

Integrative Structure Validation Report ?

March 13, 2025 - 10:20 AM PDT

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	9A08
PDB-Dev ID	PDBDEV_00000044
Structure Title	Structures of multiple states of the T4 lysozyme resolved by FRET with kinetics for free enzyme state
Structure Authors	Dimura M; Peulen TO; Sanabria H; Rodnin D; Hemmen K; Hanke CA; Seidel CAM; Gohlke H; Sanabria H ; Peulen T; Felekyan S; Fleissner MR; Koberling F; Kuehnemuth R; Hubbell W
Deposited on	2020-02-12

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

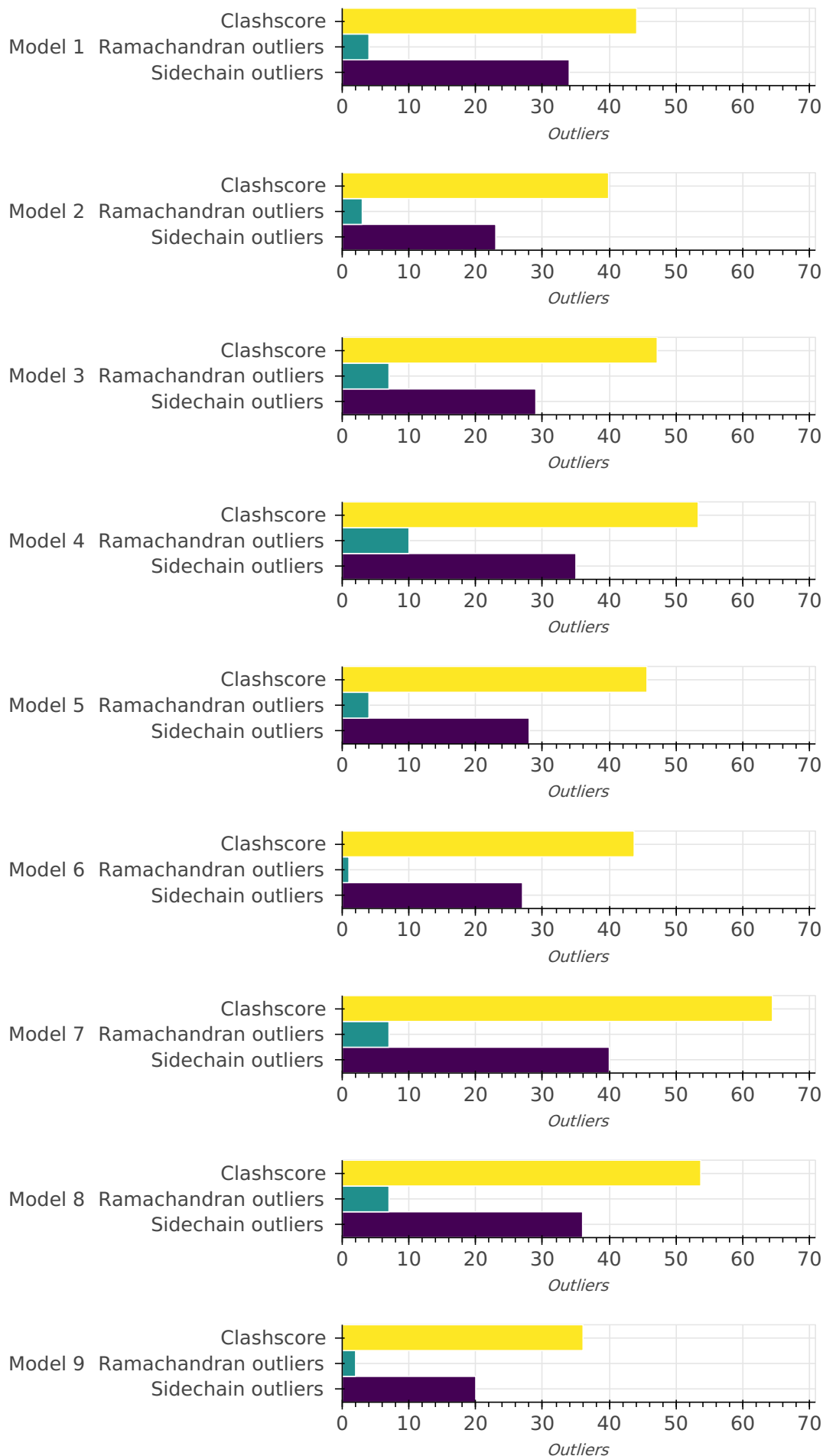
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

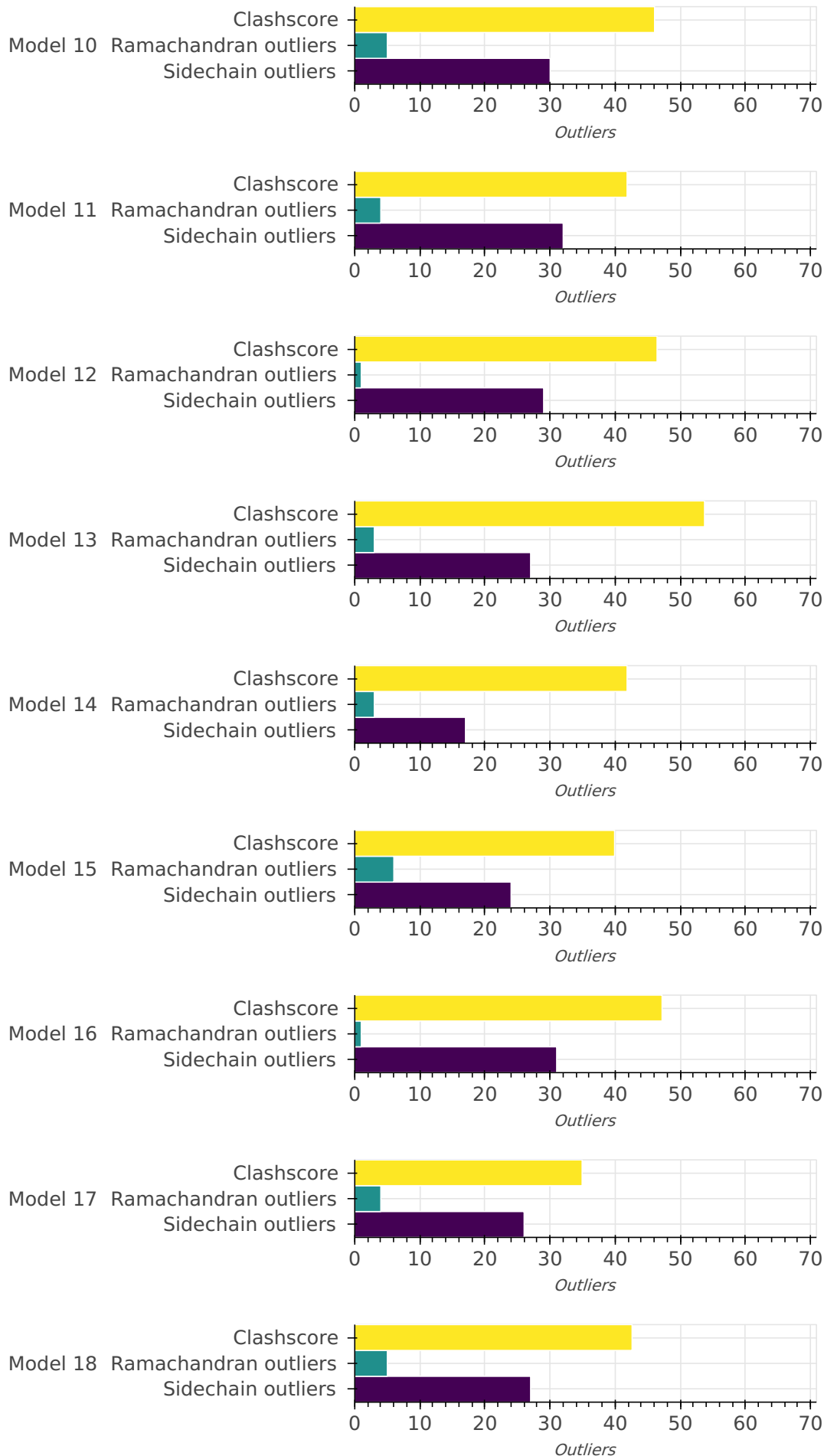
List of references used to build this report is available [here](#).

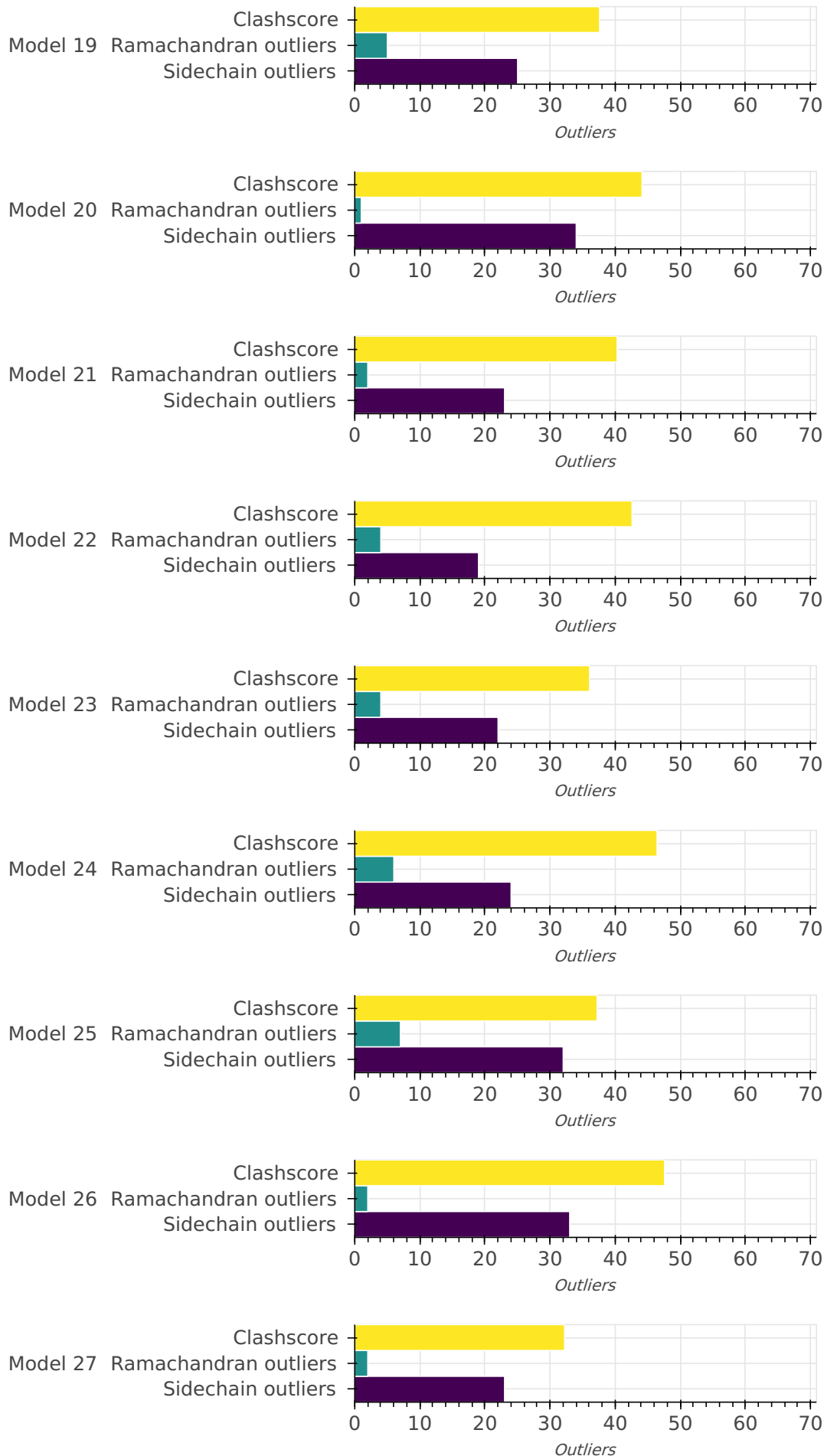
Overall quality ?

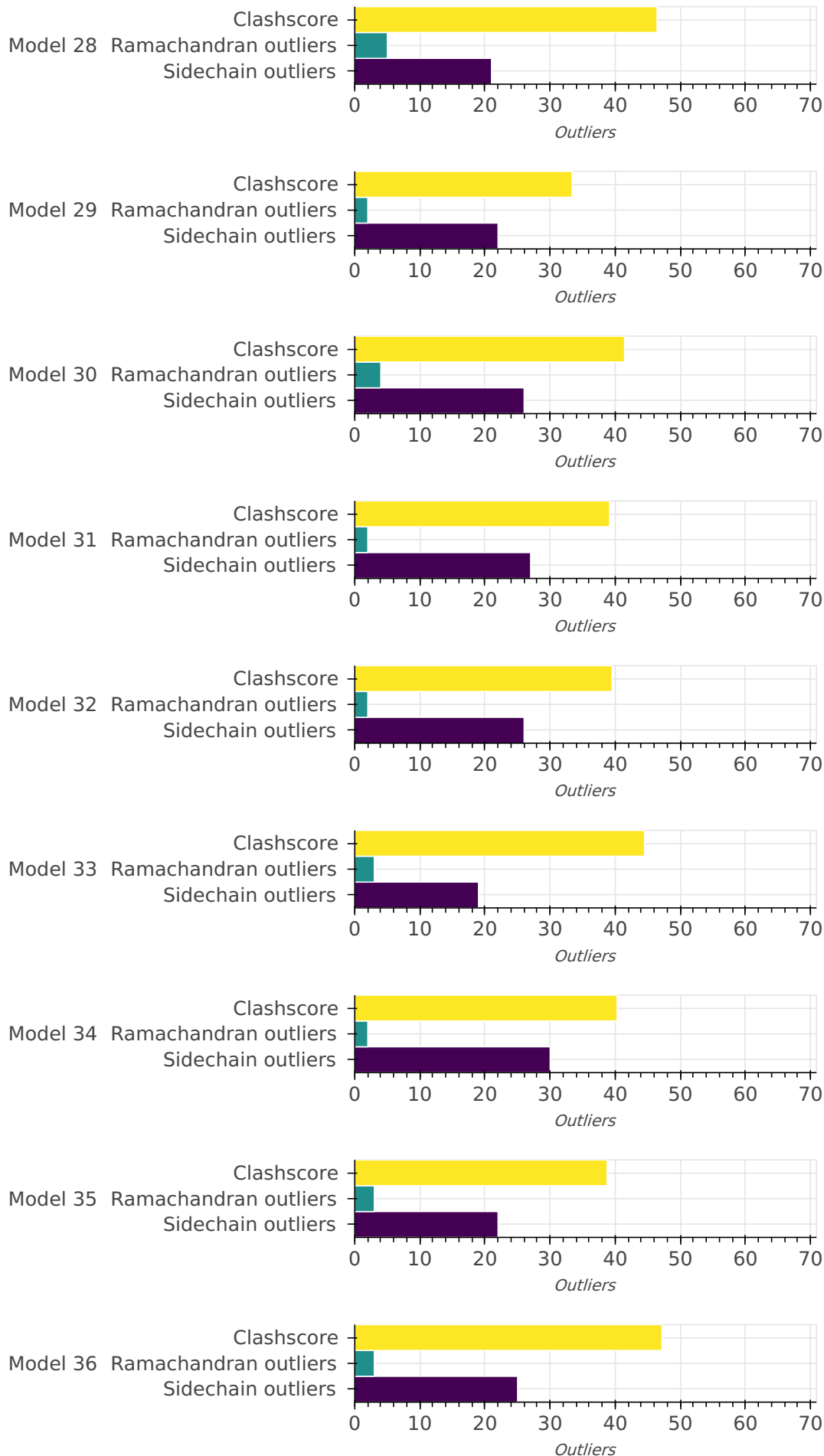
This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

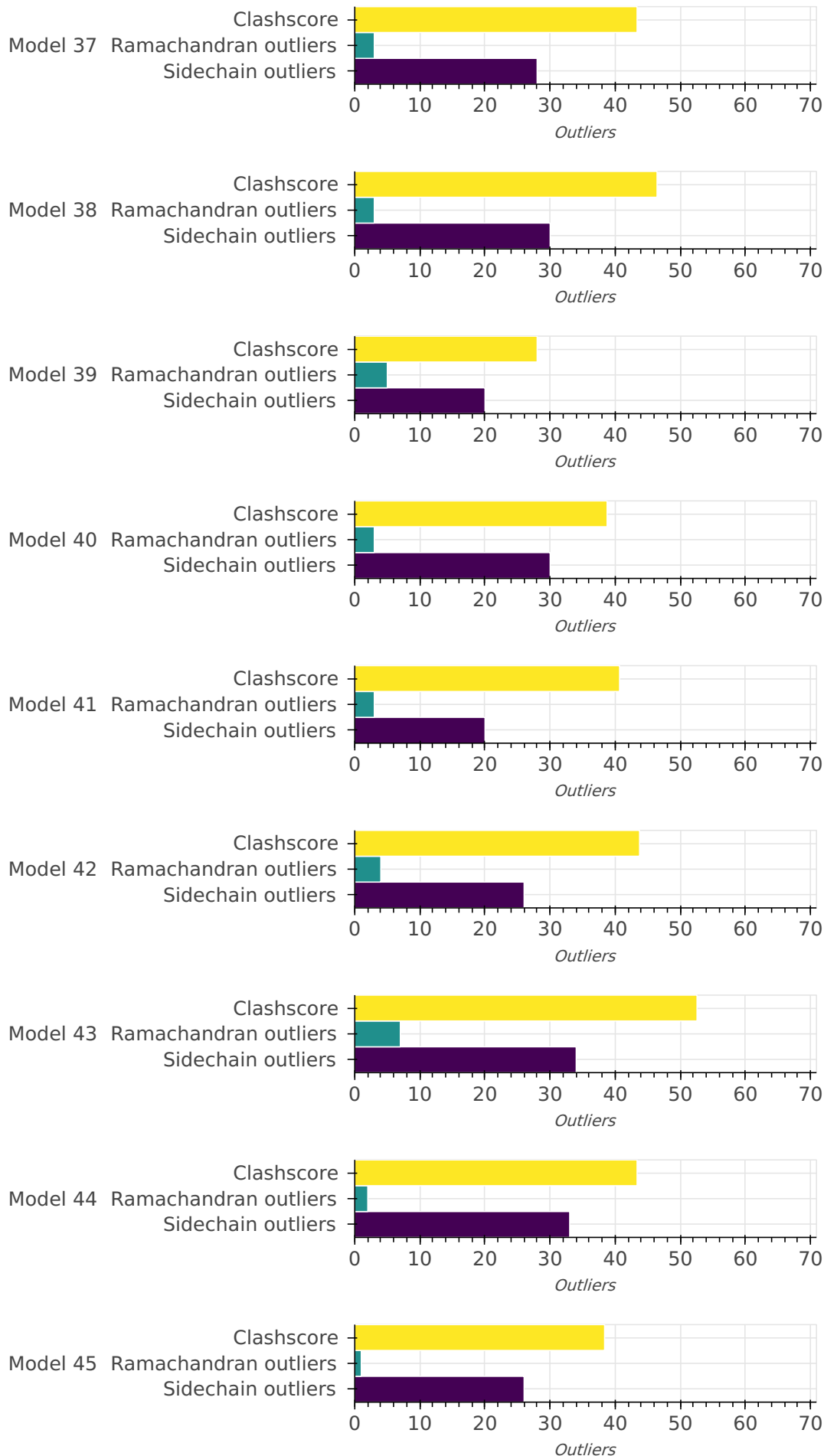
Model Quality: MolProbity Analysis

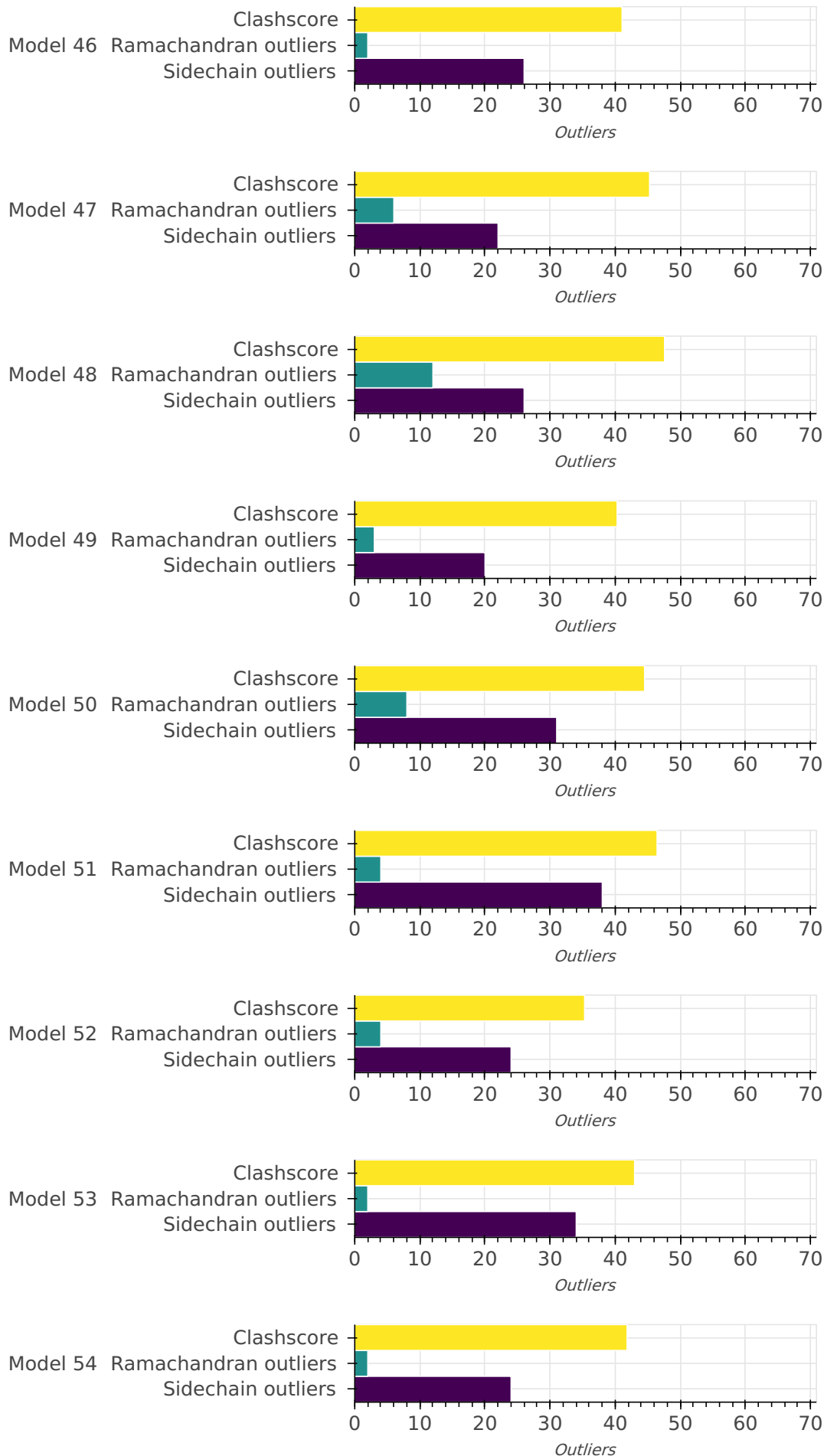


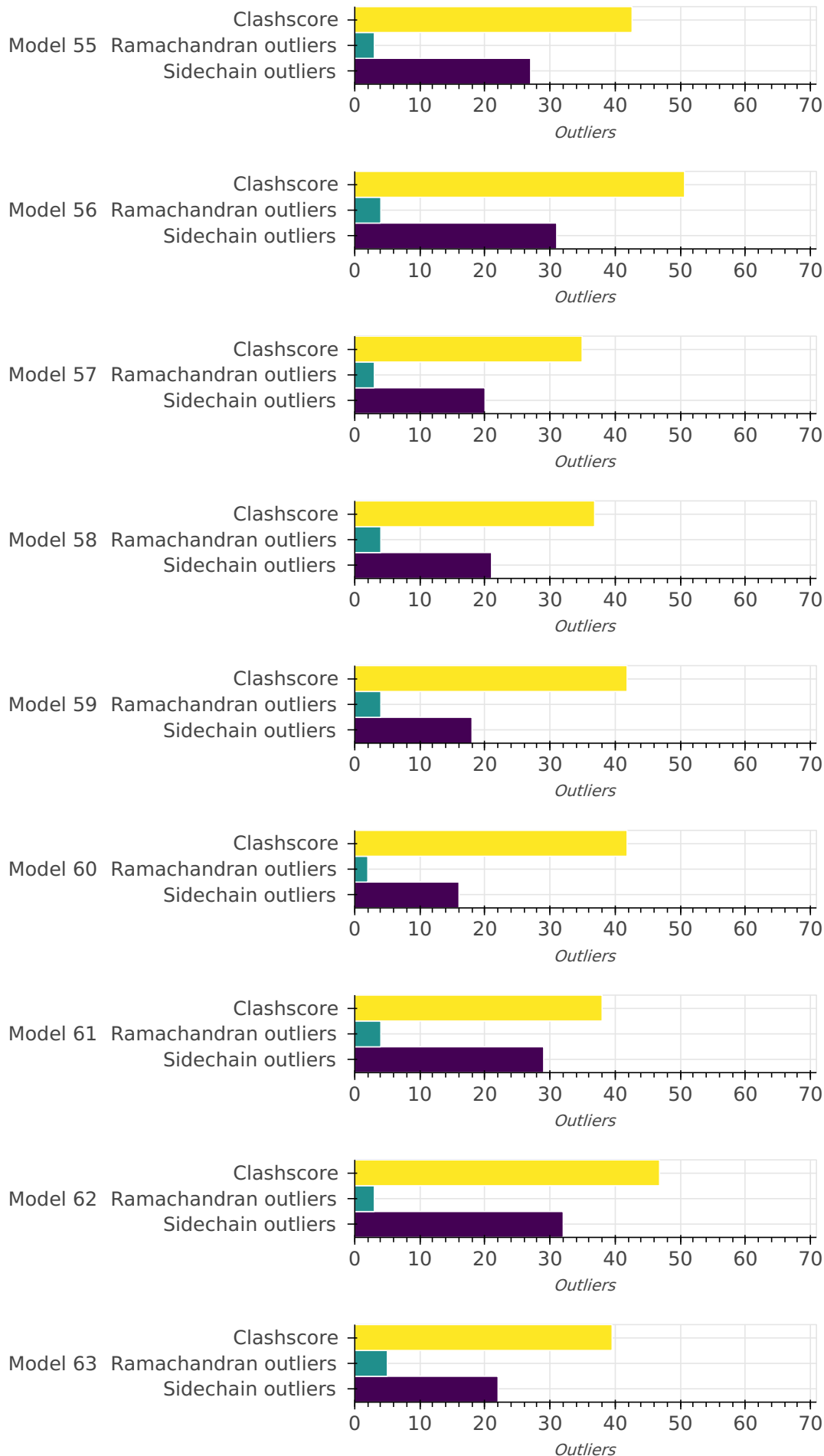


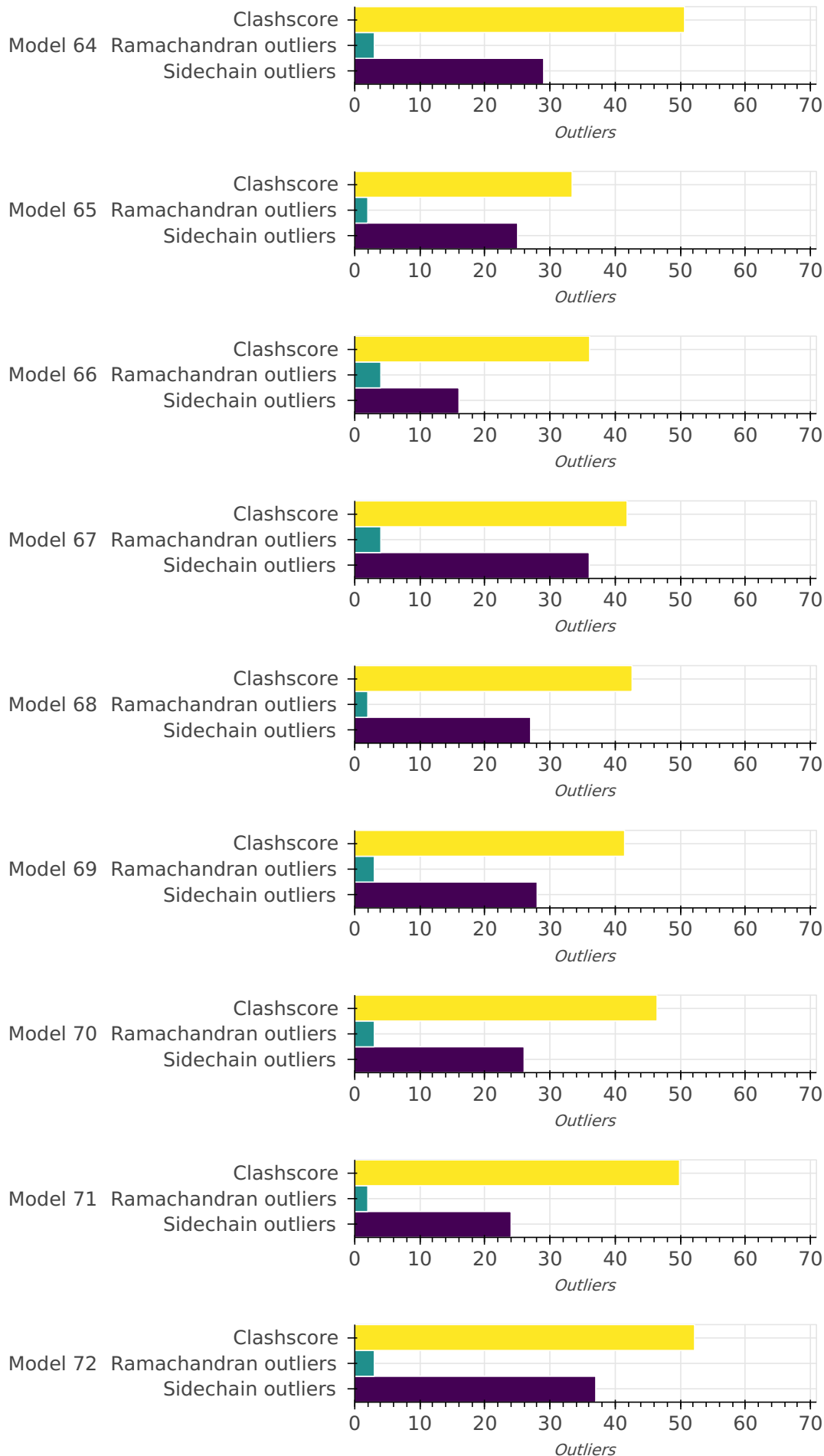


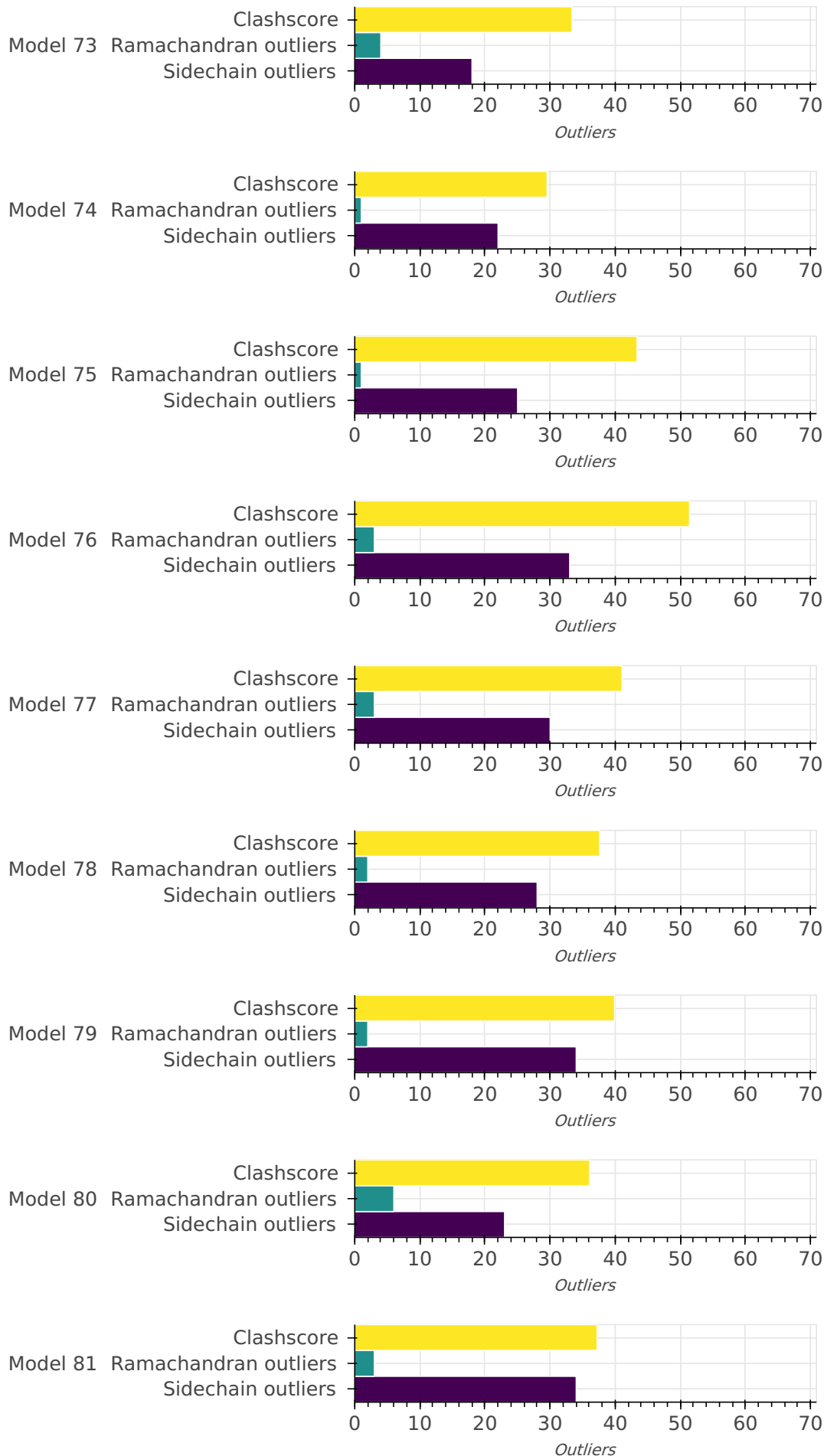


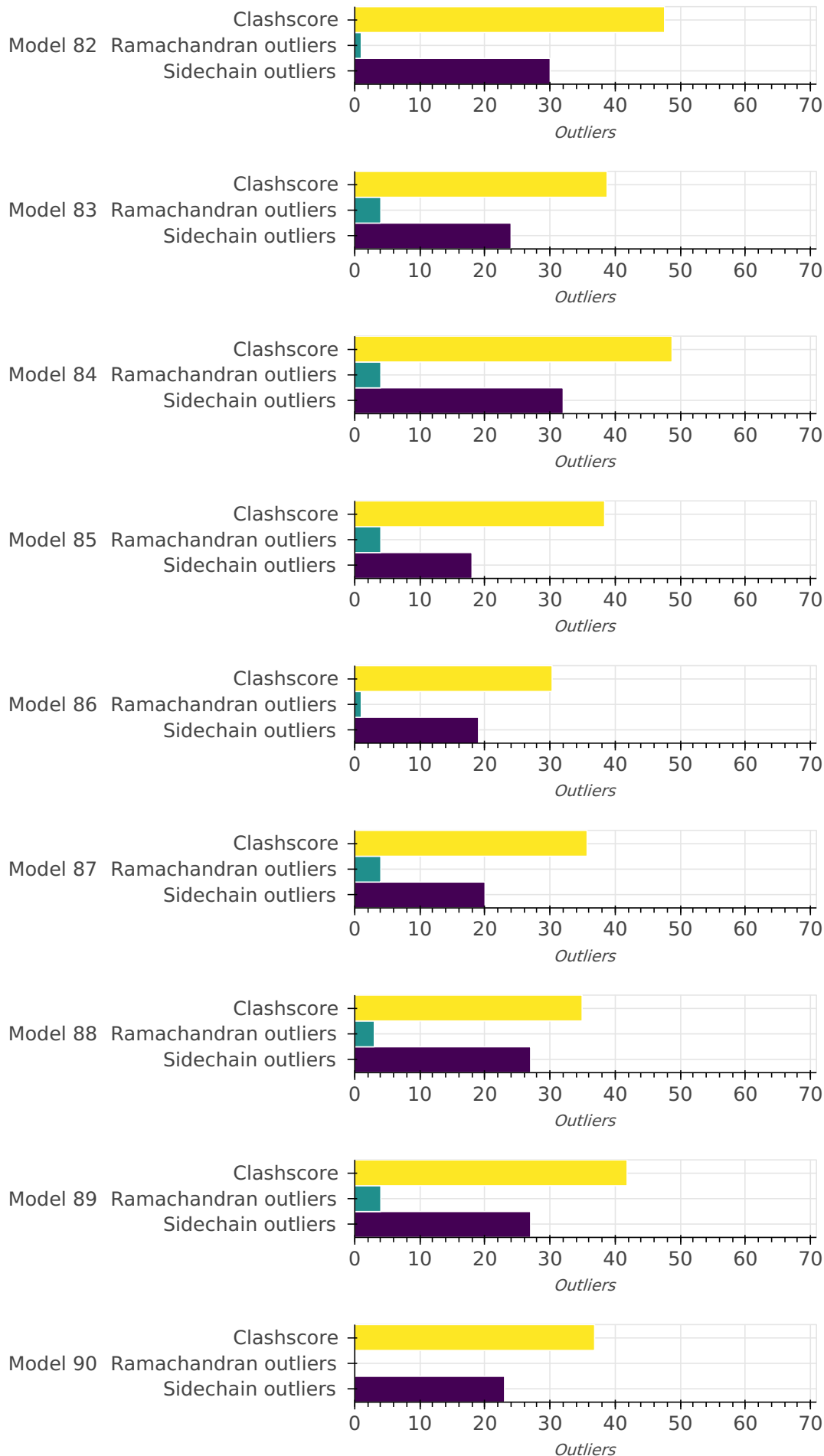


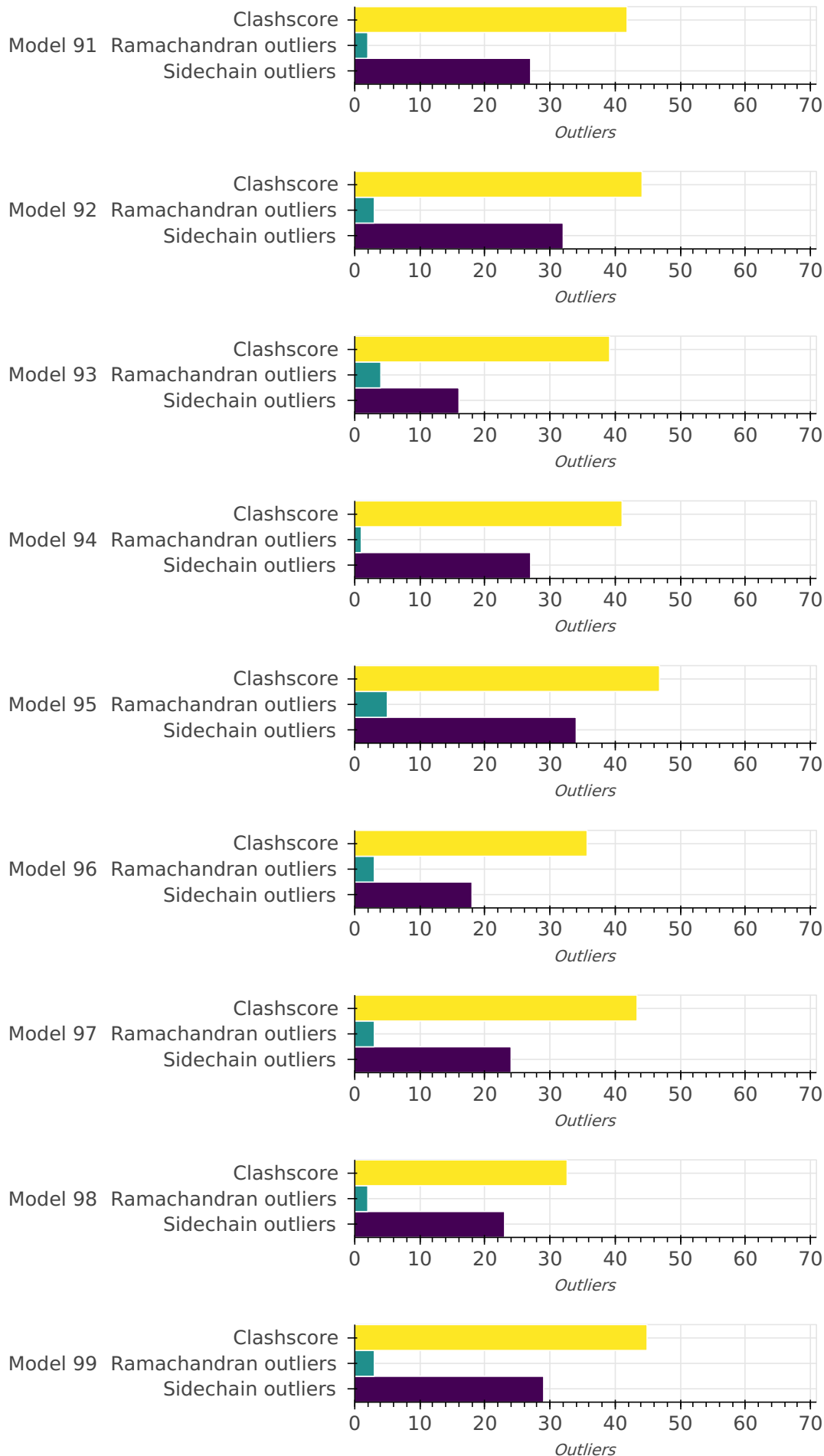


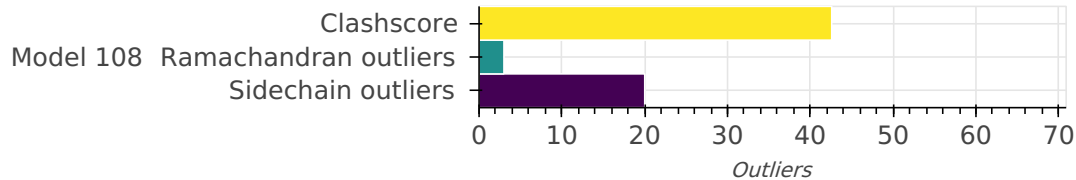
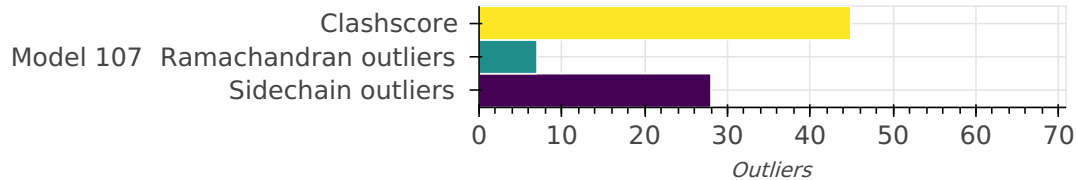
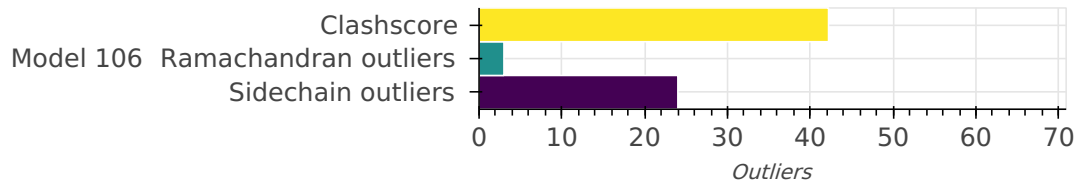
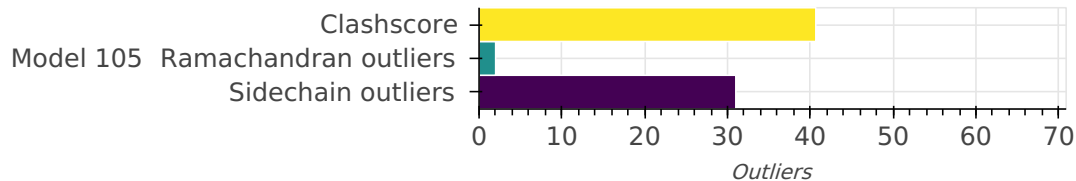
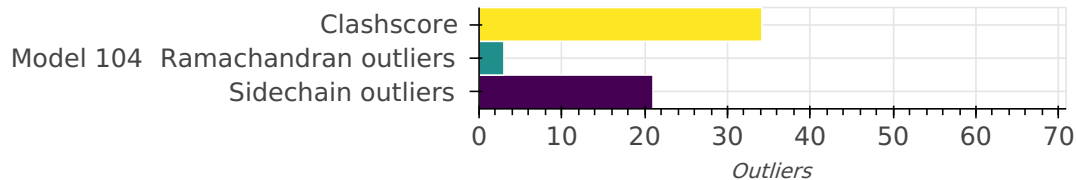
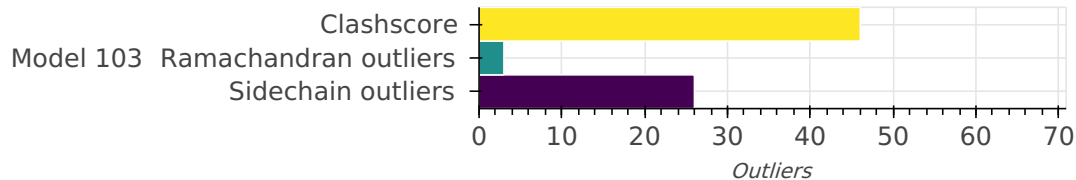
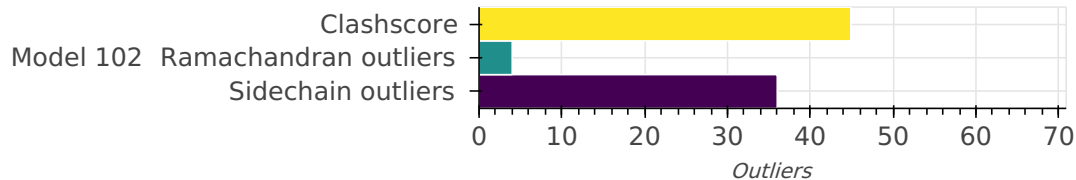
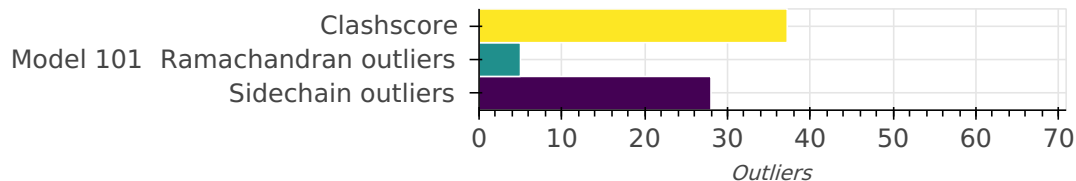
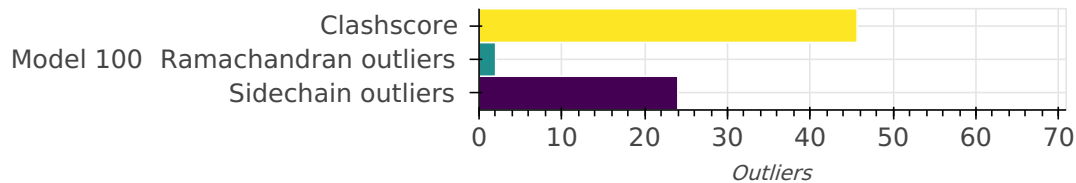


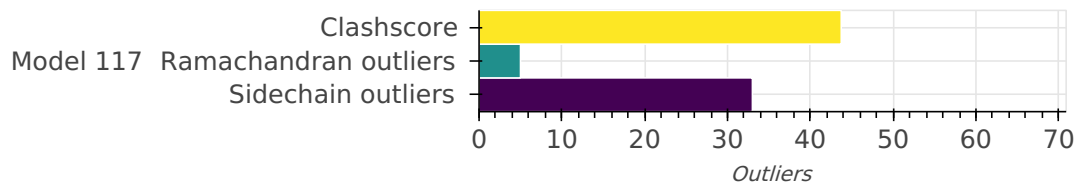
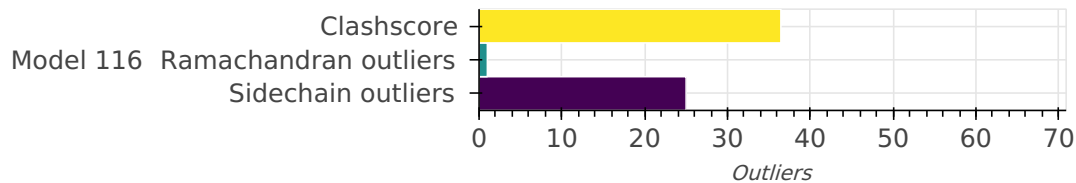
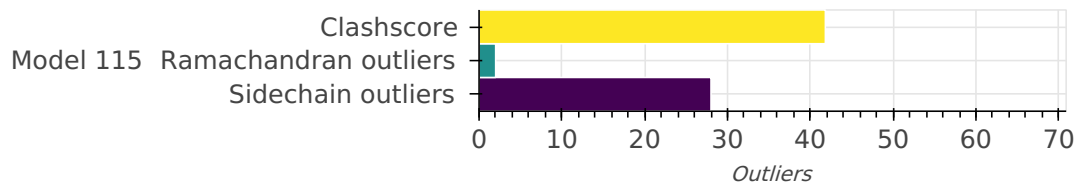
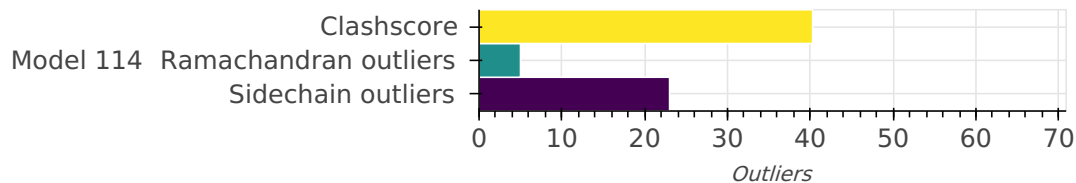
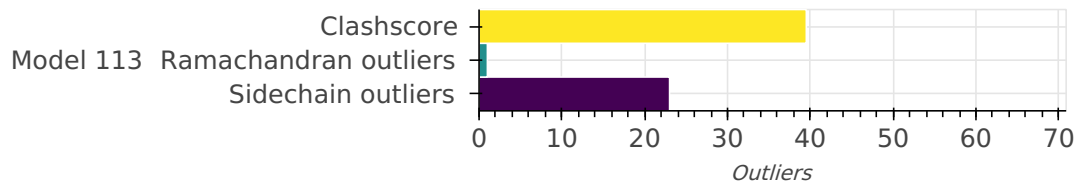
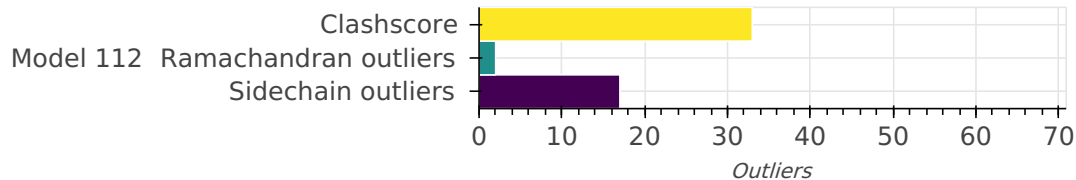
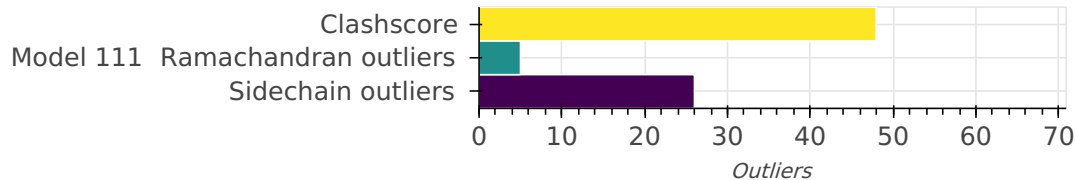
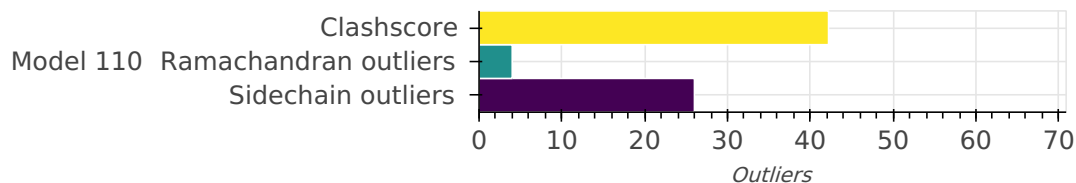
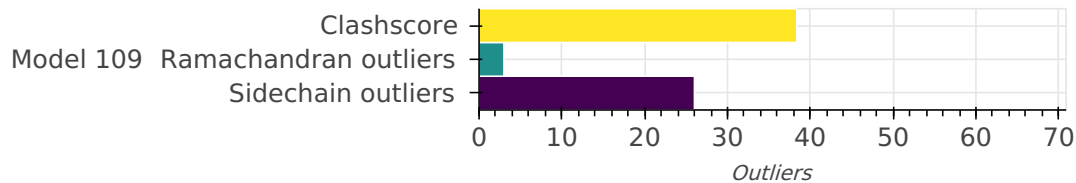


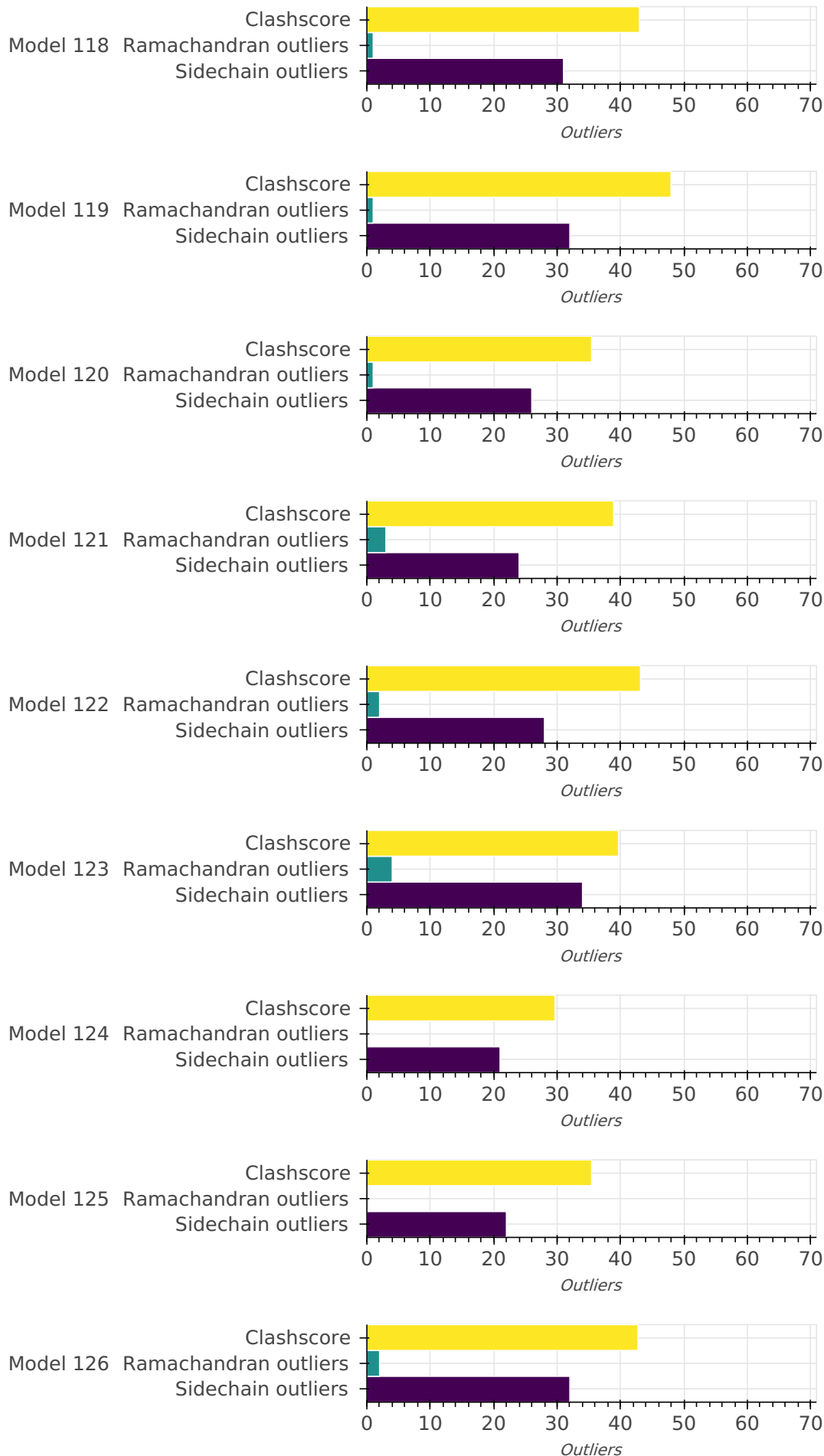


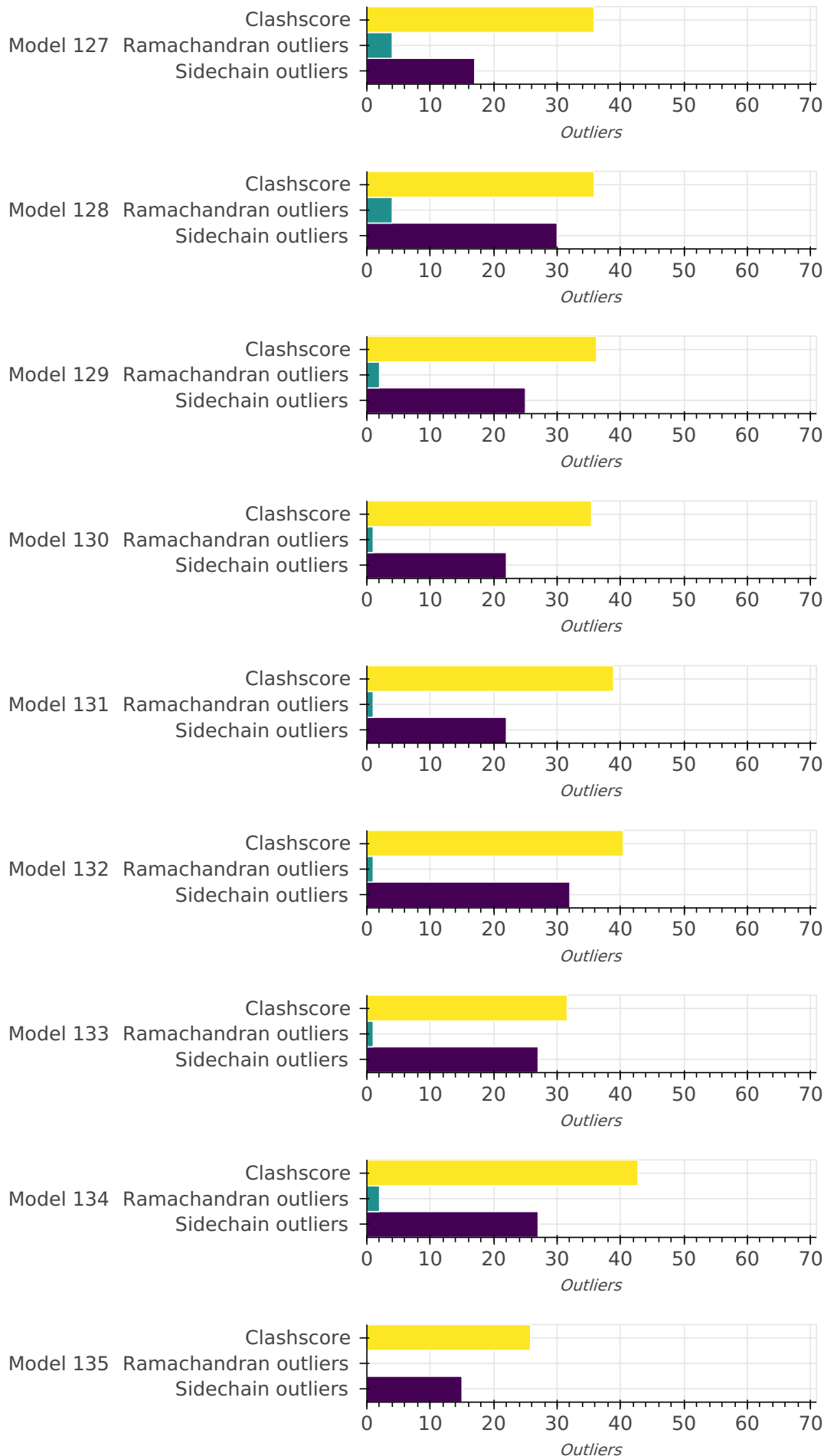


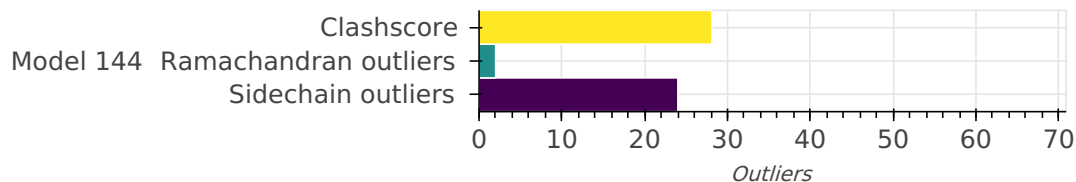
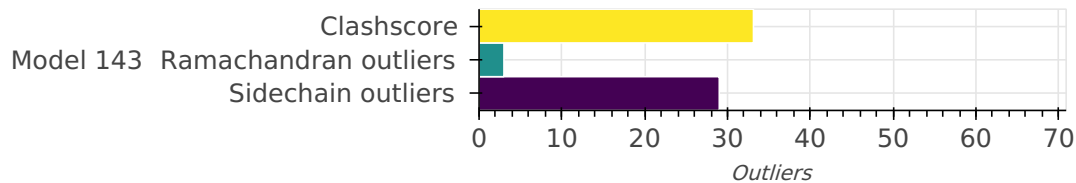
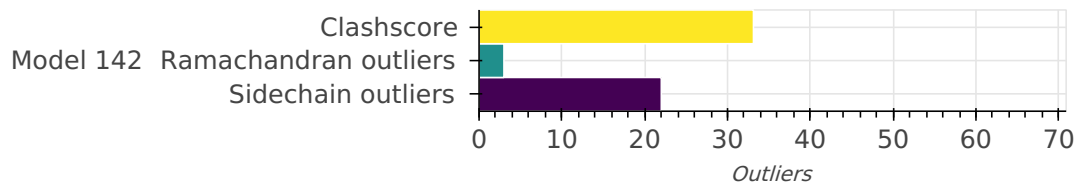
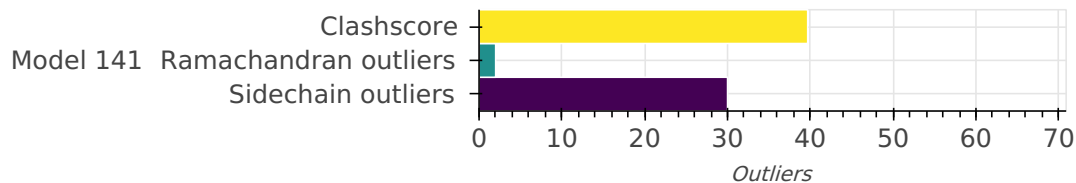
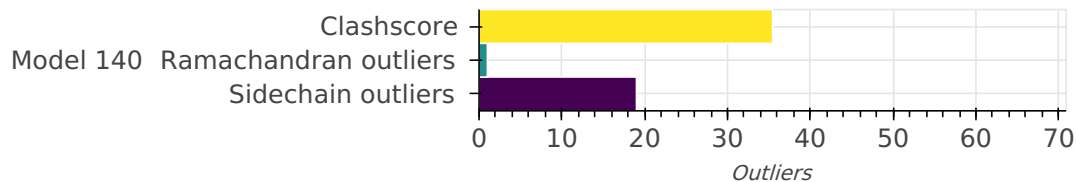
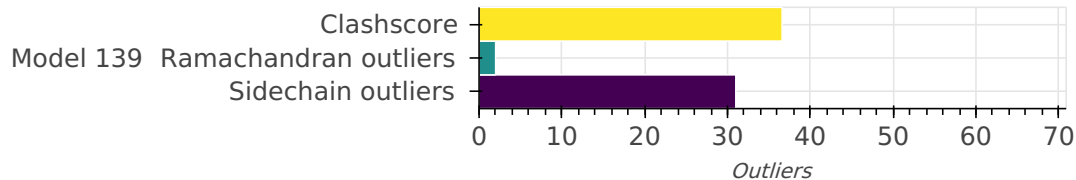
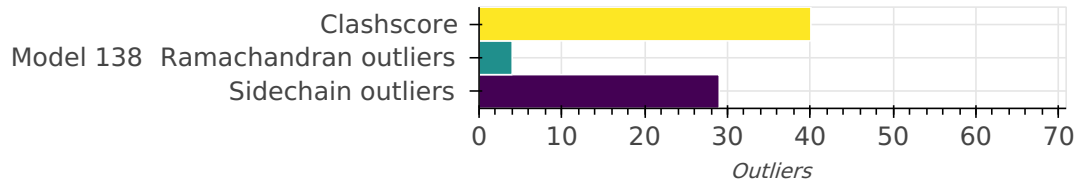
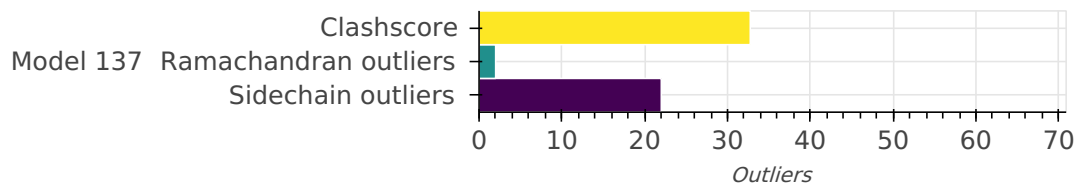
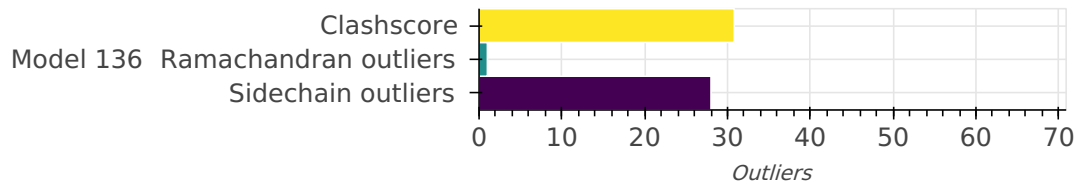


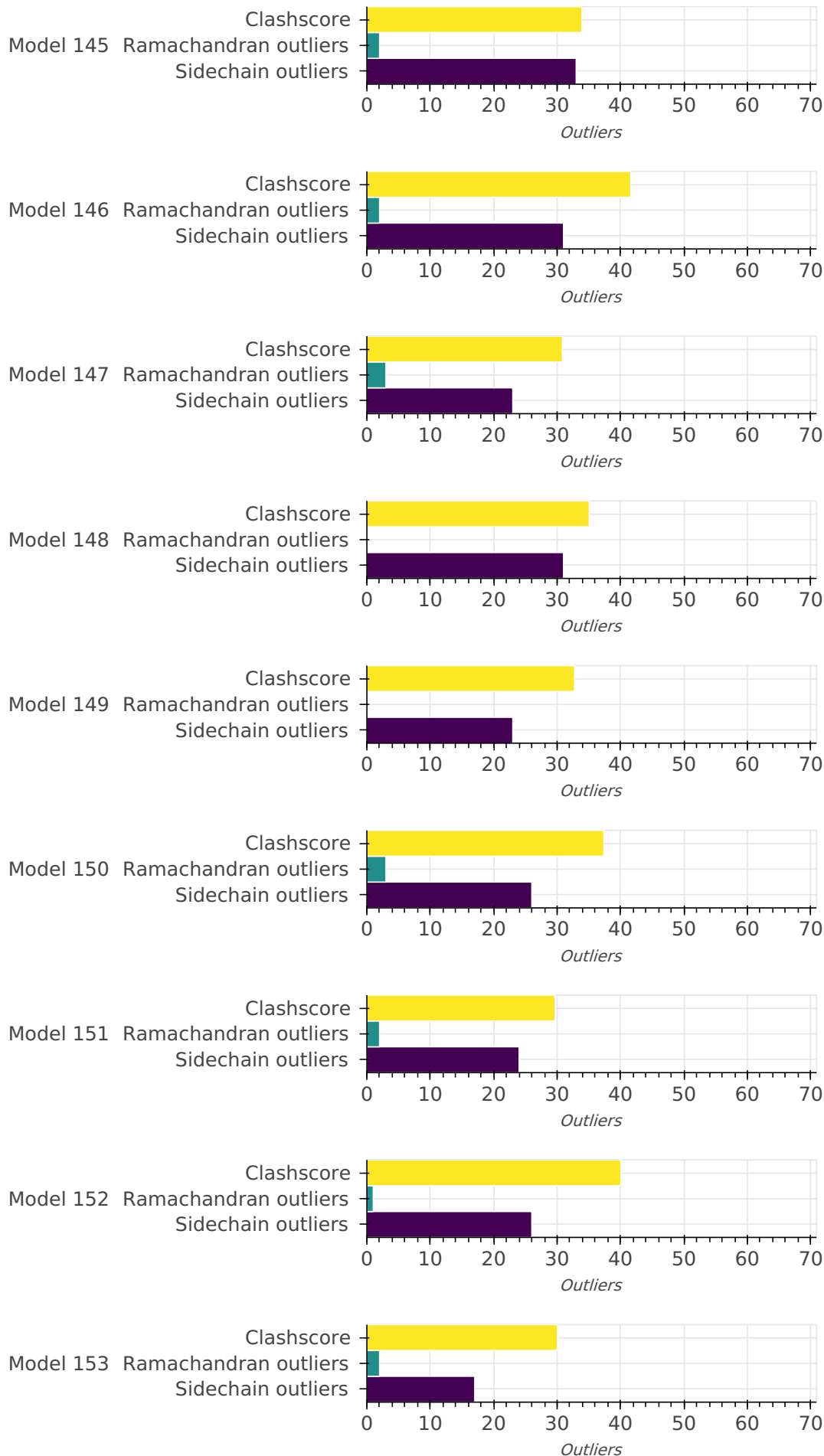


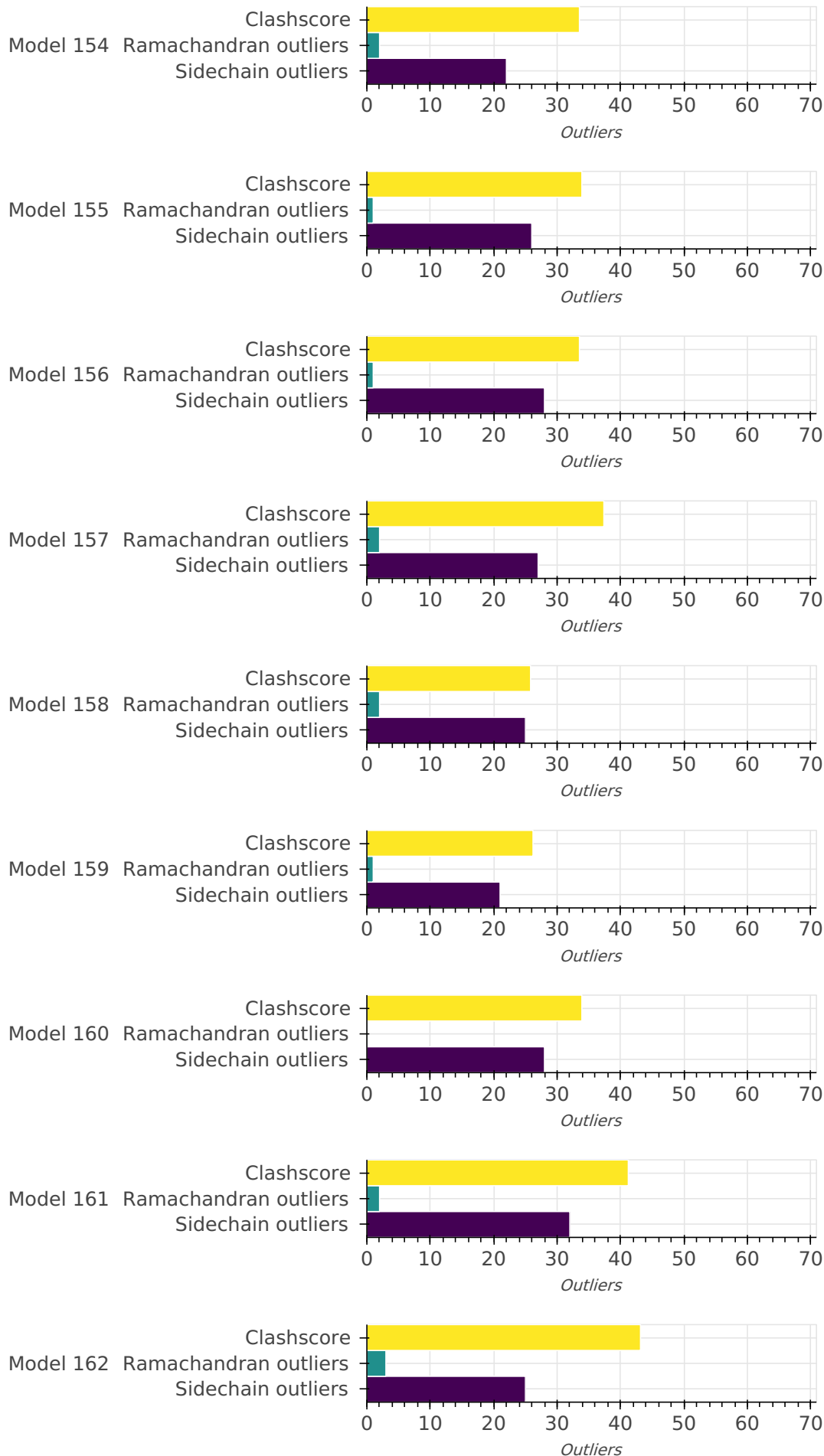


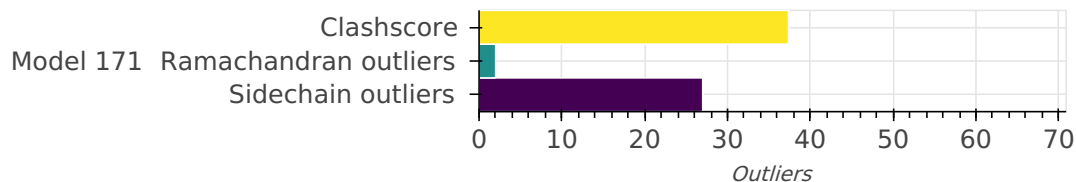
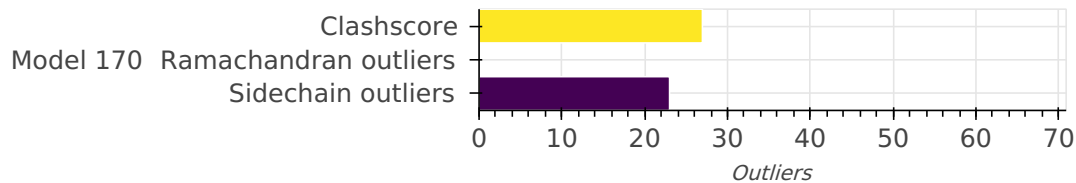
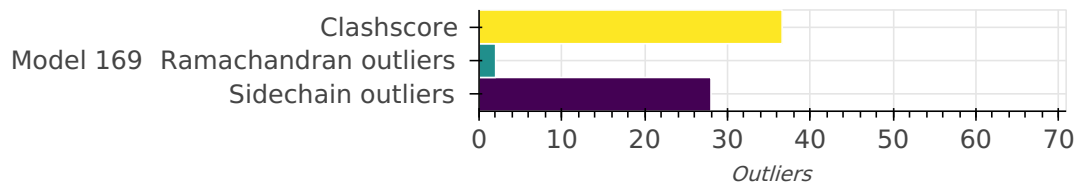
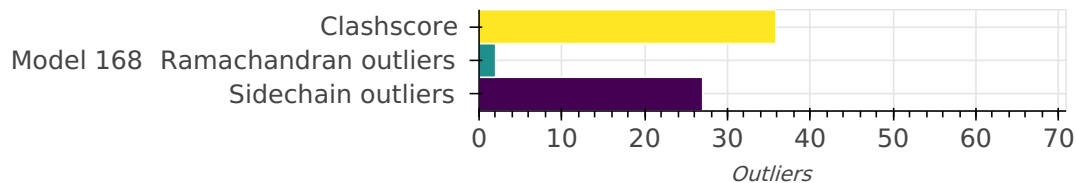
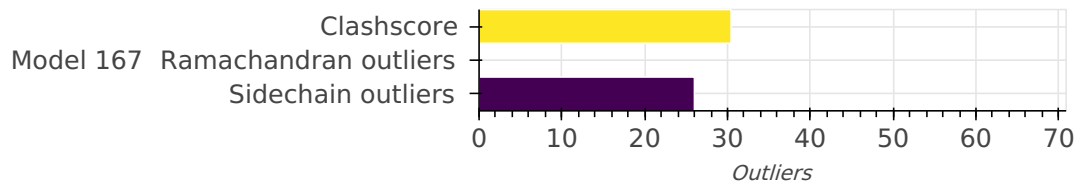
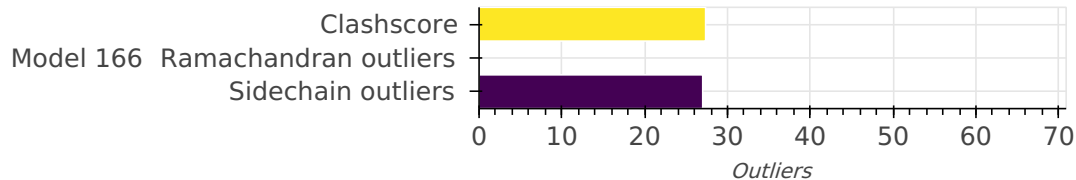
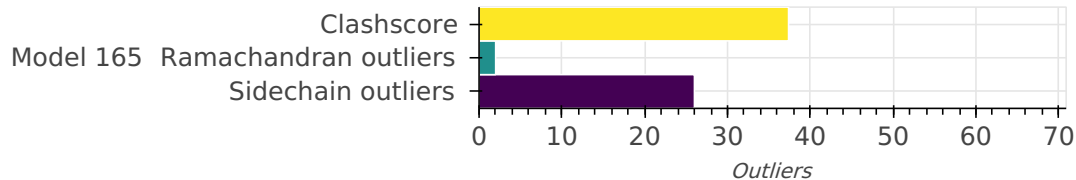
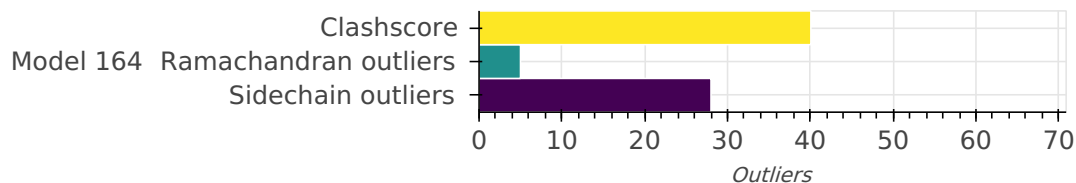
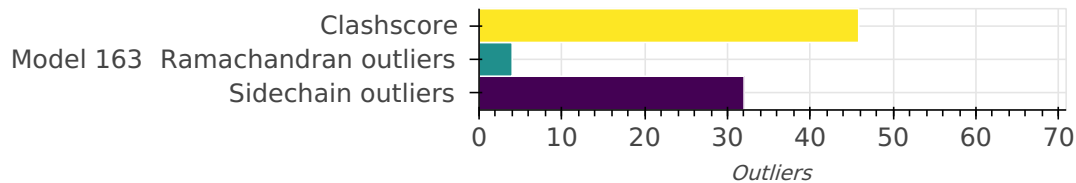


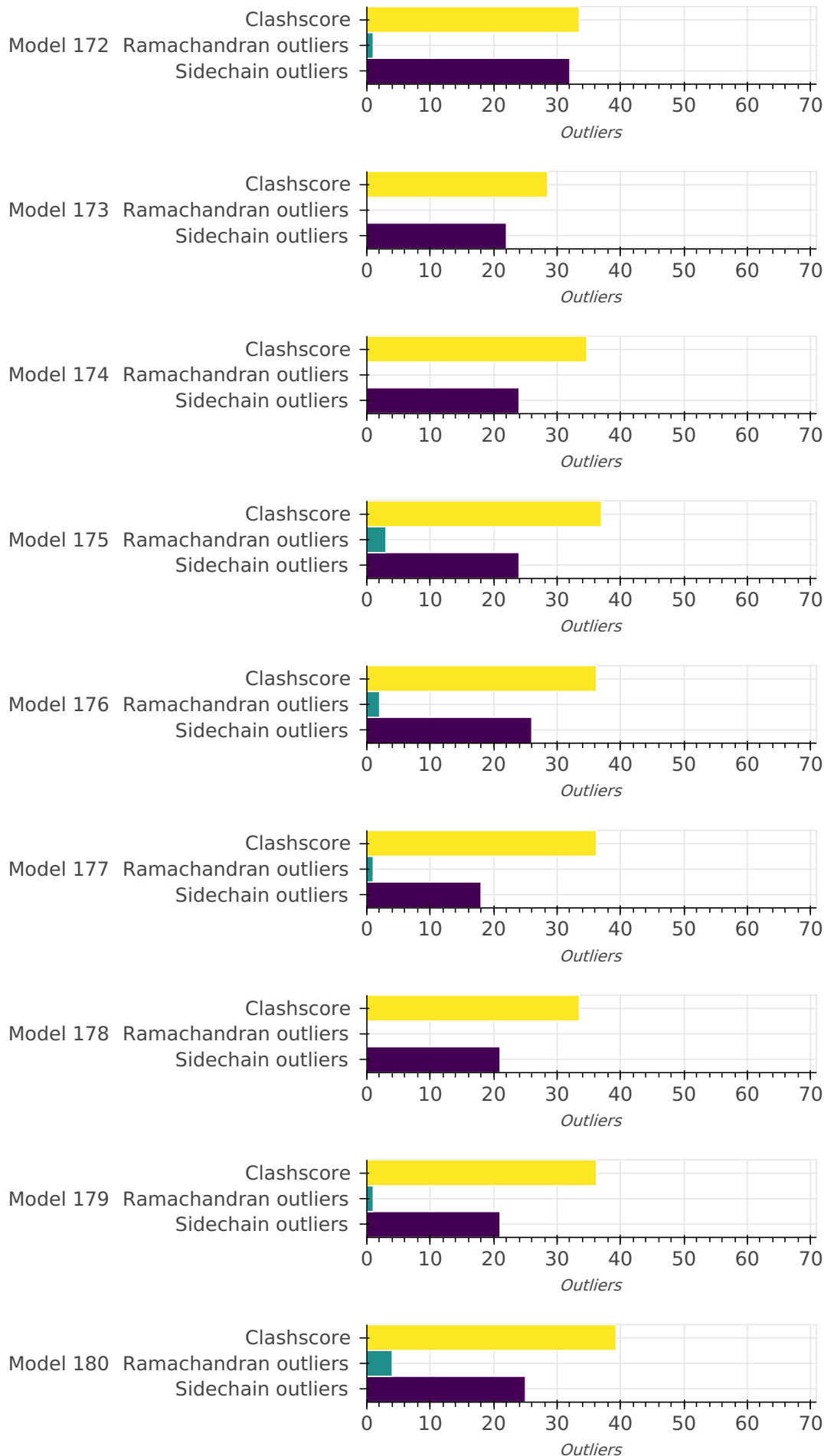


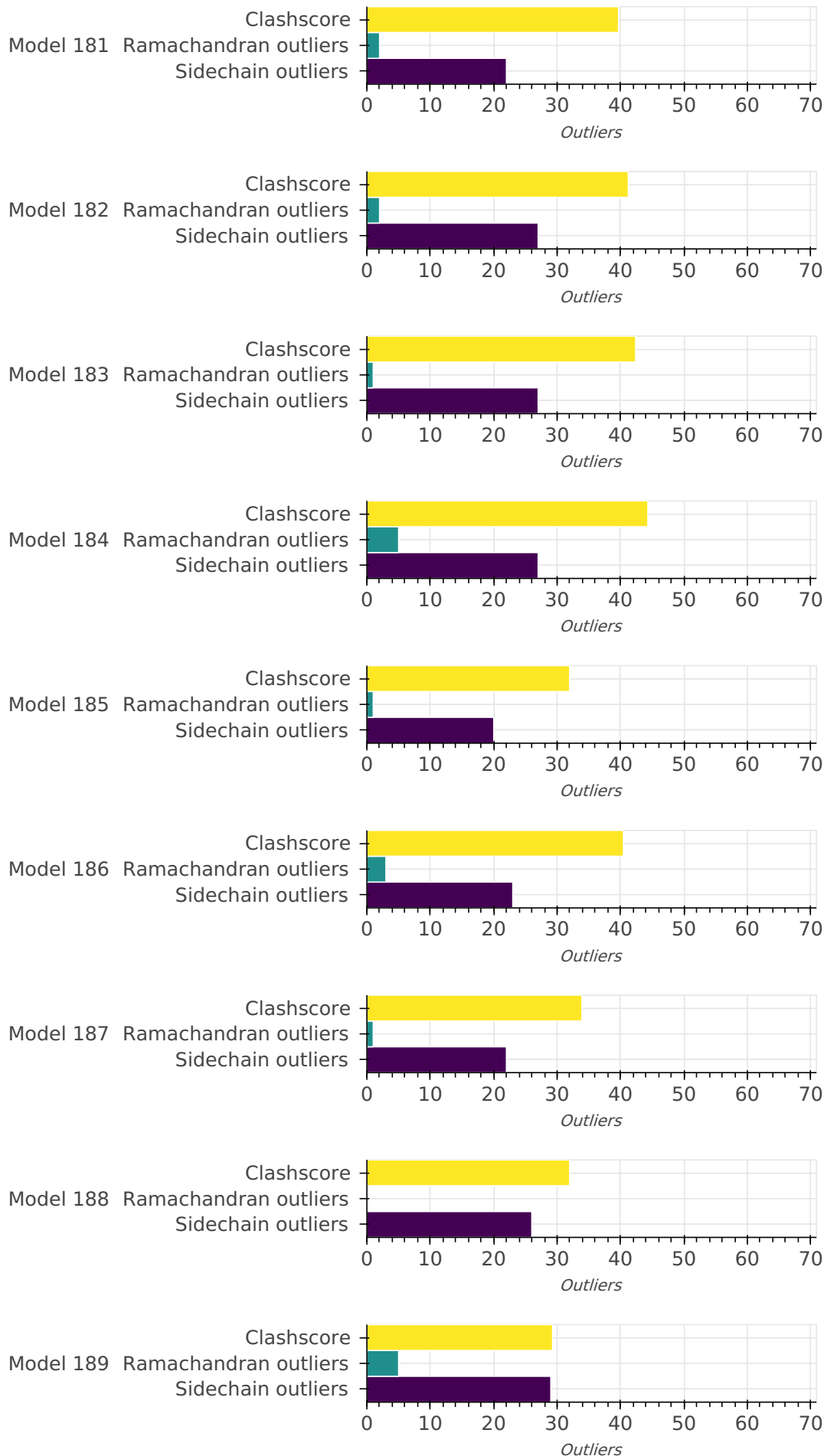


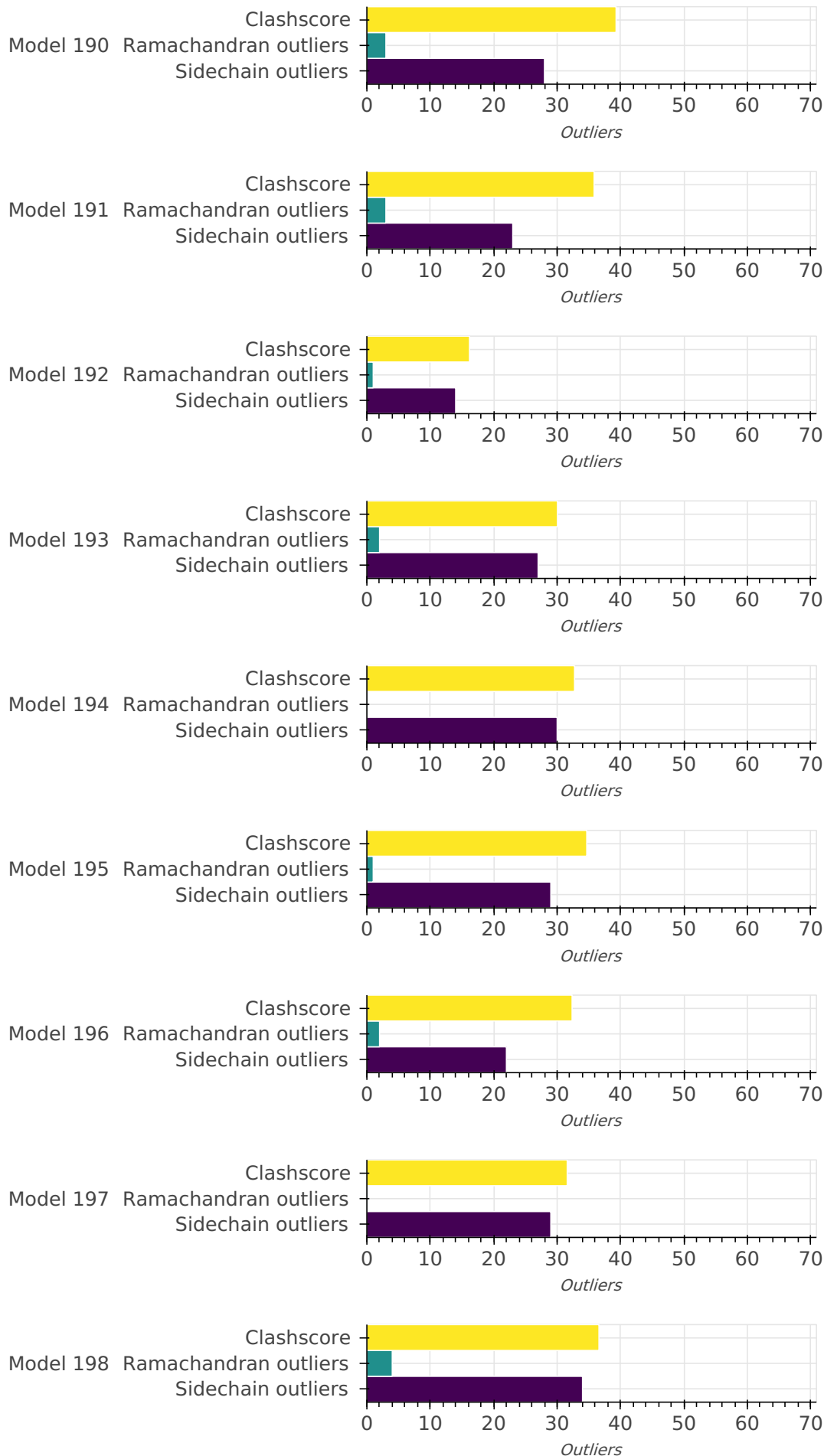


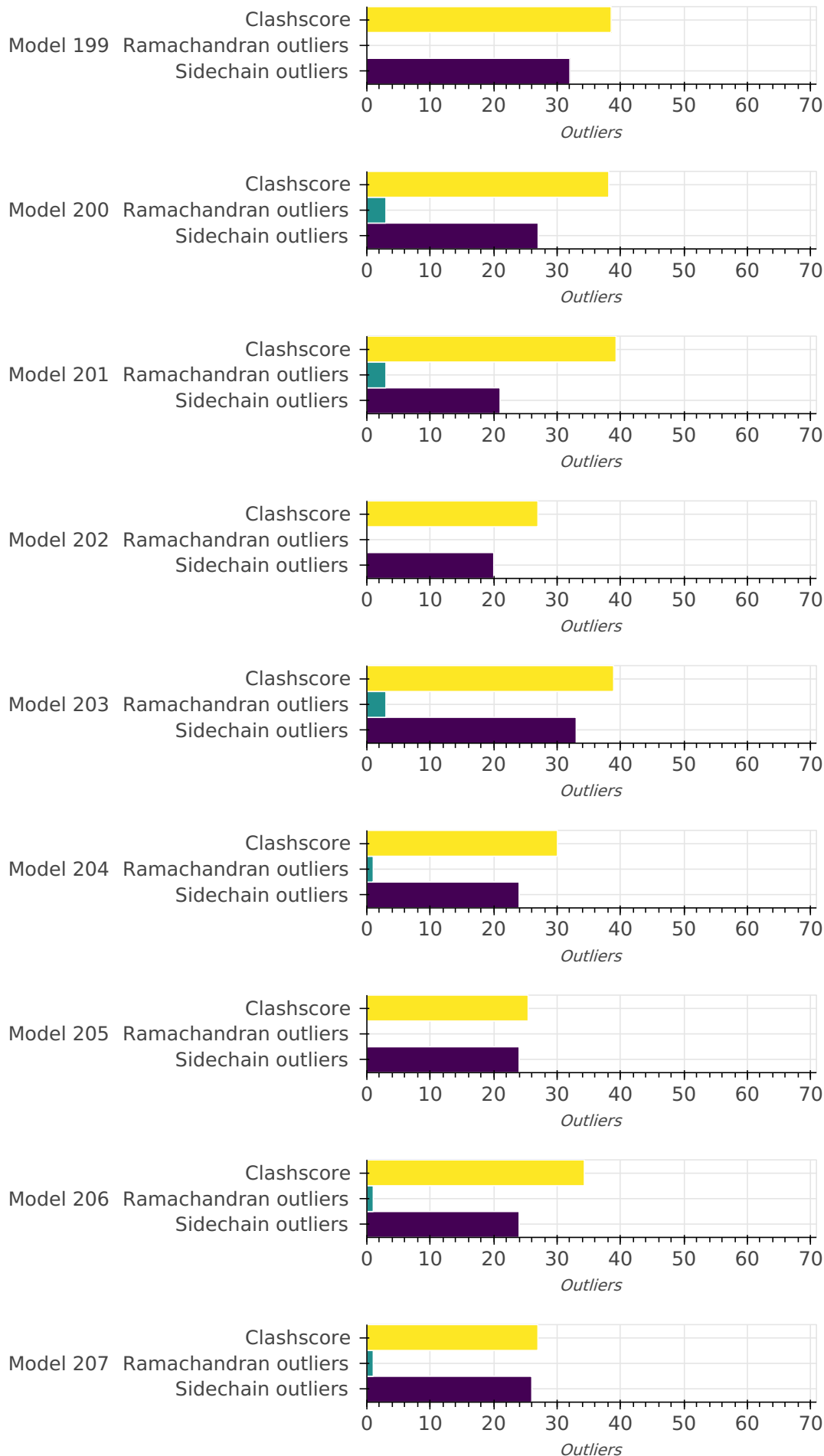


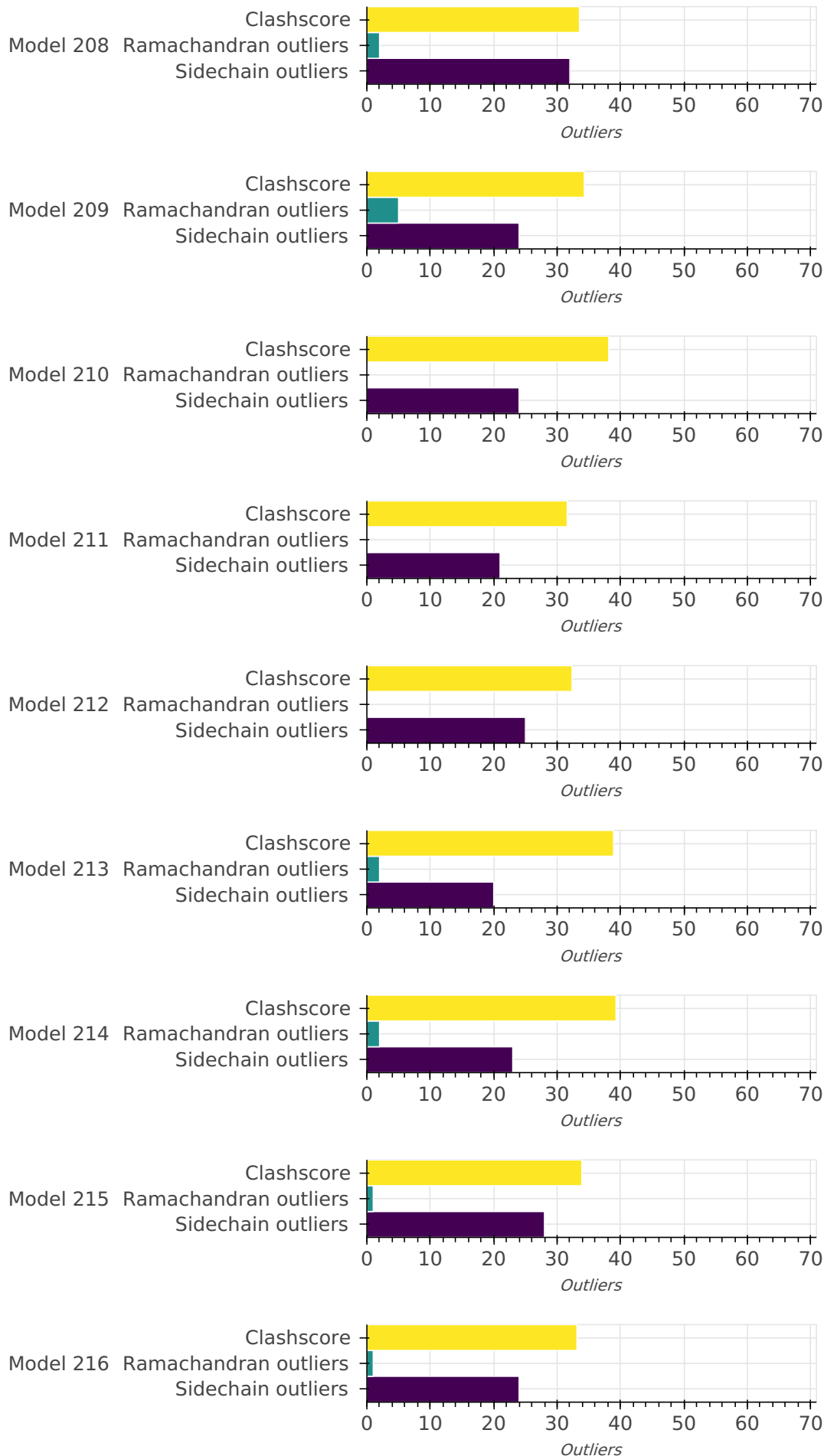


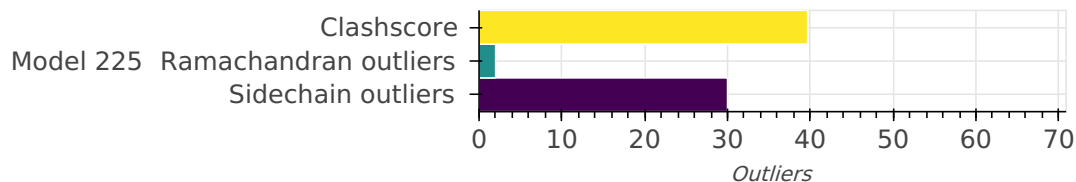
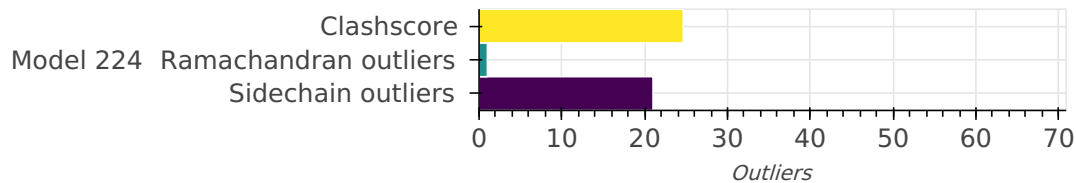
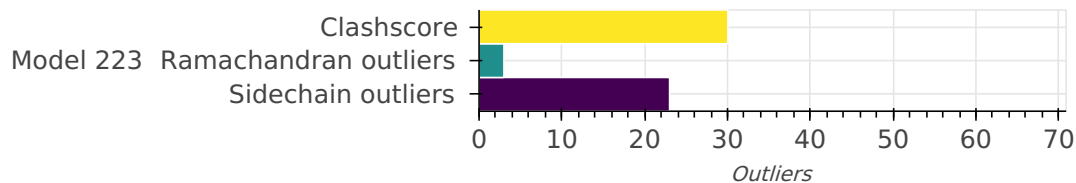
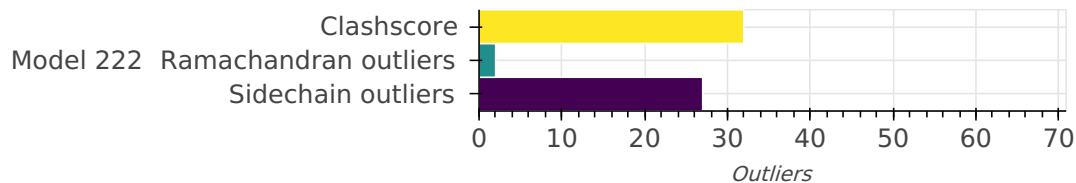
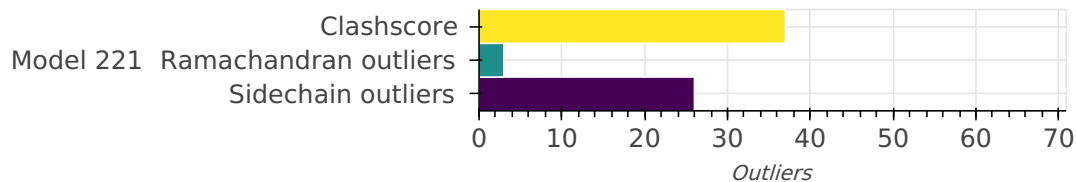
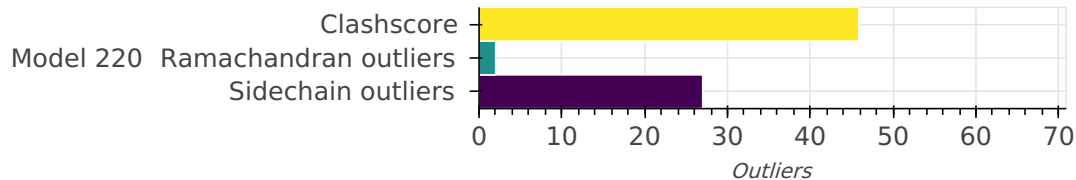
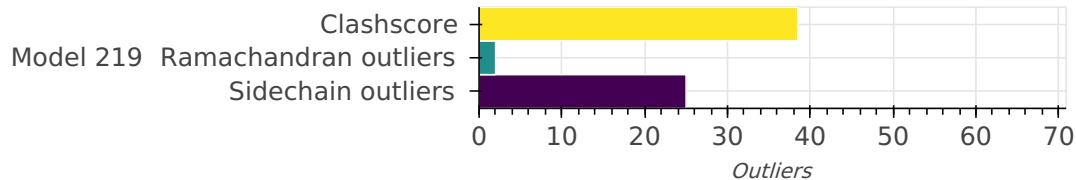
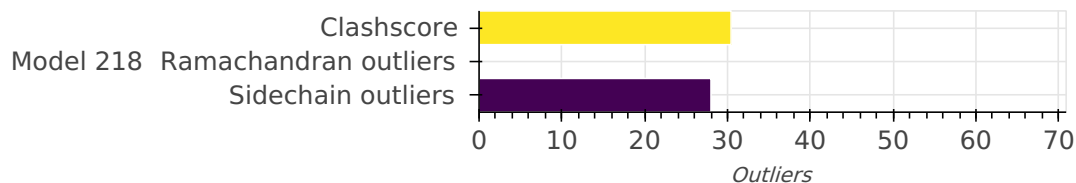
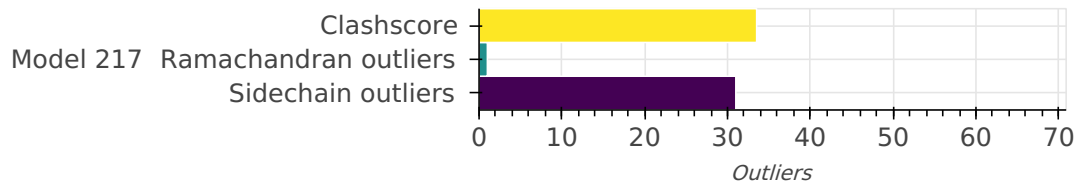


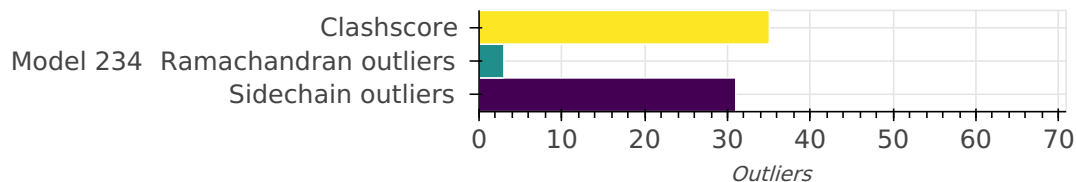
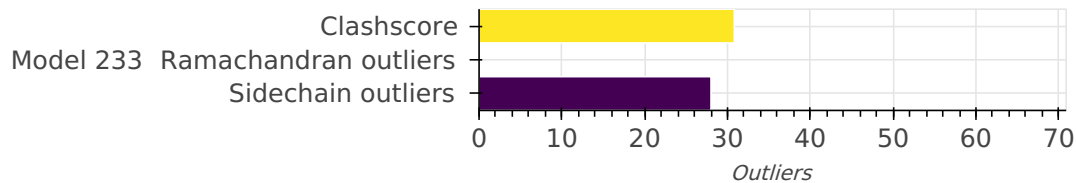
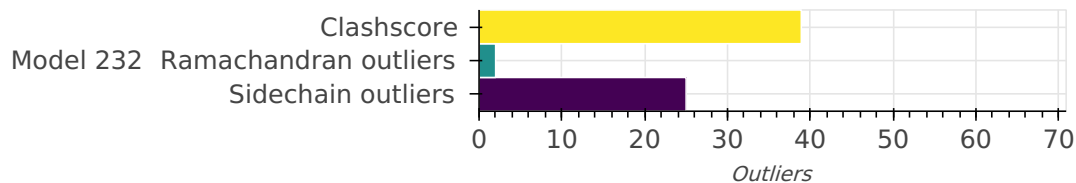
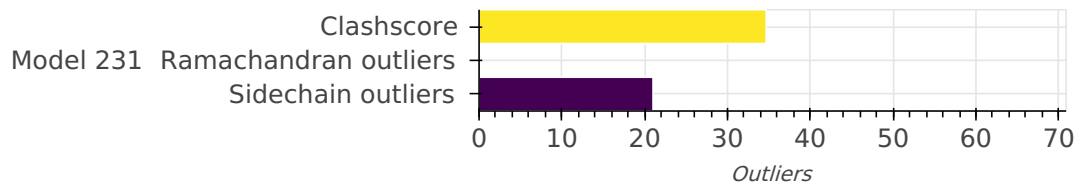
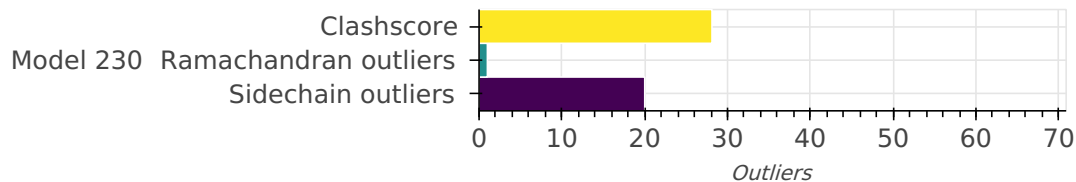
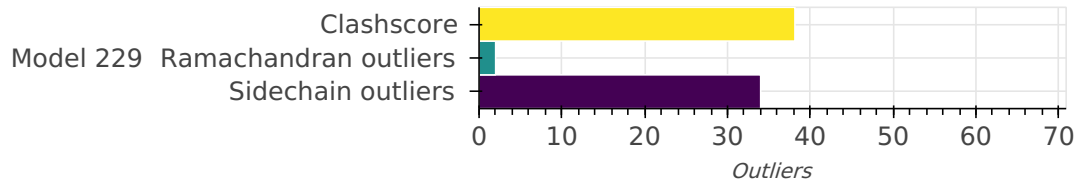
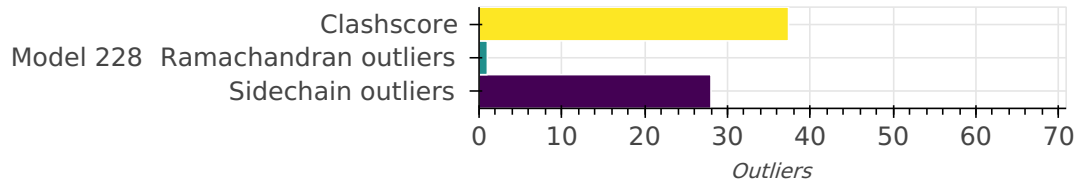
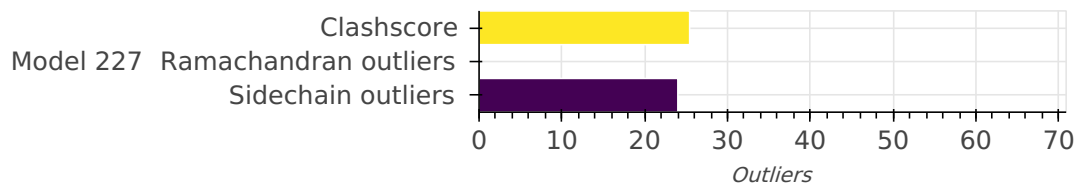
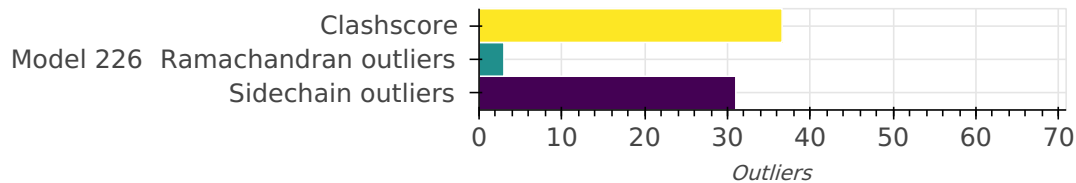


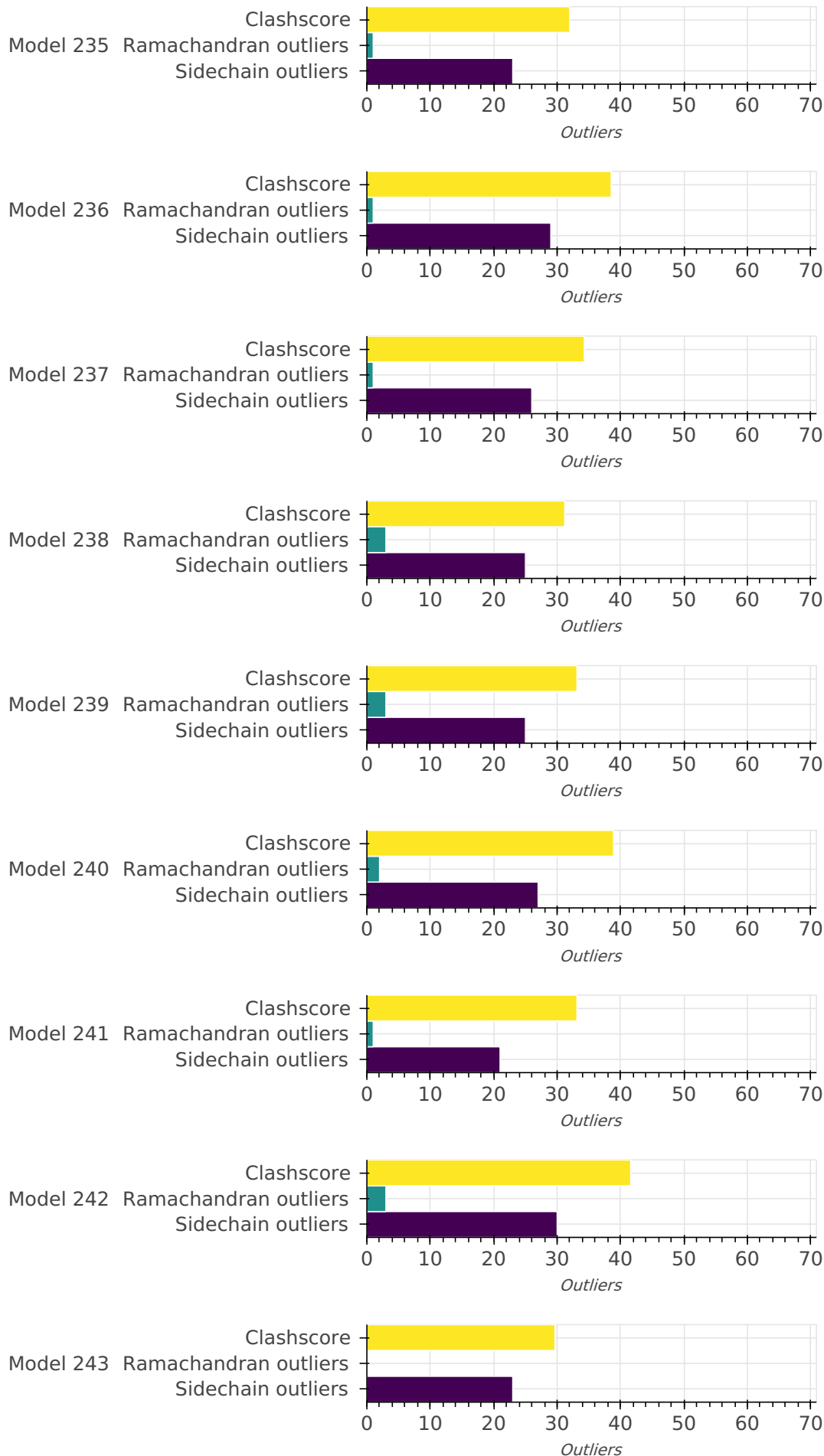


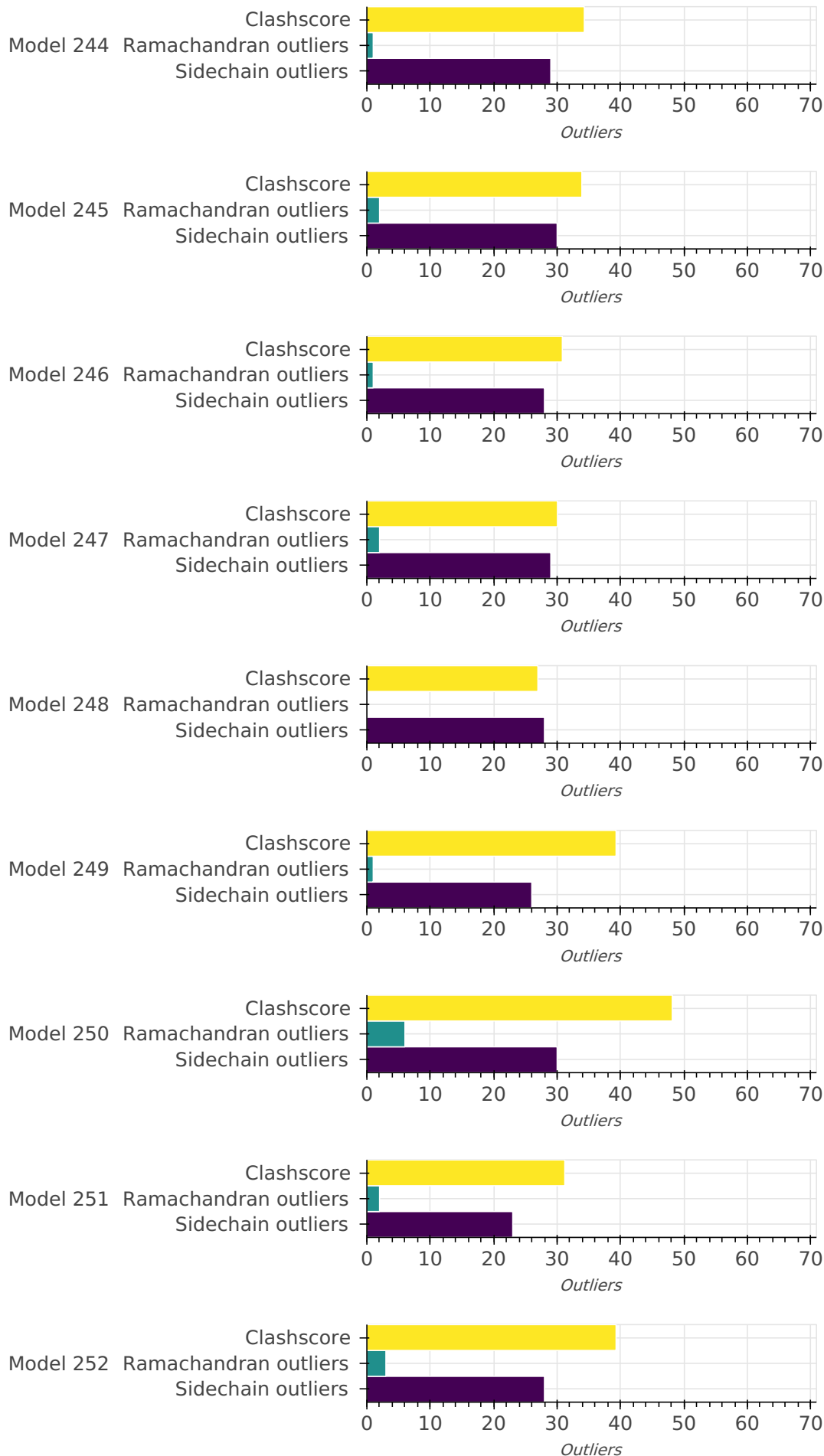


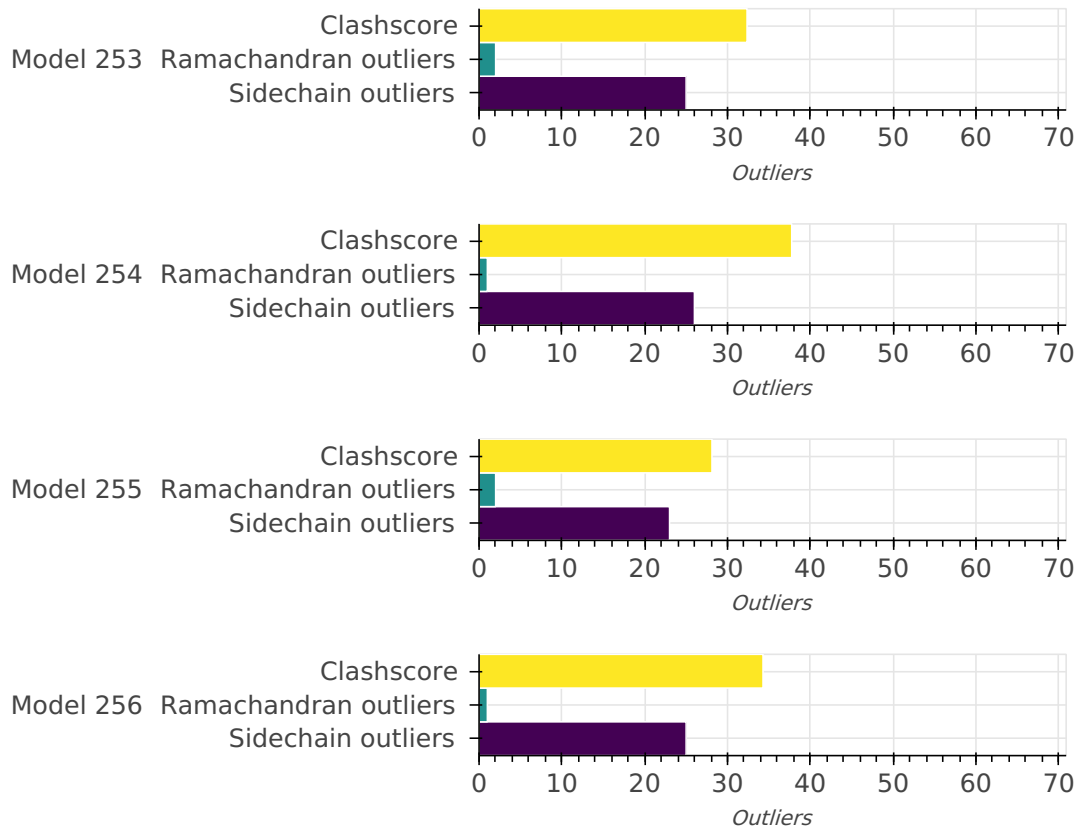












Ensemble information ?

This entry consists of 2 distinct ensemble(s).

Summary ?

This entry consists of 283 model(s). A total of 37 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	1-283	1	T4L	A	164	-	1-162, 1-162	98.78 / 100.00	Atomic

Datasets used for modeling ?

There are 37 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
2	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
3	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
4	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
5	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
6	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
7	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
8	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
9	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
10	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
11	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
12	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
13	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
14	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
15	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
16	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
17	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
18	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
19	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
20	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
21	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
22	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
23	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
24	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
25	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
26	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
27	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
28	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
29	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
30	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
31	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527

ID	Dataset type	Database name	Data access code
32	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
33	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
34	Ensemble FRET data	Zenodo	10.5281/zenodo.3376527
35	Experimental model	PDB	172L
36	Experimental model	PDB	148L
37	Single molecule FRET data	Zenodo	10.5281/zenodo.3376527

Methodology and software ?

This entry is a result of 2 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	free NMSim	None	None	None	True	False
2	1	FRET-guided NMSim	None	None	None	True	False
3	1	FRET screening	None	None	None	True	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Olga	Not available	model building and validation	https://github.com/Fluorescence-Tools/Olga
2	NMSim	Not available	model building	http://www.nmsim.de

Data quality ?

Single molecule FRET

Validation for this section is under development.

Ensemble 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 2754 bond length outliers in this entry (0.74% of 370521 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	82	ALA	C-N	9.77	1.19	1.33	282	161
A	137	ARG	CD-NE	7.39	1.56	1.46	7	51
A	24	TYR	C-N	7.38	1.43	1.33	3	21
A	68	ASN	CG-OD1	6.80	1.36	1.23	279	164
A	53	ASN	CG-OD1	6.78	1.36	1.23	44	82
A	83	LYS	CA-CB	6.70	1.40	1.53	198	3
A	135	LYS	C-N	6.62	1.42	1.33	7	3
A	77	GLY	C-N	6.27	1.42	1.33	8	2
A	51	GLY	C-N	6.18	1.24	1.33	144	145
A	132	ASN	CG-OD1	6.10	1.35	1.23	69	22
A	134	ALA	C-N	6.09	1.41	1.33	7	1
A	102	MET	C-N	6.07	1.41	1.33	7	1
A	69	GLN	CD-OE1	6.03	1.35	1.23	279	164
A	141	GLN	CD-OE1	5.94	1.34	1.23	24	119
A	56	GLY	C-N	5.92	1.25	1.33	176	147
A	144	ASN	CG-OD1	5.76	1.34	1.23	271	164
A	22	GLU	C-N	5.68	1.25	1.33	9	6
A	123	GLN	CD-OE1	5.67	1.34	1.23	124	164
A	25	TYR	C-N	5.52	1.41	1.33	8	3
A	122	GLN	CD-OE1	5.49	1.34	1.23	207	164
A	57	VAL	C-N	5.49	1.41	1.33	283	24
A	91	LEU	C-N	5.42	1.25	1.33	176	1
A	58	ILE	C-N	5.34	1.40	1.33	10	5
A	52	ARG	C-N	5.28	1.40	1.33	10	2
A	69	GLN	C-N	5.28	1.40	1.33	89	11
A	53	ASN	CG-ND2	5.17	1.22	1.33	70	82
A	100	ILE	C-N	5.09	1.26	1.33	184	4
A	144	ASN	C-N	5.02	1.40	1.33	99	3
A	122	GLN	CD-NE2	4.97	1.22	1.33	271	156
A	123	GLN	CD-NE2	4.90	1.23	1.33	273	154

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	22	GLU	CA-C	4.89	1.63	1.52	7	9
A	71	VAL	C-N	4.76	1.40	1.33	43	4
A	16	LYS	C-N	4.68	1.39	1.33	3	1
A	104	PHE	C-N	4.67	1.39	1.33	3	8
A	60	LYS	C-N	4.65	1.26	1.33	172	2
A	89	ASP	C-N	4.65	1.26	1.33	253	9
A	23	GLY	C-N	4.63	1.39	1.33	15	4
A	37	PRO	C-N	4.63	1.26	1.33	182	1
A	142	THR	N-CA	4.63	1.55	1.46	70	2
A	21	THR	C-N	4.61	1.39	1.33	4	3
A	144	ASN	CG-ND2	4.60	1.23	1.33	250	148
A	91	LEU	CB-CG	4.59	1.44	1.53	183	2
A	132	ASN	CG-ND2	4.57	1.23	1.33	73	22
A	55	ASN	C-N	4.55	1.27	1.33	271	1
A	19	LYS	CA-C	4.52	1.62	1.52	271	25
A	19	LYS	C-N	4.51	1.27	1.33	148	50
A	8	ARG	CD-NE	4.48	1.52	1.46	76	24
A	123	GLN	C-N	4.48	1.39	1.33	26	7
A	84	LEU	CB-CG	4.47	1.44	1.53	148	4
A	76	ARG	C-N	4.47	1.27	1.33	231	16
A	76	ARG	CD-NE	4.42	1.52	1.46	62	32
A	30	GLY	C-N	4.41	1.39	1.33	107	12
A	49	ALA	C-N	4.39	1.39	1.33	105	1
A	78	ILE	C-N	4.37	1.27	1.33	164	1
A	27	ILE	C-N	4.37	1.27	1.33	272	7
A	46	LEU	C-N	4.33	1.39	1.33	35	1
A	89	ASP	CG-OD2	4.33	1.33	1.25	250	21
A	68	ASN	C-N	4.33	1.39	1.33	3	1
A	159	ASP	CG-OD2	4.30	1.33	1.25	279	12
A	141	GLN	CD-NE2	4.30	1.24	1.33	108	49
A	86	PRO	C-N	4.28	1.39	1.33	149	19
A	62	GLU	CD-OE2	4.26	1.33	1.25	282	33
A	54	THR	C-N	4.26	1.27	1.33	250	7
A	69	GLN	CD-NE2	4.25	1.24	1.33	220	53
A	11	GLU	CD-OE1	4.24	1.33	1.25	224	26

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	141	GLN	C-N	4.24	1.39	1.33	254	3
A	67	PHE	CA-CB	4.21	1.45	1.53	203	1
A	62	GLU	CD-OE1	4.20	1.33	1.25	207	9
A	61	ASP	CG-OD2	4.20	1.33	1.25	147	20
A	119	ARG	NE-CZ	4.20	1.37	1.33	271	3
A	119	ARG	CD-NE	4.19	1.52	1.46	9	10
A	160	ALA	C-N	4.17	1.27	1.33	133	5
A	65	LYS	C-N	4.17	1.39	1.33	43	1
A	5	GLU	CD-OE1	4.14	1.33	1.25	153	19
A	45	GLU	CD-OE1	4.14	1.33	1.25	214	8
A	45	GLU	CD-OE2	4.13	1.33	1.25	177	17
A	149	VAL	C-N	4.08	1.39	1.33	118	2
A	80	ARG	CD-NE	4.08	1.52	1.46	22	1
A	84	LEU	CA-CB	4.05	1.45	1.53	131	2
A	68	ASN	CG-ND2	4.05	1.24	1.33	271	1
A	62	GLU	C-N	4.04	1.39	1.33	114	2
A	72	ASP	CG-OD2	4.04	1.33	1.25	156	2
A	87	VAL	C-N	4.01	1.39	1.33	89	1
A	66	LEU	C-N	4.00	1.39	1.33	144	1

Standard geometry: angle outliers ?

There are 6513 bond angle outliers in this entry (1.30% of 499122 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	54	THR	C-N-CA	15.26	149.18	121.70	10	119
A	22	GLU	C-N-CA	11.92	143.15	121.70	9	47
A	138	TRP	CA-CB-CG	8.31	129.40	113.60	8	32
A	85	LYS	CA-C-N	8.25	129.28	116.90	26	168
A	20	ASP	CA-CB-CG	8.07	120.67	112.60	99	80
A	2	ASN	CA-CB-CG	8.05	120.65	112.60	221	162
A	31	HIS	CA-CB-CG	8.01	105.79	113.80	183	164
A	137	ARG	C-N-CA	7.47	135.14	121.70	38	57
A	40	ASN	CA-CB-CG	7.35	105.25	112.60	271	166
A	20	ASP	C-N-CA	7.31	134.86	121.70	52	80
A	132	ASN	CA-CB-CG	7.25	105.35	112.60	43	119

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	80	ARG	C-N-CA	7.22	134.69	121.70	222	75
A	53	ASN	CA-CB-CG	6.96	119.56	112.60	10	28
A	140	ASN	CA-CB-CG	6.90	105.70	112.60	198	220
A	24	TYR	C-N-CA	6.60	133.57	121.70	48	9
A	4	PHE	CA-CB-CG	6.44	120.24	113.80	172	122
A	61	ASP	CA-CB-CG	6.27	106.33	112.60	189	149
A	27	ILE	C-N-CA	6.21	132.88	121.70	80	98
A	21	THR	C-N-CA	6.16	132.79	121.70	237	108
A	54	THR	CA-C-O	6.08	110.46	120.80	50	5
A	15	LEU	C-N-CA	5.94	132.40	121.70	134	69
A	68	ASN	N-CA-CB	5.90	120.52	110.50	146	164
A	54	THR	CA-C-N	5.89	127.97	116.20	3	118
A	133	LEU	C-N-CA	5.78	132.11	121.70	7	1
A	14	ARG	C-N-CA	5.78	132.10	121.70	271	3
A	54	THR	C-CA-CB	5.69	121.62	109.10	10	2
A	68	ASN	CA-CB-CG	5.69	118.29	112.60	184	155
A	67	PHE	CA-CB-CG	5.54	108.26	113.80	144	23
A	29	ILE	C-N-CA	5.54	131.67	121.70	240	24
A	145	ARG	CA-CB-CG	5.53	125.16	114.10	53	22
A	64	GLU	C-CA-CB	5.50	120.55	110.10	271	164
A	10	ASP	CA-CB-CG	5.50	107.10	112.60	159	77
A	147	LYS	CB-CG-CD	5.48	123.91	111.30	8	47
A	145	ARG	C-CA-CB	5.47	120.50	110.10	20	119
A	124	LYS	CA-CB-CG	5.46	103.18	114.10	242	155
A	142	THR	CA-C-N	5.42	125.03	116.90	56	117
A	99	LEU	CD1-CG-CD2	5.35	99.02	110.80	56	119
A	114	PHE	CA-CB-CG	5.34	108.46	113.80	158	185
A	107	GLY	C-N-CA	5.33	131.30	121.70	89	86
A	22	GLU	O-C-N	5.33	131.52	123.00	9	5
A	34	THR	CA-CB-OG1	5.29	117.53	109.60	3	34
A	123	GLN	C-N-CA	5.27	131.19	121.70	34	40
A	90	SER	CA-C-O	5.27	111.85	120.80	269	12
A	39	LEU	N-CA-CB	5.22	119.38	110.50	250	5

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	75	VAL	CA-CB-CG2	5.21	101.55	110.40	148	164
A	25	TYR	CA-CB-CG	5.20	104.54	113.90	242	159
A	86	PRO	N-CA-CB	5.19	108.71	103.00	232	127
A	5	GLU	CB-CG-CD	5.17	103.80	112.60	236	153
A	63	ALA	C-CA-CB	5.17	102.74	110.50	252	93
A	31	HIS	CB-CG-ND1	5.14	114.98	122.70	49	109
A	95	ARG	NE-CZ-NH2	5.09	123.78	119.20	271	78
A	26	THR	CA-CB-CG2	5.07	119.13	110.50	71	87
A	141	GLN	CG-CD-NE2	5.07	124.01	116.40	33	80
A	36	SER	CA-C-N	5.07	124.50	116.90	29	60
A	20	ASP	C-CA-CB	5.06	119.72	110.10	7	92
A	51	GLY	C-N-CA	5.04	130.77	121.70	92	1
A	144	ASN	CA-CB-CG	5.02	107.58	112.60	48	38
A	126	TRP	CB-CG-CD2	5.00	133.80	126.80	265	148
A	124	LYS	CB-CG-CD	4.96	122.71	111.30	140	1
A	134	ALA	O-C-N	4.96	115.07	123.00	7	1
A	54	THR	O-C-N	4.95	115.08	123.00	50	36
A	120	MET	CG-SD-CE	4.93	90.05	100.90	6	119
A	55	ASN	N-CA-CB	4.92	118.87	110.50	271	113
A	22	GLU	CA-C-O	4.88	112.50	120.80	7	4
A	91	LEU	C-CA-CB	4.88	100.84	110.10	184	42
A	24	TYR	N-CA-CB	4.75	118.58	110.50	183	54
A	15	LEU	O-C-N	4.72	130.55	123.00	176	16
A	81	ASN	C-CA-CB	4.71	119.05	110.10	137	60
A	68	ASN	CB-CG-ND2	4.69	123.43	116.40	271	5
A	37	PRO	C-N-CA	4.67	130.11	121.70	8	1
A	159	ASP	CA-CB-CG	4.66	107.94	112.60	266	48
A	74	ALA	C-CA-CB	4.65	103.53	110.50	236	141
A	39	LEU	C-CA-CB	4.62	118.88	110.10	276	20
A	26	THR	C-N-CA	4.62	130.01	121.70	2	2
A	13	LEU	C-N-CA	4.61	130.00	121.70	271	2
A	72	ASP	CA-CB-CG	4.60	108.00	112.60	168	41
A	142	THR	O-C-N	4.59	115.66	123.00	8	59
A	66	LEU	C-N-CA	4.56	113.49	121.70	203	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	85	LYS	O-C-N	4.56	115.70	123.00	8	4
A	29	ILE	N-CA-CB	4.54	119.21	111.50	148	1
A	131	VAL	C-CA-CB	4.52	102.81	111.40	197	67
A	54	THR	N-CA-C	4.51	123.62	111.00	83	38
A	126	TRP	C-CA-CB	4.50	118.65	110.10	167	95
A	134	ALA	C-N-CA	4.50	113.61	121.70	7	1
A	25	TYR	O-C-N	4.47	115.84	123.00	8	1
A	124	LYS	N-CA-CB	4.45	118.07	110.50	140	1
A	56	GLY	C-N-CA	4.44	129.69	121.70	29	4
A	62	GLU	C-CA-CB	4.42	118.50	110.10	121	64
A	14	ARG	CB-CG-CD	4.39	121.41	111.30	225	32
A	59	THR	O-C-N	4.39	115.97	123.00	4	1
A	36	SER	O-C-N	4.37	116.00	123.00	43	3
A	52	ARG	O-C-N	4.36	116.02	123.00	10	1
A	44	SER	N-CA-CB	4.35	117.90	110.50	251	64
A	96	ARG	CA-C-O	4.35	113.41	120.80	215	1
A	8	ARG	CD-NE-CZ	4.34	130.48	124.40	271	1
A	25	TYR	N-CA-CB	4.33	117.86	110.50	28	1
A	63	ALA	N-CA-CB	4.30	103.95	110.40	214	4
A	52	ARG	CA-CB-CG	4.30	122.70	114.10	31	1
A	78	ILE	CA-CB-CG2	4.28	117.78	110.50	269	3
A	151	THR	CA-CB-OG1	4.27	103.20	109.60	138	46

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	44.11	115
2	39.89	104
3	47.18	123
4	53.32	139
5	45.65	119
6	43.73	114
7	64.44	168

Model ID	Clash score	Number of clashes
8	53.70	140
9	36.07	94
10	46.03	120
11	41.81	109
12	46.41	121
13	53.70	140
14	41.81	109
15	39.89	104
16	47.18	123
17	34.91	91
18	42.58	111
19	37.59	98
20	44.11	115
21	40.28	105
22	42.58	111
23	36.06	94
24	46.41	121
25	37.21	97
26	47.56	124
27	32.22	84
28	46.41	121
29	33.37	87
30	41.43	108
31	39.13	102
32	39.51	103
33	44.50	116
34	40.28	105
35	38.74	101
36	47.18	123
37	43.34	113
38	46.41	121
39	28.00	73
40	38.74	101
41	40.66	106
42	43.73	114

Model ID	Clash score	Number of clashes
43	52.55	137
44	43.34	113
45	38.36	100
46	41.04	107
47	45.26	118
48	47.56	124
49	40.28	105
50	44.50	116
51	46.41	121
52	35.29	92
53	42.96	112
54	41.81	109
55	42.58	111
56	50.63	132
57	34.91	91
58	36.82	96
59	41.81	109
60	41.81	109
61	37.97	99
62	46.80	122
63	39.51	103
64	50.63	132
65	33.37	87
66	36.06	94
67	41.81	109
68	42.58	111
69	41.43	108
70	46.41	121
71	49.87	130
72	52.17	136
73	33.37	87
74	29.54	77
75	43.34	113
76	51.40	134
77	41.04	107

Model ID	Clash score	Number of clashes
78	37.59	98
79	39.89	104
80	36.06	94
81	37.21	97
82	47.56	124
83	38.74	101
84	48.71	127
85	38.36	100
86	30.30	79
87	35.67	93
88	34.91	91
89	41.81	109
90	36.82	96
91	41.81	109
92	44.11	115
93	39.13	102
94	41.04	107
95	46.80	122
96	35.67	93
97	43.34	113
98	32.60	85
99	44.88	117
100	45.65	119
101	37.21	97
102	44.88	117
103	46.03	120
104	34.14	89
105	40.66	106
106	42.19	110
107	44.88	117
108	42.58	111
109	38.36	100
110	42.19	110
111	47.95	125
112	32.99	86

Model ID	Clash score	Number of clashes
113	39.51	103
114	40.28	105
115	41.81	109
116	36.44	95
117	43.73	114
118	42.96	112
119	47.95	125
120	35.44	92
121	38.91	101
122	43.14	112
123	39.68	103
124	29.66	77
125	35.44	92
126	42.76	111
127	35.82	93
128	35.82	93
129	36.21	94
130	35.44	92
131	38.91	101
132	40.45	105
133	31.59	82
134	42.76	111
135	25.81	67
136	30.82	80
137	32.74	85
138	40.06	104
139	36.59	95
140	35.44	92
141	39.68	103
142	33.13	86
143	33.13	86
144	28.12	73
145	33.90	88
146	41.60	108
147	30.82	80

Model ID	Clash score	Number of clashes
148	35.05	91
149	32.74	85
150	37.37	97
151	29.66	77
152	40.06	104
153	30.05	78
154	33.51	87
155	33.90	88
156	33.51	87
157	37.37	97
158	25.81	67
159	26.19	68
160	33.90	88
161	41.22	107
162	43.14	112
163	45.84	119
164	40.06	104
165	37.37	97
166	27.35	71
167	30.43	79
168	35.82	93
169	36.59	95
170	26.96	70
171	37.37	97
172	33.51	87
173	28.51	74
174	34.67	90
175	36.98	96
176	36.21	94
177	36.21	94
178	33.51	87
179	36.21	94
180	39.29	102
181	39.68	103
182	41.22	107

Model ID	Clash score	Number of clashes
183	42.37	110
184	44.30	115
185	31.97	83
186	40.45	105
187	33.90	88
188	31.97	83
189	29.28	76
190	39.29	102
191	35.82	93
192	16.18	42
193	30.05	78
194	32.74	85
195	34.67	90
196	32.36	84
197	31.59	82
198	36.59	95
199	38.52	100
200	38.14	99
201	39.29	102
202	26.96	70
203	38.91	101
204	30.05	78
205	25.42	66
206	34.28	89
207	26.96	70
208	33.51	87
209	34.28	89
210	38.14	99
211	31.59	82
212	32.36	84
213	38.91	101
214	39.29	102
215	33.90	88
216	33.13	86
217	33.51	87

Model ID	Clash score	Number of clashes
218	30.43	79
219	38.52	100
220	45.84	119
221	36.98	96
222	31.97	83
223	30.05	78
224	24.65	64
225	39.68	103
226	36.59	95
227	25.42	66
228	37.37	97
229	38.14	99
230	28.12	73
231	34.67	90
232	38.91	101
233	30.82	80
234	35.05	91
235	31.97	83
236	38.52	100
237	34.28	89
238	31.20	81
239	33.13	86
240	38.91	101
241	33.13	86
242	41.60	108
243	29.66	77
244	34.28	89
245	33.90	88
246	30.82	80
247	30.05	78
248	26.96	70
249	39.29	102
250	48.15	125
251	31.20	81
252	39.29	102

Model ID	Clash score	Number of clashes
253	32.36	84
254	37.75	98
255	28.12	73
256	34.28	89
257	36.98	96
258	29.66	77
259	36.98	96
260	32.74	85
261	32.36	84
262	29.66	77
263	34.28	89
264	30.82	80
265	33.90	88
266	44.30	115
267	39.68	103
268	37.37	97
269	35.44	92
270	38.91	101
271	35.05	91
272	42.37	110
273	32.74	85
274	29.28	76
275	38.14	99
276	34.28	89
277	42.76	111
278	32.74	85
279	41.22	107
280	40.45	105
281	36.98	96
282	32.74	85
283	38.91	101

There are 27892 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:130:ALA:HB1	A:150:ILE:HG23	1.21	67	179
A:17:ILE:HD12	A:43:LYS:HD3	1.20	164	64
A:16:LYS:HG3	A:57:VAL:HG22	1.19	272	69
A:58:ILE:HD13	A:63:ALA:HB2	1.19	137	34
A:16:LYS:HG2	A:57:VAL:HG22	1.18	206	97
A:81:ASN:HB3	A:84:LEU:HB2	1.18	42	115
A:15:LEU:HD12	A:58:ILE:HG13	1.18	98	44
A:13:LEU:HD23	A:29:ILE:HG13	1.18	7	39
A:102:MET:HE3	A:111:VAL:HG13	1.18	87	48
A:13:LEU:HG	A:29:ILE:HG23	1.18	138	63
A:27:ILE:HG21	A:46:LEU:HD21	1.18	156	17
A:103:VAL:HG22	A:111:VAL:HG21	1.17	274	117
A:1:MET:HB3	A:158:TRP:HB3	1.17	84	32
A:141:GLN:HG2	A:142:THR:HG23	1.17	91	9
A:91:LEU:HD11	A:121:LEU:HD12	1.17	119	25
A:50:ILE:HD13	A:66:LEU:HD13	1.17	5	6
A:120:MET:HB3	A:125:ARG:HB2	1.16	6	31
A:151:THR:HG22	A:160:ALA:HB1	1.16	90	8
A:1:MET:HE1	A:9:ILE:HD12	1.16	110	52
A:7:LEU:HD12	A:11:GLU:HB2	1.16	277	58
A:79:LEU:HD23	A:85:LYS:HG3	1.16	147	35
A:79:LEU:HD22	A:85:LYS:HG3	1.15	255	13
A:121:LEU:HD21	A:153:PHE:HE1	1.15	109	17
A:50:ILE:HG23	A:62:GLU:HG2	1.15	93	8
A:120:MET:HB3	A:125:ARG:HB3	1.15	23	18
A:15:LEU:HD11	A:29:ILE:HG13	1.15	226	52
A:121:LEU:HD13	A:126:TRP:HZ3	1.14	12	59
A:151:THR:HG21	A:160:ALA:HB3	1.14	199	25
A:8:ARG:HG3	A:67:PHE:HE2	1.14	114	23
A:78:ILE:HG12	A:103:VAL:HG21	1.14	46	56
A:130:ALA:HB3	A:154:ARG:HG3	1.14	48	8
A:130:ALA:HB2	A:150:ILE:HG21	1.14	268	7
A:17:ILE:HD11	A:43:LYS:HB3	1.14	54	12
A:33:LEU:HD21	A:46:LEU:HG	1.14	252	33
A:58:ILE:HD12	A:63:ALA:HB2	1.14	24	93

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:17:ILE:HD12	A:43:LYS:HD2	1.14	239	15
A:17:ILE:HG12	A:27:ILE:HG22	1.13	272	45
A:1:MET:HG3	A:5:GLU:HB2	1.13	241	58
A:17:ILE:HG21	A:42:ALA:HB1	1.13	111	13
A:102:MET:HG2	A:111:VAL:HG22	1.12	60	51
A:87:VAL:HG22	A:118:LEU:HD11	1.12	199	2
A:1:MET:HE3	A:6:MET:HB2	1.12	206	37
A:24:TYR:HD1	A:35:LYS:HG3	1.12	119	3
A:75:VAL:HG13	A:79:LEU:HD12	1.12	183	6
A:27:ILE:HD13	A:46:LEU:HD21	1.11	70	14
A:27:ILE:HD11	A:58:ILE:HG21	1.11	8	4
A:10:ASP:HB3	A:145:ARG:HG2	1.11	277	43
A:87:VAL:HG21	A:118:LEU:HD21	1.11	121	20
A:79:LEU:HD12	A:85:LYS:HG3	1.11	120	20
A:91:LEU:HD12	A:99:LEU:HD11	1.11	57	35
A:27:ILE:HG23	A:33:LEU:HD22	1.11	281	78
A:10:ASP:HB3	A:145:ARG:HG3	1.10	246	40
A:7:LEU:HB3	A:67:PHE:HZ	1.10	110	73
A:114:PHE:HB3	A:118:LEU:HD23	1.10	183	7
A:27:ILE:HD11	A:58:ILE:HG12	1.10	212	38
A:13:LEU:HG	A:29:ILE:HG22	1.10	266	2
A:94:VAL:HG12	A:152:THR:HG23	1.10	241	31
A:13:LEU:HD23	A:29:ILE:HD11	1.10	21	73
A:29:ILE:HD12	A:67:PHE:HE2	1.10	175	4
A:50:ILE:HD11	A:66:LEU:HD21	1.09	216	23
A:102:MET:HE2	A:106:MET:HE1	1.09	124	68
A:7:LEU:HD23	A:67:PHE:HE1	1.09	23	30
A:88:TYR:HD1	A:99:LEU:HD13	1.08	99	54
A:120:MET:HG2	A:125:ARG:HB2	1.08	27	24
A:78:ILE:HD11	A:84:LEU:HD12	1.08	147	12
A:84:LEU:HD12	A:99:LEU:HD21	1.08	183	5
A:34:THR:HG21	A:42:ALA:HB2	1.08	279	14
A:46:LEU:HD11	A:58:ILE:HG23	1.08	50	34
A:79:LEU:HD13	A:85:LYS:HG3	1.07	137	16
A:34:THR:HG21	A:42:ALA:HB1	1.07	150	18

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:46:LEU:HD11	A:58:ILE:HG21	1.07	93	22
A:46:LEU:HD12	A:50:ILE:HG13	1.07	4	22
A:102:MET:HE1	A:133:LEU:HB3	1.06	159	63
A:7:LEU:HD21	A:71:VAL:HG21	1.06	77	4
A:1:MET:SD	A:5:GLU:HB3	1.06	79	62
A:102:MET:HE1	A:133:LEU:HG	1.06	263	66
A:14:ARG:HB2	A:18:TYR:HE2	1.06	208	17
A:139:TYR:HE2	A:150:ILE:HD12	1.06	9	7
A:87:VAL:HG21	A:118:LEU:HD23	1.05	226	4
A:4:PHE:HZ	A:64:GLU:HG3	1.05	248	6
A:50:ILE:HG21	A:54:THR:SG	1.05	263	89
A:13:LEU:HD21	A:63:ALA:HB1	1.05	107	17
A:24:TYR:HB2	A:32:LEU:HD21	1.05	119	34
A:50:ILE:HG13	A:54:THR:SG	1.05	182	50
A:8:ARG:HB3	A:13:LEU:HB2	1.04	279	3
A:25:TYR:HE1	A:39:LEU:HD12	1.04	48	1
A:78:ILE:HG21	A:88:TYR:HD2	1.04	262	15
A:121:LEU:HD22	A:126:TRP:HE3	1.03	43	51
A:17:ILE:HG22	A:25:TYR:HD1	1.03	195	34
A:79:LEU:HD12	A:85:LYS:HG2	1.03	272	13
A:84:LEU:HG	A:118:LEU:HD13	1.03	53	2
A:25:TYR:HE2	A:39:LEU:HD13	1.03	33	8
A:1:MET:HG3	A:158:TRP:CE3	1.03	25	52
A:84:LEU:HG	A:108:GLU:HB3	1.02	114	19
A:7:LEU:HB3	A:67:PHE:CZ	1.02	33	84
A:17:ILE:HD13	A:43:LYS:HB3	1.02	64	4
A:151:THR:HG21	A:160:ALA:HB2	1.02	250	34
A:78:ILE:HG13	A:103:VAL:HG21	1.02	104	58
A:91:LEU:HD22	A:126:TRP:CH2	1.02	20	2
A:24:TYR:HB3	A:32:LEU:HD23	1.02	85	6

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	160	140	16	4

Model ID	Analysed	Favored	Allowed	Outliers
2	160	142	15	3
3	160	140	13	7
4	160	130	20	10
5	160	148	8	4
6	160	142	17	1
7	160	130	23	7
8	160	128	25	7
9	160	147	11	2
10	160	139	16	5
11	160	137	19	4
12	160	144	15	1
13	160	147	10	3
14	160	145	12	3
15	160	144	10	6
16	160	142	17	1
17	160	151	5	4
18	160	143	12	5
19	160	147	8	5
20	160	141	18	1
21	160	151	7	2
22	160	150	6	4
23	160	142	14	4
24	160	143	11	6
25	160	145	8	7
26	160	144	14	2
27	160	146	12	2
28	160	138	17	5
29	160	146	12	2
30	160	147	9	4
31	160	149	9	2
32	160	145	13	2
33	160	148	9	3
34	160	150	8	2
35	160	149	8	3
36	160	142	15	3

Model ID	Analysed	Favored	Allowed	Outliers
37	160	146	11	3
38	160	137	20	3
39	160	146	9	5
40	160	147	10	3
41	160	150	7	3
42	160	141	15	4
43	160	137	16	7
44	160	141	17	2
45	160	152	7	1
46	160	143	15	2
47	160	144	10	6
48	160	134	14	12
49	160	146	11	3
50	160	142	10	8
51	160	141	15	4
52	160	148	8	4
53	160	140	18	2
54	160	148	10	2
55	160	145	12	3
56	160	134	22	4
57	160	151	6	3
58	160	146	10	4
59	160	142	14	4
60	160	149	9	2
61	160	149	7	4
62	160	135	22	3
63	160	147	8	5
64	160	150	7	3
65	160	152	6	2
66	160	146	10	4
67	160	148	8	4
68	160	148	10	2
69	160	149	8	3
70	160	142	15	3
71	160	141	17	2

Model ID	Analysed	Favored	Allowed	Outliers
72	160	136	21	3
73	160	146	10	4
74	160	154	5	1
75	160	147	12	1
76	160	137	20	3
77	160	146	11	3
78	160	150	8	2
79	160	144	14	2
80	160	142	12	6
81	160	144	13	3
82	160	151	8	1
83	160	147	9	4
84	160	147	9	4
85	160	141	15	4
86	160	152	7	1
87	160	149	7	4
88	160	141	16	3
89	160	143	13	4
90	160	151	9	0
91	160	143	15	2
92	160	140	17	3
93	160	140	16	4
94	160	142	17	1
95	160	138	17	5
96	160	147	10	3
97	160	141	16	3
98	160	148	10	2
99	160	146	11	3
100	160	147	11	2
101	160	142	13	5
102	160	140	16	4
103	160	150	7	3
104	160	148	9	3
105	160	130	28	2
106	160	150	7	3

Model ID	Analysed	Favored	Allowed	Outliers
107	160	134	19	7
108	160	148	9	3
109	160	149	8	3
110	160	144	12	4
111	160	149	6	5
112	160	150	8	2
113	160	154	5	1
114	160	143	12	5
115	160	139	19	2
116	160	148	11	1
117	160	143	12	5
118	160	140	19	1
119	160	148	11	1
120	160	151	8	1
121	160	140	17	3
122	160	139	19	2
123	160	145	11	4
124	160	153	7	0
125	160	151	9	0
126	160	139	19	2
127	160	149	7	4
128	160	146	10	4
129	160	147	11	2
130	160	147	12	1
131	160	145	14	1
132	160	142	17	1
133	160	150	9	1
134	160	144	14	2
135	160	156	4	0
136	160	143	16	1
137	160	146	12	2
138	160	139	17	4
139	160	150	8	2
140	160	145	14	1
141	160	146	12	2

Model ID	Analysed	Favored	Allowed	Outliers
142	160	146	11	3
143	160	145	12	3
144	160	149	9	2
145	160	145	13	2
146	160	148	10	2
147	160	147	10	3
148	160	142	18	0
149	160	151	9	0
150	160	146	11	3
151	160	149	9	2
152	160	144	15	1
153	160	144	14	2
154	160	144	14	2
155	160	152	7	1
156	160	152	7	1
157	160	147	11	2
158	160	150	8	2
159	160	152	7	1
160	160	154	6	0
161	160	148	10	2
162	160	148	9	3
163	160	147	9	4
164	160	140	15	5
165	160	144	14	2
166	160	148	12	0
167	160	149	11	0
168	160	144	14	2
169	160	148	10	2
170	160	154	6	0
171	160	143	15	2
172	160	143	16	1
173	160	149	11	0
174	160	147	13	0
175	160	146	11	3
176	160	141	17	2

Model ID	Analysed	Favored	Allowed	Outliers
177	160	139	20	1
178	160	152	8	0
179	160	147	12	1
180	160	138	18	4
181	160	143	15	2
182	160	142	16	2
183	160	146	13	1
184	160	139	16	5
185	160	151	8	1
186	160	142	15	3
187	160	148	11	1
188	160	148	12	0
189	160	143	12	5
190	160	143	14	3
191	160	146	11	3
192	160	156	3	1
193	160	145	13	2
194	160	148	12	0
195	160	149	10	1
196	160	153	5	2
197	160	150	10	0
198	160	145	11	4
199	160	147	13	0
200	160	142	15	3
201	160	144	13	3
202	160	151	9	0
203	160	144	13	3
204	160	150	9	1
205	160	150	10	0
206	160	150	9	1
207	160	153	6	1
208	160	150	8	2
209	160	140	15	5
210	160	151	9	0
211	160	154	6	0

Model ID	Analysed	Favored	Allowed	Outliers
212	160	143	17	0
213	160	145	13	2
214	160	145	13	2
215	160	144	15	1
216	160	152	7	1
217	160	144	15	1
218	160	152	8	0
219	160	153	5	2
220	160	151	7	2
221	160	149	8	3
222	160	147	11	2
223	160	140	17	3
224	160	146	13	1
225	160	146	12	2
226	160	148	9	3
227	160	150	10	0
228	160	149	10	1
229	160	148	10	2
230	160	148	11	1
231	160	151	9	0
232	160	144	14	2
233	160	147	13	0
234	160	143	14	3
235	160	151	8	1
236	160	144	15	1
237	160	146	13	1
238	160	140	17	3
239	160	146	11	3
240	160	150	8	2
241	160	154	5	1
242	160	141	16	3
243	160	147	13	0
244	160	146	13	1
245	160	148	10	2
246	160	143	16	1

Model ID	Analysed	Favored	Allowed	Outliers
247	160	149	9	2
248	160	155	5	0
249	160	151	8	1
250	160	137	17	6
251	160	146	12	2
252	160	145	12	3
253	160	147	11	2
254	160	145	14	1
255	160	146	12	2
256	160	151	8	1
257	160	149	9	2
258	160	149	11	0
259	160	151	9	0
260	160	145	13	2
261	160	152	8	0
262	160	152	7	1
263	160	147	13	0
264	160	152	7	1
265	160	146	13	1
266	160	142	17	1
267	160	149	8	3
268	160	148	11	1
269	160	138	20	2
270	160	145	13	2
271	160	137	18	5
272	160	139	19	2
273	160	154	6	0
274	160	153	5	2
275	160	149	9	2
276	160	149	10	1
277	160	150	9	1
278	160	146	13	1
279	160	137	19	4
280	160	146	14	0
281	160	146	10	4

Model ID	Analysed	Favored	Allowed	Outliers
282	160	151	6	3
283	160	142	17	1

There are 58 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	30	GLY	116
A	124	LYS	57
A	12	GLY	51
A	138	TRP	45
A	55	ASN	44
A	28	GLY	43
A	54	THR	39
A	37	PRO	33
A	80	ARG	20
A	143	PRO	18
A	23	GLY	17
A	59	THR	16
A	92	ASP	11
A	142	THR	11
A	134	ALA	10
A	25	TYR	9
A	38	SER	9
A	53	ASN	9
A	58	ILE	8
A	114	PHE	8
A	17	ILE	7
A	90	SER	7
A	14	ARG	6
A	22	GLU	6
A	56	GLY	6
A	81	ASN	6
A	136	SER	6
A	52	ARG	5
A	91	LEU	5
A	16	LYS	4

Chain	Res	Type	Models (Total)
A	57	VAL	4
A	78	ILE	4
A	113	GLY	4
A	29	ILE	3
A	107	GLY	3
A	110	GLY	3
A	15	LEU	2
A	33	LEU	2
A	34	THR	2
A	49	ALA	2
A	83	LYS	2
A	85	LYS	2
A	108	GLU	2
A	6	MET	1
A	8	ARG	1
A	9	ILE	1
A	13	LEU	1
A	20	ASP	1
A	21	THR	1
A	32	LEU	1
A	42	ALA	1
A	51	GLY	1
A	77	GLY	1
A	79	LEU	1
A	104	PHE	1
A	123	GLN	1
A	133	LEU	1
A	159	ASP	1

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	134	77	23	34
2	134	83	28	23
3	134	81	24	29

Model ID	Analysed	Favored	Allowed	Outliers
4	134	81	18	35
5	134	84	22	28
6	134	88	19	27
7	134	72	22	40
8	134	75	23	36
9	134	87	27	20
10	134	79	25	30
11	134	82	20	32
12	134	87	18	29
13	134	86	21	27
14	134	90	27	17
15	134	85	25	24
16	134	84	19	31
17	134	83	25	26
18	134	92	15	27
19	134	82	27	25
20	134	72	28	34
21	134	94	17	23
22	134	86	29	19
23	134	89	23	22
24	134	84	26	24
25	134	76	26	32
26	134	79	22	33
27	134	94	17	23
28	134	83	30	21
29	134	89	23	22
30	134	83	25	26
31	134	81	26	27
32	134	82	26	26
33	134	85	30	19
34	134	81	23	30
35	134	85	27	22
36	134	82	27	25
37	134	85	21	28
38	134	78	26	30

Model ID	Analysed	Favored	Allowed	Outliers
39	134	88	26	20
40	134	80	24	30
41	134	94	20	20
42	134	85	23	26
43	134	73	27	34
44	134	79	22	33
45	134	83	25	26
46	134	90	18	26
47	134	88	24	22
48	134	82	26	26
49	134	84	30	20
50	134	79	24	31
51	134	80	16	38
52	134	84	26	24
53	134	72	28	34
54	134	87	23	24
55	134	88	19	27
56	134	82	21	31
57	134	91	23	20
58	134	75	38	21
59	134	90	26	18
60	134	94	24	16
61	134	80	25	29
62	134	77	25	32
63	134	93	19	22
64	134	86	19	29
65	134	88	21	25
66	134	96	22	16
67	134	82	16	36
68	134	90	17	27
69	134	81	25	28
70	134	89	19	26
71	134	89	21	24
72	134	78	19	37
73	134	90	26	18

Model ID	Analysed	Favored	Allowed	Outliers
74	134	86	26	22
75	134	87	22	25
76	134	80	21	33
77	134	82	22	30
78	134	83	23	28
79	134	82	18	34
80	134	95	16	23
81	134	75	25	34
82	134	84	20	30
83	134	92	18	24
84	134	69	33	32
85	134	84	32	18
86	134	93	22	19
87	134	88	26	20
88	134	82	25	27
89	134	80	27	27
90	134	84	27	23
91	134	89	18	27
92	134	77	25	32
93	134	94	24	16
94	134	86	21	27
95	134	74	26	34
96	134	93	23	18
97	134	87	23	24
98	134	90	21	23
99	134	89	16	29
100	134	88	22	24
101	134	86	20	28
102	134	71	27	36
103	134	82	26	26
104	134	82	31	21
105	134	87	16	31
106	134	91	19	24
107	134	75	31	28
108	134	90	24	20

Model ID	Analysed	Favored	Allowed	Outliers
109	134	87	21	26
110	134	86	22	26
111	134	91	17	26
112	134	89	28	17
113	134	86	25	23
114	134	85	26	23
115	134	80	26	28
116	134	91	18	25
117	134	71	30	33
118	134	79	24	31
119	134	84	18	32
120	133	80	27	26
121	133	80	29	24
122	133	72	33	28
123	133	74	25	34
124	133	87	25	21
125	133	80	31	22
126	133	77	24	32
127	133	86	30	17
128	133	76	27	30
129	133	80	28	25
130	133	90	21	22
131	133	81	30	22
132	133	83	18	32
133	133	81	25	27
134	133	81	25	27
135	133	97	21	15
136	133	76	29	28
137	133	82	29	22
138	133	76	28	29
139	133	81	21	31
140	133	84	30	19
141	133	79	24	30
142	133	85	26	22
143	133	82	22	29

Model ID	Analysed	Favored	Allowed	Outliers
144	133	86	23	24
145	133	71	29	33
146	133	74	28	31
147	133	95	15	23
148	133	76	26	31
149	133	85	25	23
150	133	85	22	26
151	133	81	28	24
152	133	80	27	26
153	133	87	29	17
154	133	85	26	22
155	133	86	21	26
156	133	79	26	28
157	133	83	23	27
158	133	82	26	25
159	133	89	23	21
160	133	83	22	28
161	133	74	27	32
162	133	82	26	25
163	133	71	30	32
164	133	71	34	28
165	133	80	27	26
166	133	82	24	27
167	133	84	23	26
168	133	88	18	27
169	133	85	20	28
170	133	86	24	23
171	133	86	20	27
172	133	71	30	32
173	133	85	26	22
174	133	80	29	24
175	133	82	27	24
176	133	77	30	26
177	133	84	31	18
178	133	87	25	21

Model ID	Analysed	Favored	Allowed	Outliers
179	133	86	26	21
180	133	78	30	25
181	133	85	26	22
182	133	81	25	27
183	133	86	20	27
184	133	86	20	27
185	133	86	27	20
186	133	86	24	23
187	133	85	26	22
188	133	79	28	26
189	133	76	28	29
190	133	80	25	28
191	133	90	20	23
192	133	99	20	14
193	133	79	27	27
194	133	79	24	30
195	133	87	17	29
196	133	87	24	22
197	133	82	22	29
198	133	73	26	34
199	133	72	29	32
200	133	74	32	27
201	133	87	25	21
202	133	91	22	20
203	133	68	32	33
204	133	82	27	24
205	133	86	23	24
206	133	90	19	24
207	133	80	27	26
208	133	77	24	32
209	133	89	20	24
210	133	86	23	24
211	133	90	22	21
212	133	68	40	25
213	133	88	25	20

Model ID	Analysed	Favored	Allowed	Outliers
214	133	77	33	23
215	133	88	17	28
216	133	80	29	24
217	133	72	30	31
218	133	82	23	28
219	133	77	31	25
220	133	86	20	27
221	133	80	27	26
222	133	83	23	27
223	133	89	21	23
224	133	89	23	21
225	133	74	29	30
226	133	83	19	31
227	133	87	22	24
228	133	83	22	28
229	133	75	24	34
230	133	84	29	20
231	133	90	22	21
232	133	82	26	25
233	133	80	25	28
234	133	77	25	31
235	133	83	27	23
236	133	79	25	29
237	133	87	20	26
238	133	78	30	25
239	133	83	25	25
240	133	87	19	27
241	133	85	27	21
242	133	79	24	30
243	133	82	28	23
244	133	85	19	29
245	133	77	26	30
246	133	76	29	28
247	133	73	31	29
248	133	77	28	28

Model ID	Analysed	Favored	Allowed	Outliers
249	133	89	18	26
250	133	73	30	30
251	133	92	18	23
252	133	79	26	28
253	133	88	20	25
254	133	80	27	26
255	133	81	29	23
256	133	78	30	25
257	133	81	20	32
258	133	78	22	33
259	133	86	25	22
260	133	83	24	26
261	133	91	21	21
262	133	92	15	26
263	133	81	25	27
264	133	86	29	18
265	133	88	23	22
266	133	85	29	19
267	133	77	31	25
268	133	89	24	20
269	133	86	23	24
270	133	77	22	34
271	133	82	24	27
272	133	84	27	22
273	133	81	25	27
274	133	90	23	20
275	133	78	24	31
276	133	91	19	23
277	133	84	23	26
278	133	89	24	20
279	133	75	28	30
280	133	79	28	26
281	133	81	24	28
282	133	86	26	21
283	133	82	29	22


There are 121 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	32	LEU	230
A	84	LEU	211
A	126	TRP	201
A	11	GLU	173
A	35	LYS	164
A	62	GLU	156
A	52	ARG	150
A	66	LEU	140
A	13	LEU	139
A	43	LYS	138
A	83	LYS	136
A	27	ILE	128
A	46	LEU	127
A	118	LEU	127
A	15	LEU	124
A	7	LEU	119
A	161	TYR	118
A	1	MET	117
A	106	MET	116
A	79	LEU	115
A	80	ARG	109
A	121	LEU	109
A	39	LEU	108
A	22	GLU	105
A	48	LYS	104
A	124	LYS	100
A	19	LYS	96
A	91	LEU	93
A	45	GLU	92
A	85	LYS	92
A	14	ARG	90
A	20	ASP	83
A	64	GLU	82

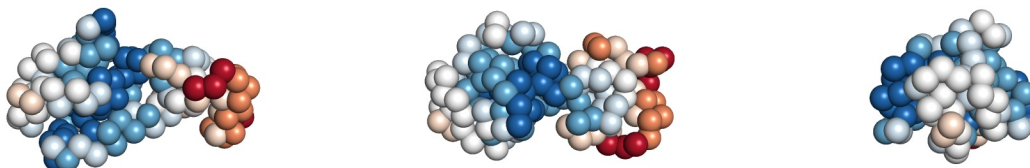
Chain	Res	Type	Models (Total)
A	162	LYS	82
A	60	LYS	81
A	65	LYS	81
A	99	LEU	81
A	16	LYS	77
A	33	LEU	77
A	128	GLU	77
A	132	ASN	77
A	67	PHE	76
A	76	ARG	74
A	26	THR	71
A	58	ILE	71
A	139	TYR	71
A	50	ILE	68
A	119	ARG	67
A	100	ILE	63
A	104	PHE	61
A	122	GLN	61
A	127	ASP	61
A	137	ARG	60
A	105	GLN	59
A	8	ARG	57
A	125	ARG	57
A	135	LYS	55
A	25	TYR	53
A	92	ASP	53
A	95	ARG	53
A	148	ARG	53
A	53	ASN	51
A	5	GLU	50
A	147	LYS	49
A	78	ILE	47
A	4	PHE	44
A	145	ARG	41
A	47	ASP	40

Chain	Res	Type	Models (Total)
A	120	MET	40
A	96	ARG	36
A	154	ARG	36
A	6	MET	34
A	55	ASN	34
A	108	GLU	34
A	115	THR	34
A	141	GLN	33
A	29	ILE	32
A	21	THR	29
A	69	GLN	29
A	133	LEU	29
A	18	TYR	28
A	89	ASP	27
A	61	ASP	26
A	72	ASP	26
A	17	ILE	25
A	151	THR	25
A	24	TYR	24
A	57	VAL	23
A	70	ASP	23
A	123	GLN	23
A	38	SER	22
A	102	MET	22
A	142	THR	22
A	31	HIS	21
A	68	ASN	20
A	88	TYR	20
A	40	ASN	16
A	159	ASP	14
A	117	SER	13
A	10	ASP	12

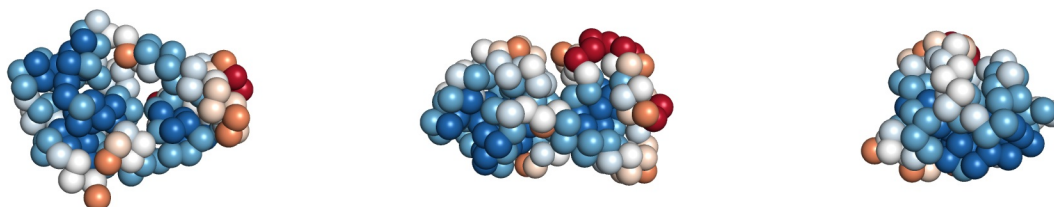
PrISM precision analysis

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: 119/119).



PrISM analysis for Ensemble 2 (models deposited/total: 164/164).



Fit of model to data used for modeling ?

Single molecule FRET

Validation for this section is under development.

Ensemble FRET

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749).

The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.