137	ASP	2
A	141	LEU	2
A	142	SER	2
A	158	ALA	2
A	165	GLN	2
A	173	SER	2
A	178	ILE	2
A	195	LEU	2

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	357	241	53	63
2	357	238	54	65
3	357	243	57	57
4	357	243	55	59
5	357	239	59	59
6	357	240	54	63
7	357	239	55	63
8	357	237	60	60
9	357	233	54	70
10	357	236	53	68
11	357	231	64	62
12	357	236	57	64
13	357	247	43	67
14	357	240	55	62
15	357	239	54	64
16	357	242	54	61
17	357	232	65	60
18	357	243	52	62
19	357	247	50	60
20	357	237	54	66
21	357	245	53	59
22	357	224	66	67
23	357	235	59	63

Model ID	Analysed	Favored	Allowed	Outliers
24	357	237	56	64
25	357	231	57	69
26	357	240	53	64
27	357	245	53	59
28	357	228	60	69
29	357	247	55	55
30	357	243	55	59
31	357	245	55	57
32	357	240	53	64
33	357	235	49	73
34	357	238	54	65
35	357	237	54	66
36	357	236	59	62
37	357	234	61	62
38	357	240	53	64
39	357	243	57	57
40	357	233	50	74
41	357	243	49	65
42	357	237	60	60
43	357	232	59	66
44	357	235	49	73
45	357	225	65	67
46	357	243	58	56
47	357	236	55	66
48	357	242	49	66
49	357	242	51	64
50	357	248	51	58
51	357	241	56	60
52	357	224	62	71
53	357	234	56	67
54	357	230	62	65
55	357	236	51	70
56	357	224	60	73
57	357	239	49	69
58	357	242	59	56

Model ID	Analysed	Favored	Allowed	Outliers
59	357	248	56	53
60	357	238	46	73
61	357	237	58	62
62	357	228	60	69
63	357	242	55	60
64	357	232	55	70
65	357	248	50	59
66	357	232	54	71
67	357	242	53	62
68	357	241	55	61
69	357	233	62	62
70	357	241	47	69
71	357	233	57	67
72	357	244	52	61
73	357	240	55	62
74	357	233	52	72
75	357	219	61	77
76	357	238	59	60
77	357	231	56	70
78	357	235	58	64
79	357	246	53	58
80	357	238	53	66
81	357	231	63	63
82	357	245	48	64
83	357	242	57	58
84	357	239	54	64
85	357	237	56	64
86	357	234	55	68
87	357	227	63	67
88	357	226	57	74
89	357	233	53	71
90	357	246	59	52
91	357	229	51	77
92	357	232	64	61
93	357	224	73	60

Model ID	Analysed	Favored	Allowed	Outliers
94	357	237	57	63
95	357	232	59	66
96	357	237	51	69
97	357	232	69	56
98	357	248	50	59
99	357	241	50	66
100	357	244	55	58
101	357	242	55	60
102	357	237	64	56
103	357	233	62	62
104	357	226	58	73
105	357	244	53	60
106	357	227	55	75
107	357	242	48	67
108	357	239	54	64
109	357	240	48	69
110	357	249	48	60
111	357	234	49	74
112	357	231	53	73
113	357	240	54	63
114	357	245	50	62
115	357	232	55	70
116	357	226	64	67
117	357	232	66	59
118	357	240	53	64
119	357	243	54	60
120	357	237	53	67
121	357	249	57	51
122	357	236	59	62
123	357	239	53	65
124	357	242	55	60
125	357	231	58	68
126	357	235	55	67
127	357	239	60	58
128	357	229	61	67

Model ID	Analysed	Favored	Allowed	Outliers
129	357	240	42	75
130	357	227	64	66
131	357	223	57	77
132	357	232	54	71
133	357	248	46	63
134	357	248	49	60
135	357	249	51	57
136	357	236	59	62
137	357	225	66	66
138	357	242	49	66
139	357	243	56	58
140	357	235	60	62
141	357	248	47	62
142	357	233	59	65
143	357	246	50	61
144	357	236	60	61
145	357	237	54	66
146	357	232	58	67
147	357	239	66	52
148	357	218	61	78
149	357	232	66	59
150	357	238	58	61
151	357	243	61	53
152	357	233	53	71
153	357	238	55	64
154	357	236	56	65
155	357	247	45	65
156	357	240	50	67
157	357	235	58	64
158	357	237	59	61
159	357	241	59	57
160	357	230	59	68
161	357	233	54	70
162	357	246	53	58
163	357	234	61	62

Model ID	Analysed	Favored	Allowed	Outliers
164	357	231	66	60
165	357	240	60	57
166	357	230	60	67
167	357	221	70	66
168	357	237	47	73
169	357	240	62	55
170	357	237	53	67
171	357	236	56	65
172	357	248	50	59
173	357	230	54	73
174	357	226	60	71
175	357	224	53	80
176	357	222	56	79
177	357	231	50	76
178	357	232	58	67
179	357	252	53	52
180	357	234	64	59
181	357	244	54	59
182	357	235	49	73
183	357	246	46	65
184	357	244	57	56
185	357	230	58	69
186	357	246	53	58
187	357	253	55	49
188	357	233	44	80
189	357	244	64	49
190	357	235	56	66
191	357	239	62	56
192	357	234	55	68
193	357	240	50	67
194	357	237	58	62
195	357	247	54	56
196	357	244	52	61
197	357	239	48	70
198	357	241	54	62

Model ID	Analysed	Favored	Allowed	Outliers
199	357	235	56	66
200	357	244	51	62


There are 211 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	237	LYS	200
A	238	ASP	200
A	260	THR	200
A	283	GLU	200
A	289	HIS	200
A	298	ASN	200
A	310	ARG	200
A	311	GLU	200
A	317	LYS	200
A	322	ASP	200
A	364	ARG	200
A	372	LYS	200
A	378	THR	200
A	379	GLU	200
A	380	CYS	200
A	417	LEU	158
A	97	ILE	147
A	109	LEU	144
A	20	ILE	140
A	219	VAL	137
A	156	ILE	129
A	176	ASP	127
A	411	VAL	126
A	181	ILE	121
A	409	ILE	120
A	9	ILE	117
A	213	VAL	112
A	7	ILE	110
A	178	ILE	110
A	34	ILE	108

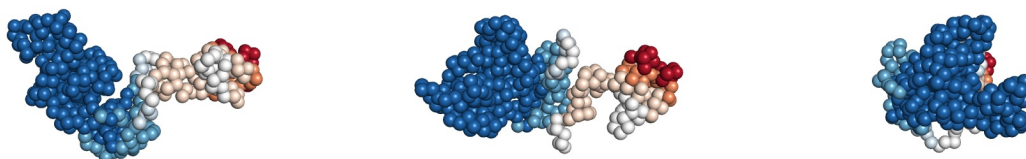
Chain	Res	Type	Models (Total)
A	106	ASN	105
A	135	THR	104
A	81	ILE	103
A	157	ASP	103
A	186	ARG	97
A	29	ILE	90
A	113	THR	90
A	21	VAL	89
A	126	ILE	89
A	104	LEU	81
A	207	GLN	80
A	94	GLU	76
A	100	LEU	76
A	152	VAL	76
A	218	THR	76
A	92	ARG	75
A	14	THR	74
A	48	LYS	74
A	72	LEU	74
A	35	LEU	73
A	116	LEU	73
A	134	LYS	73
A	89	GLU	71
A	96	LYS	71
A	82	ILE	67
A	224	VAL	67
A	42	LEU	66
A	105	MET	66
A	141	LEU	65
A	161	GLU	65
A	52	ILE	62
A	145	LEU	60
A	214	LEU	59
A	220	THR	59
A	174	GLU	58

Chain	Res	Type	Models (Total)
A	78	THR	56
A	136	LYS	56
A	62	ASN	55
A	129	LEU	55
A	191	GLU	55
A	16	LEU	54
A	31	ILE	53
A	117	ARG	53
A	2	ARG	52
A	70	ILE	52
A	222	MET	52
A	3	GLU	51
A	121	LYS	51
A	415	GLU	51
A	74	ASN	50
A	175	THR	50
A	195	LEU	50
A	215	SER	50
A	225	HIS	50
A	416	ARG	50
A	122	ARG	49
A	146	SER	49
A	155	VAL	49
A	46	LEU	48
A	160	ASP	48
A	210	GLU	48
A	211	ASP	48
A	133	ASP	47
A	140	PHE	46
A	165	GLN	46
A	184	LYS	46
A	8	VAL	45
A	13	SER	45
A	131	ASP	45
A	138	CYS	45

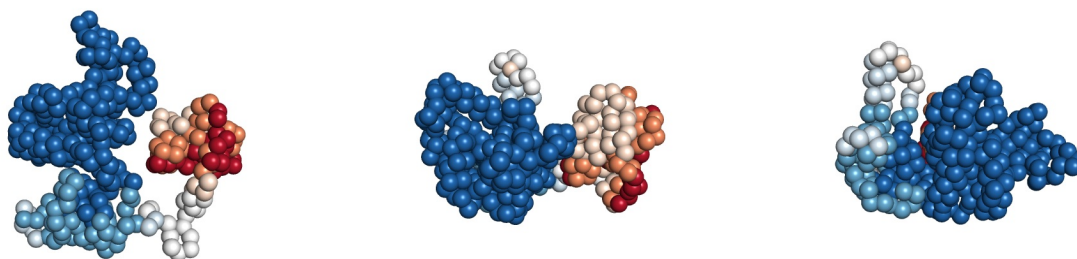
PrISM precision analysis ?

Regions of **low**  **high** precision, defined as the variability among the models that satisfy the input data and calculated as the density-weighted root mean-square fluctuation (RMSF) from the bead/atom center of density, annotated and visualized using PrISM. The per-bead precision is computed from the deposited ensemble of superposed integrative models. High- and low-precision regions are then determined by clustering beads of similar precision based on their proximity in the structure. Only coarse-grained beads (or CA atoms for atomic models) of deposited models are used for assessment and visualization, and three projections for each representative model are generated.

PrISM analysis for Ensemble 1 (models deposited/total: 100/4325).



PrISM analysis for Ensemble 2 (models deposited/total: 100/114).



Fit of model to data used for modeling ?

Single molecule FRET

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

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