Integrative Structure Validation Report

March 13, 2025 - 11:54 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
ATSAS Version 3.2.1 (r14885)
PyMOL Version 2.5.0

PDB ID	9A1G
PDB-Dev ID	PDBDEV_00000088
Structure Title	Structures of multiple states of the hGBP1 resolved by FRET, SAXS, and EPR
Structure Authors	Thomas-Otavio Peulen; Carola S. Hengstenberg; Ralf Biehl; Mykola Dimura; Charlotte Lorenz; Alessandro Valeri; Julian Folz; Christian A. Hanke; Semra Ince; Tobias Voepel; Bela Farago; Holger Gohlke; Johann P. Klare; Andreas M. Stadler; Claus A. M. Seidel; Christian Herrmann
Deposited on	2021-06-28

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

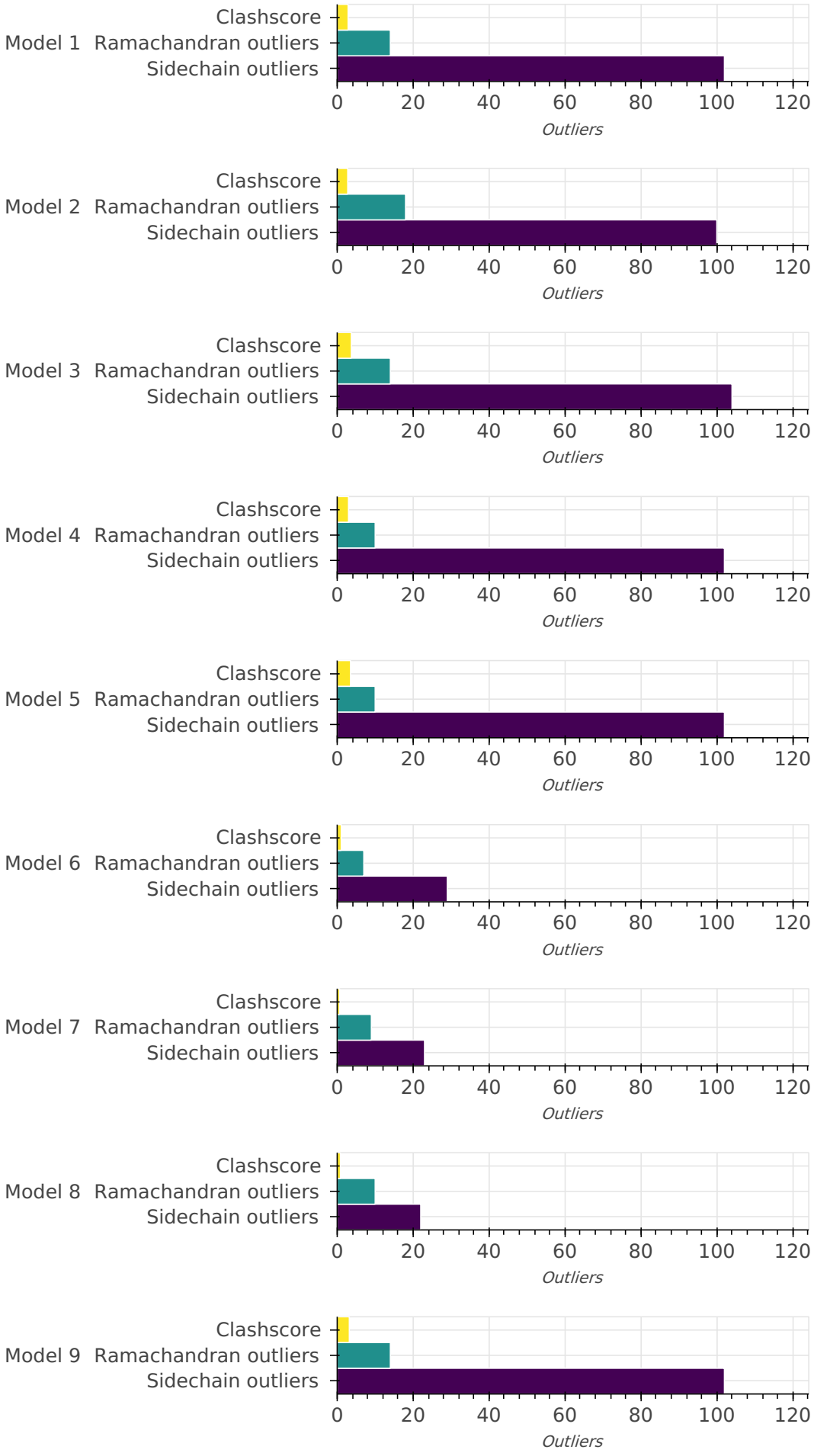
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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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Clashscore
Model 3 Ramachandran outliers
Sidechain outliers
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Outliers
Clashscore
Model 4 Ramachandran outliers
Sidechain outliers
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Outliers
Clashscore
Model 5 Ramachandran outliers
Sidechain outliers
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Model 6 Ramachandran outliers
Sidechain outliers
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Model 7 Ramachandran outliers
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Clashscore
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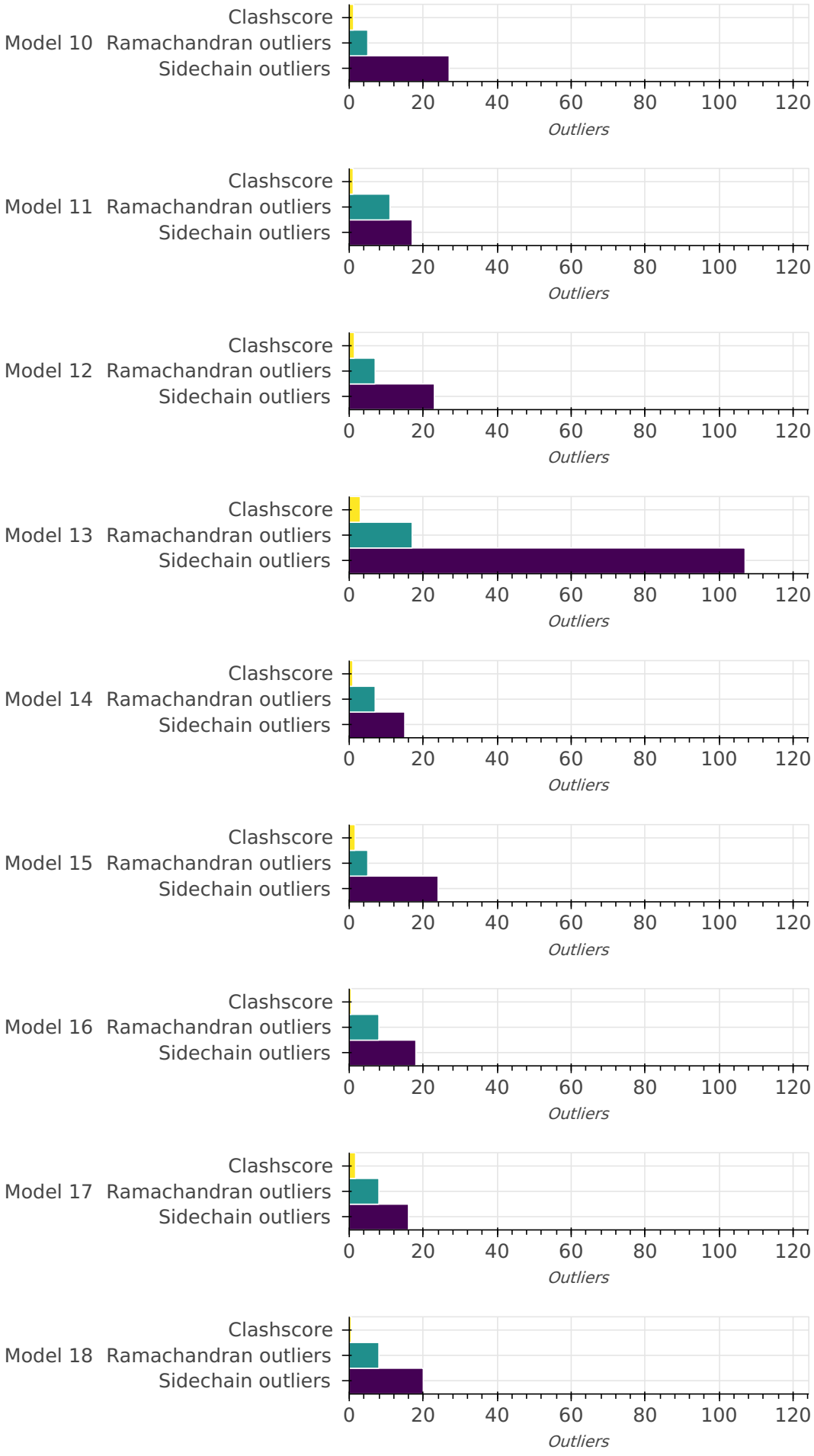
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Model 13 Ramachandran outliers
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Sidechain outliers
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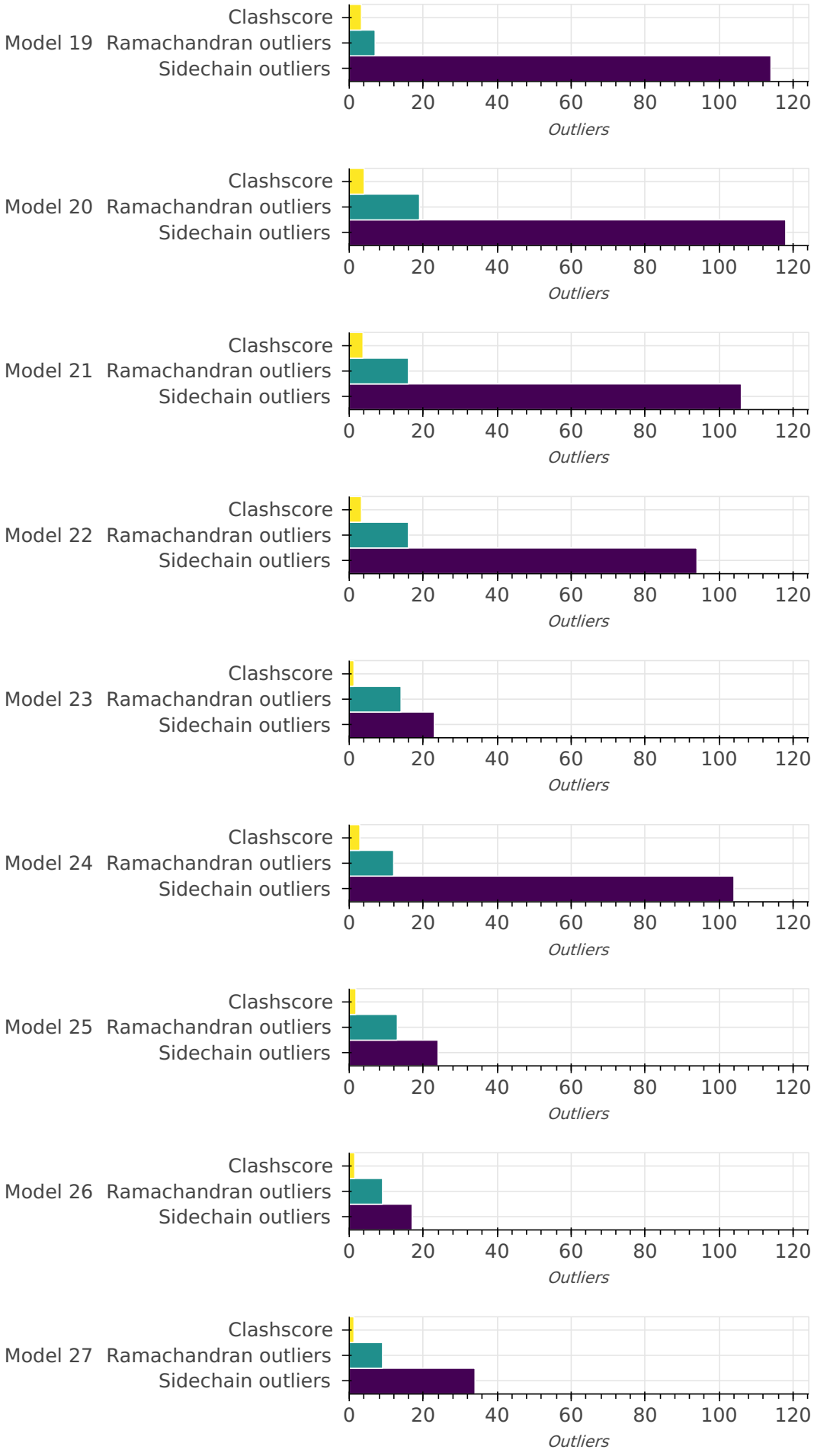
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Model 22 Ramachandran outliers
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Model 23 Ramachandran outliers
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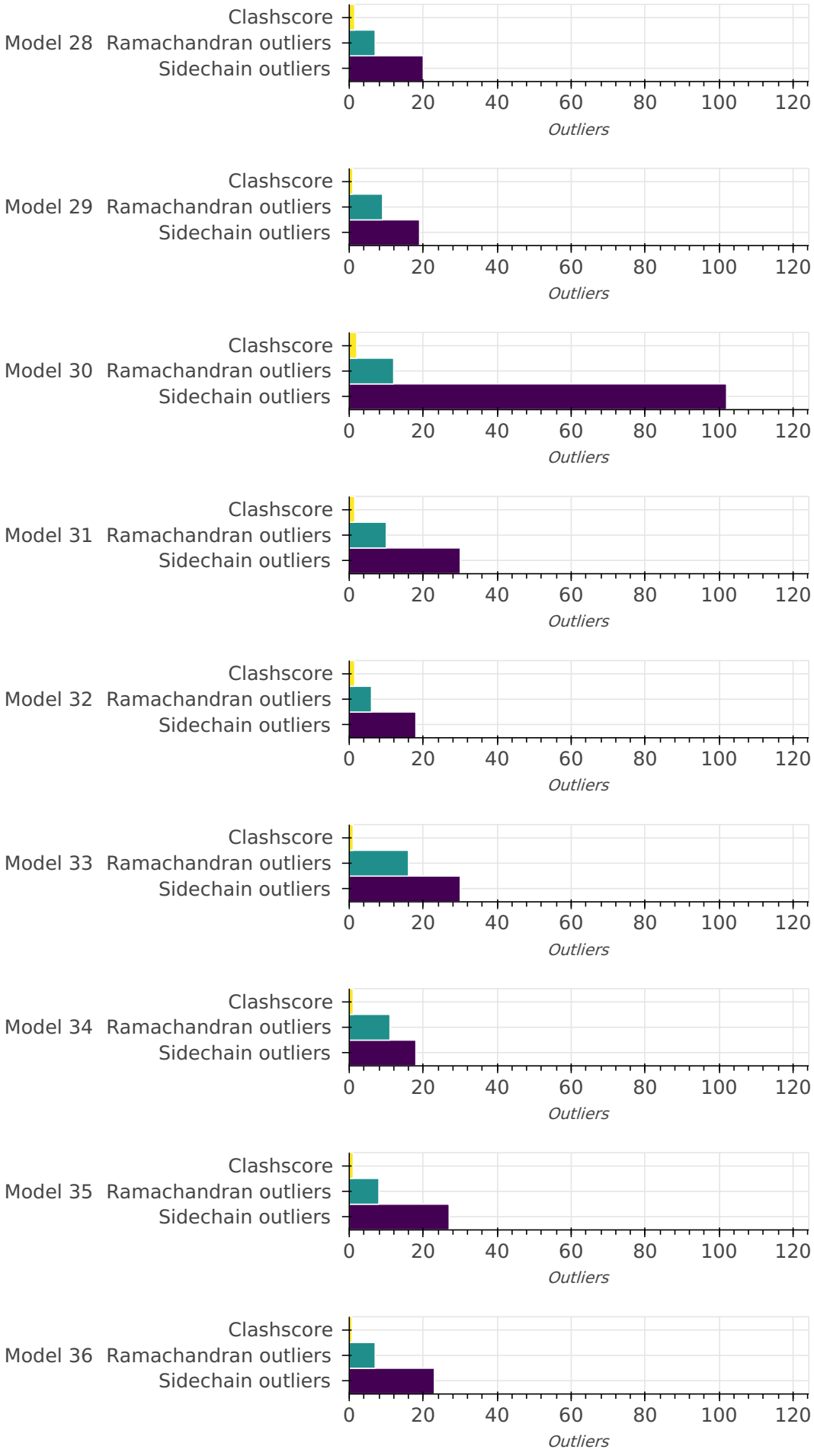
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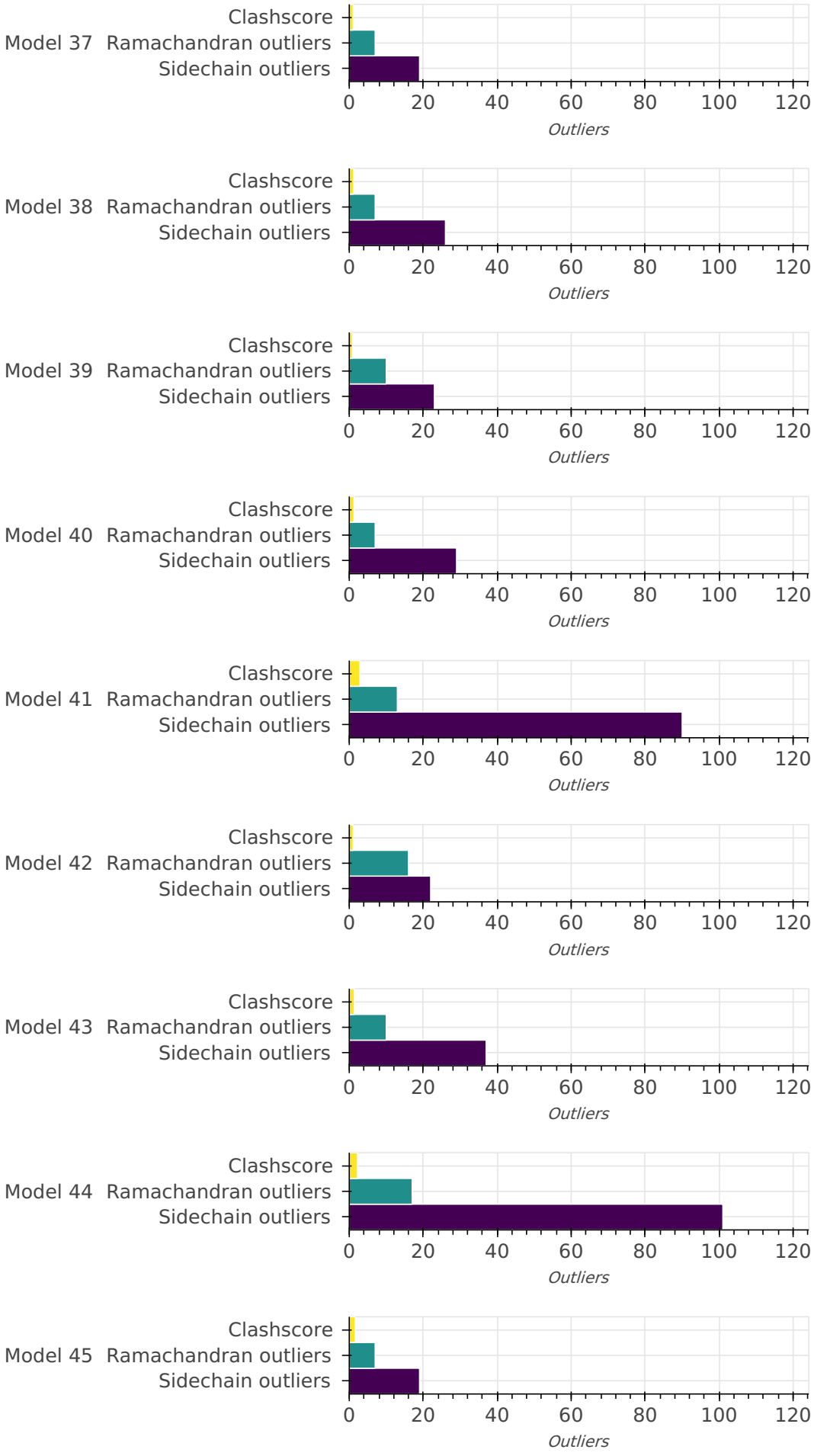
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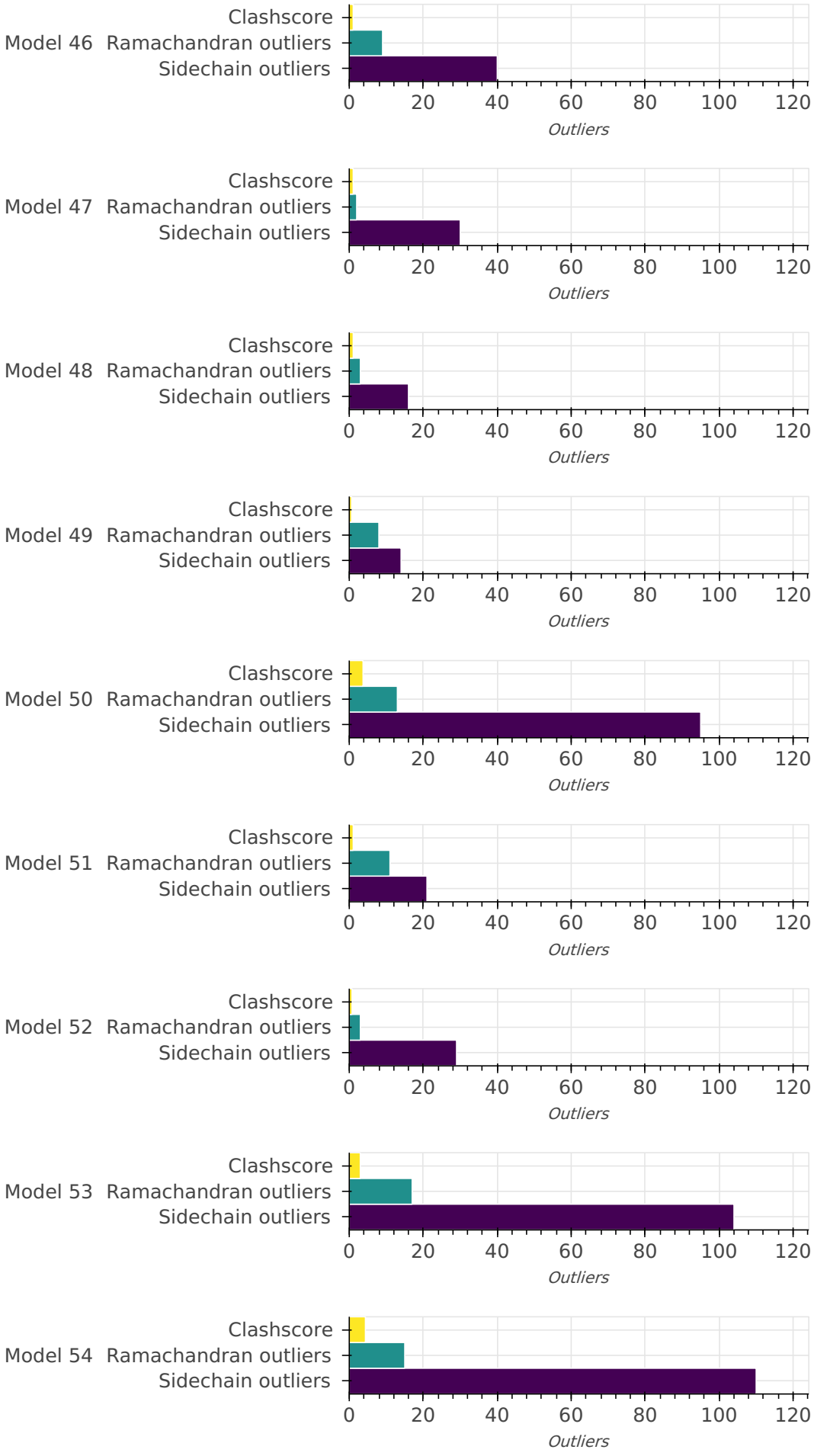
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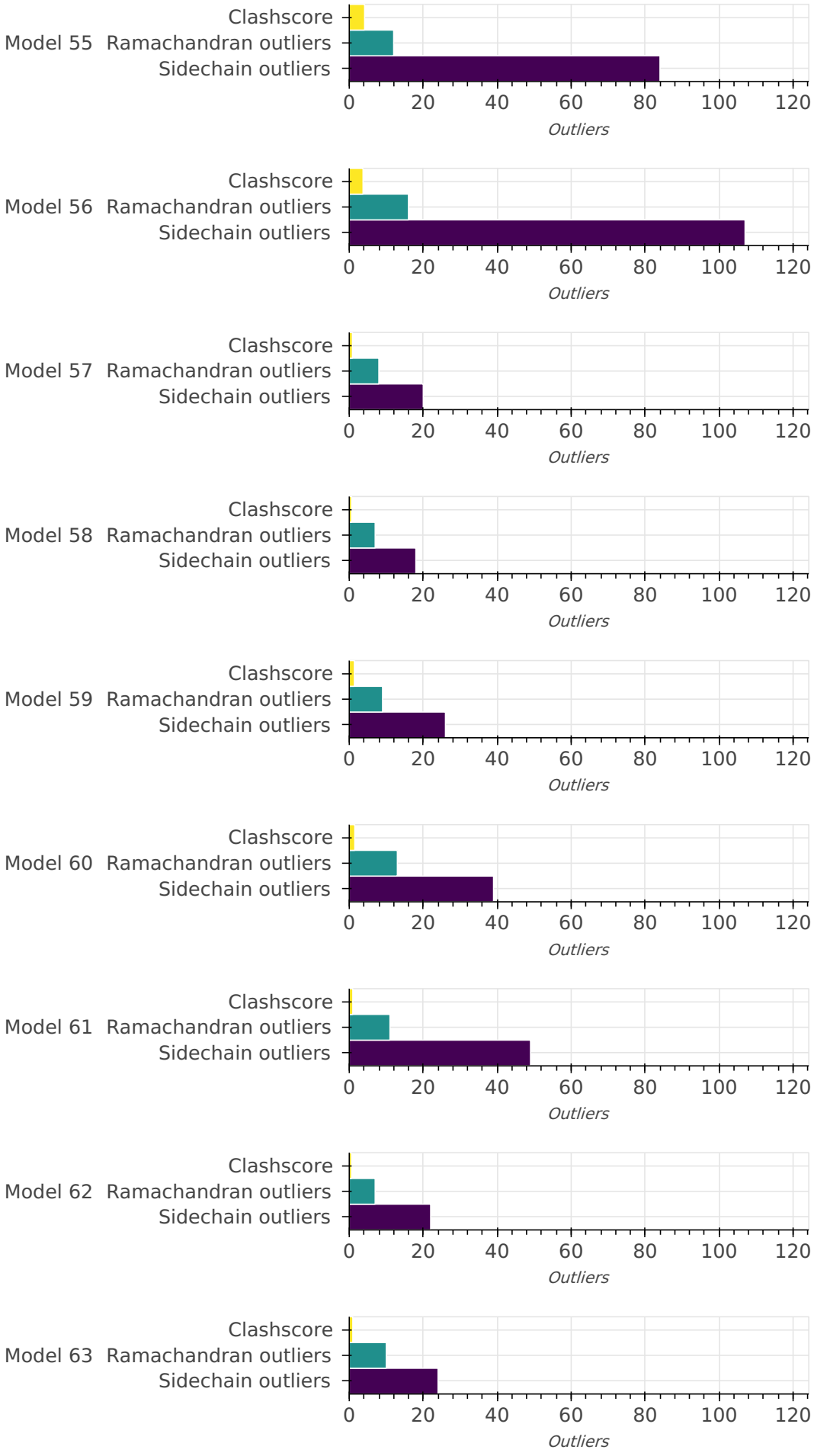
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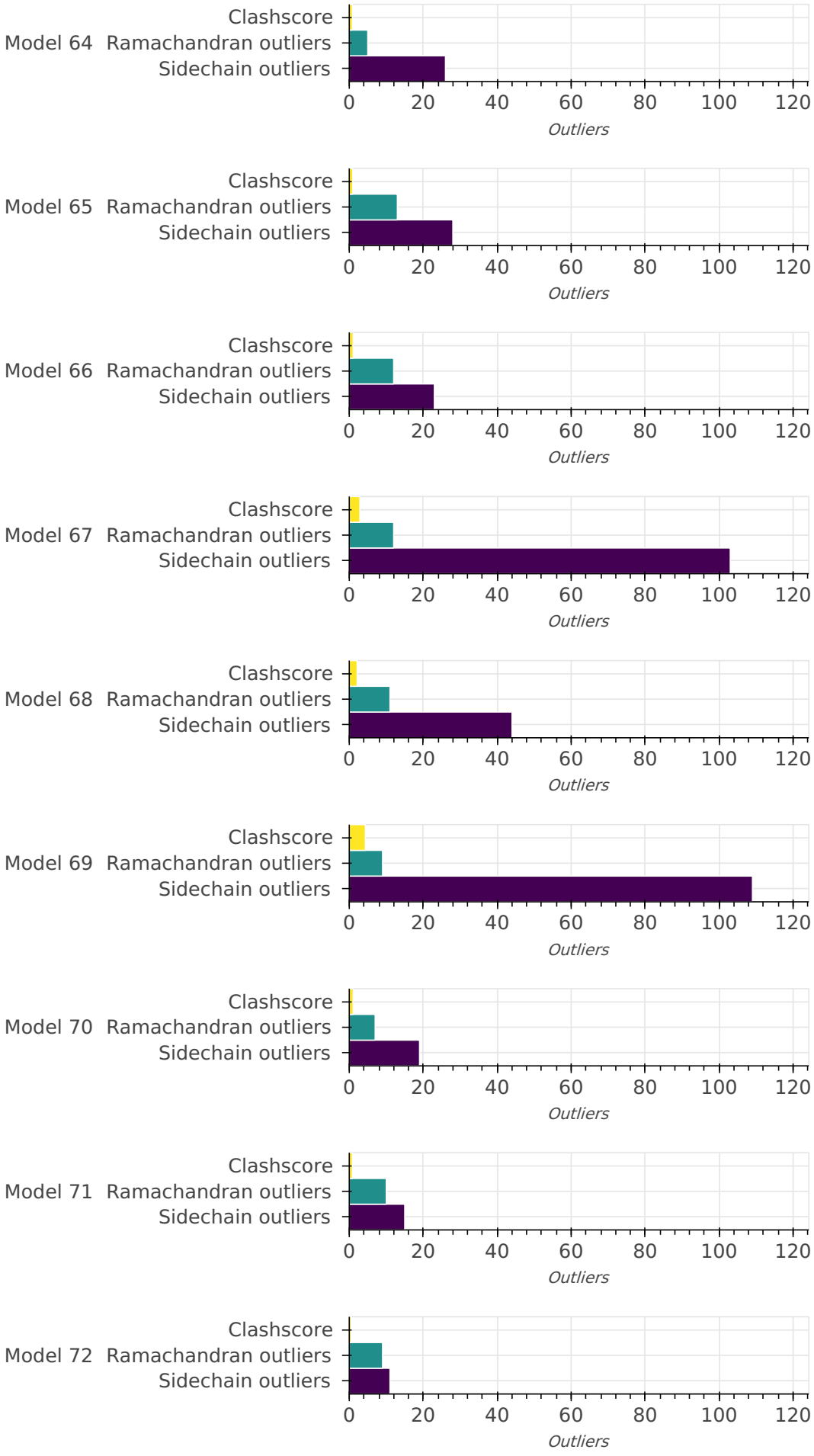
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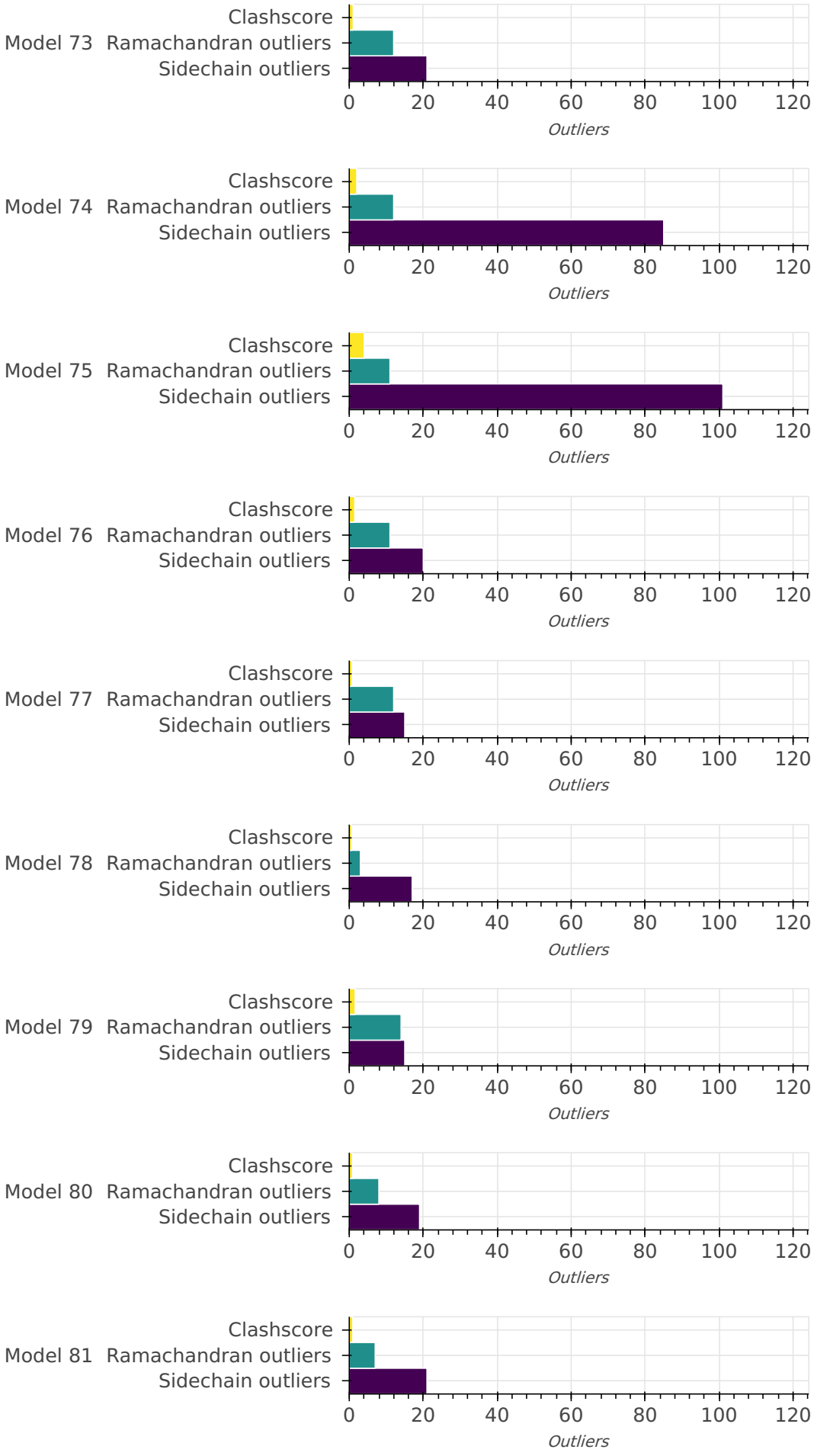
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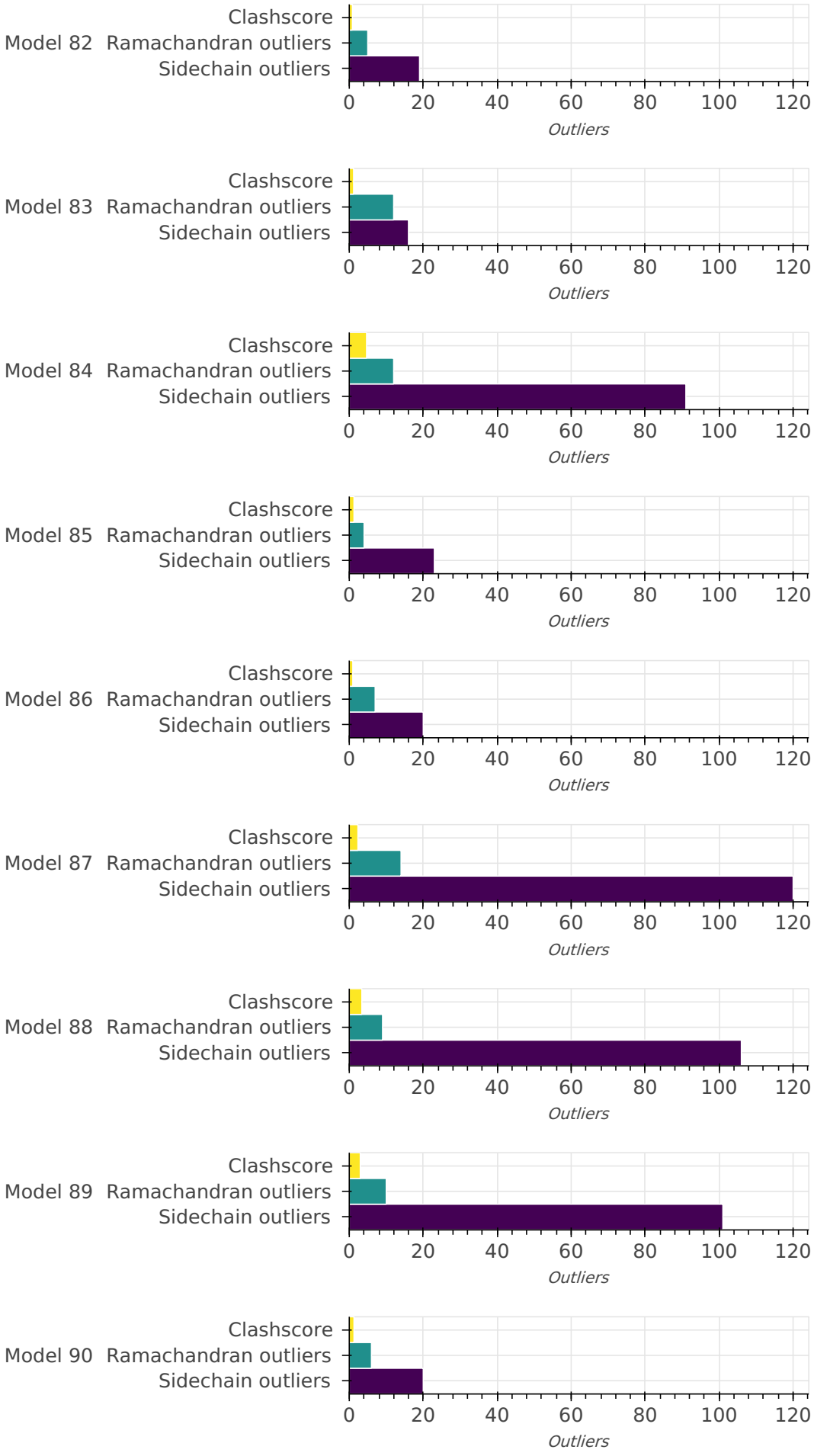
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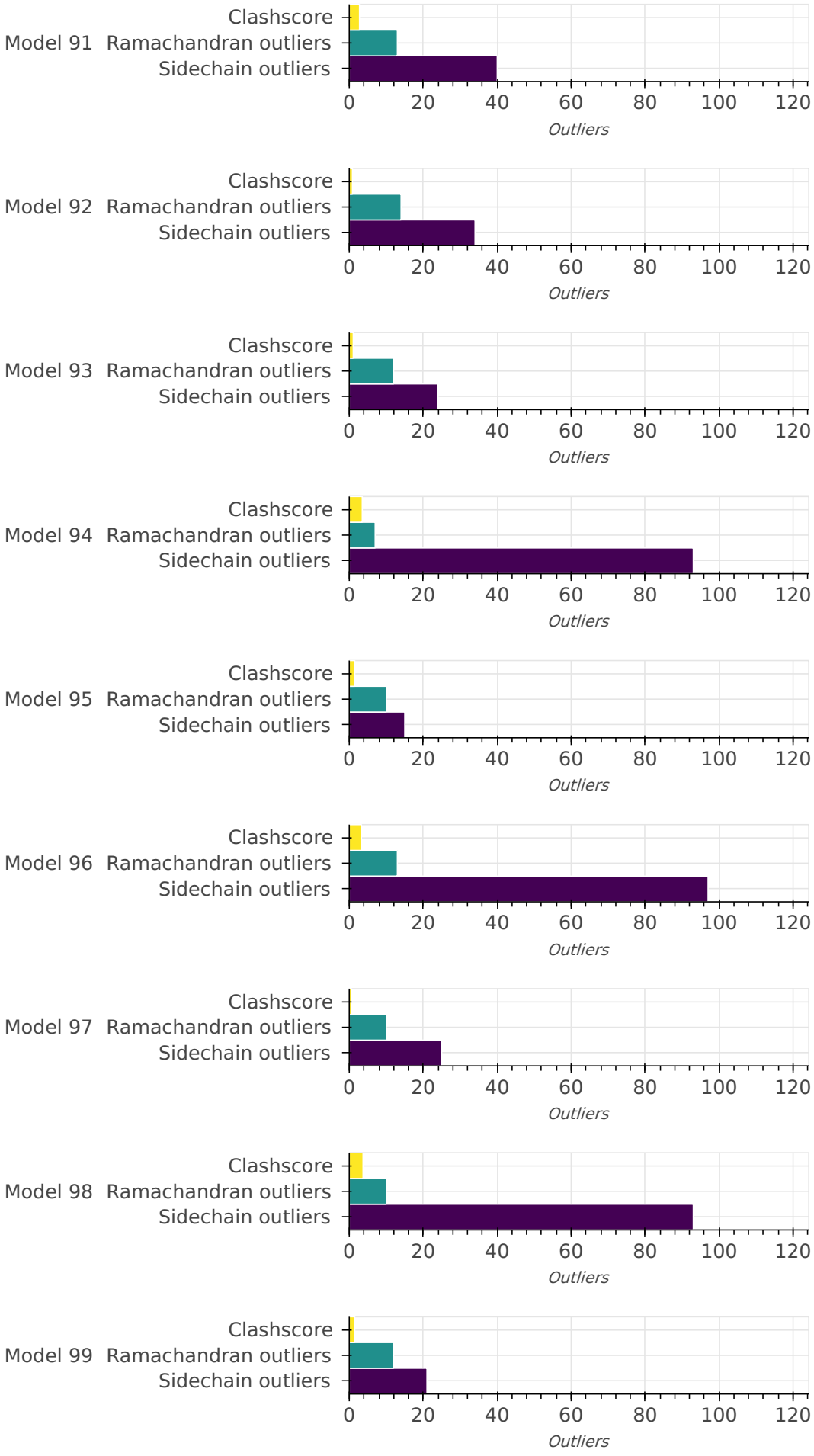
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Model 94 Ramachandran outliers
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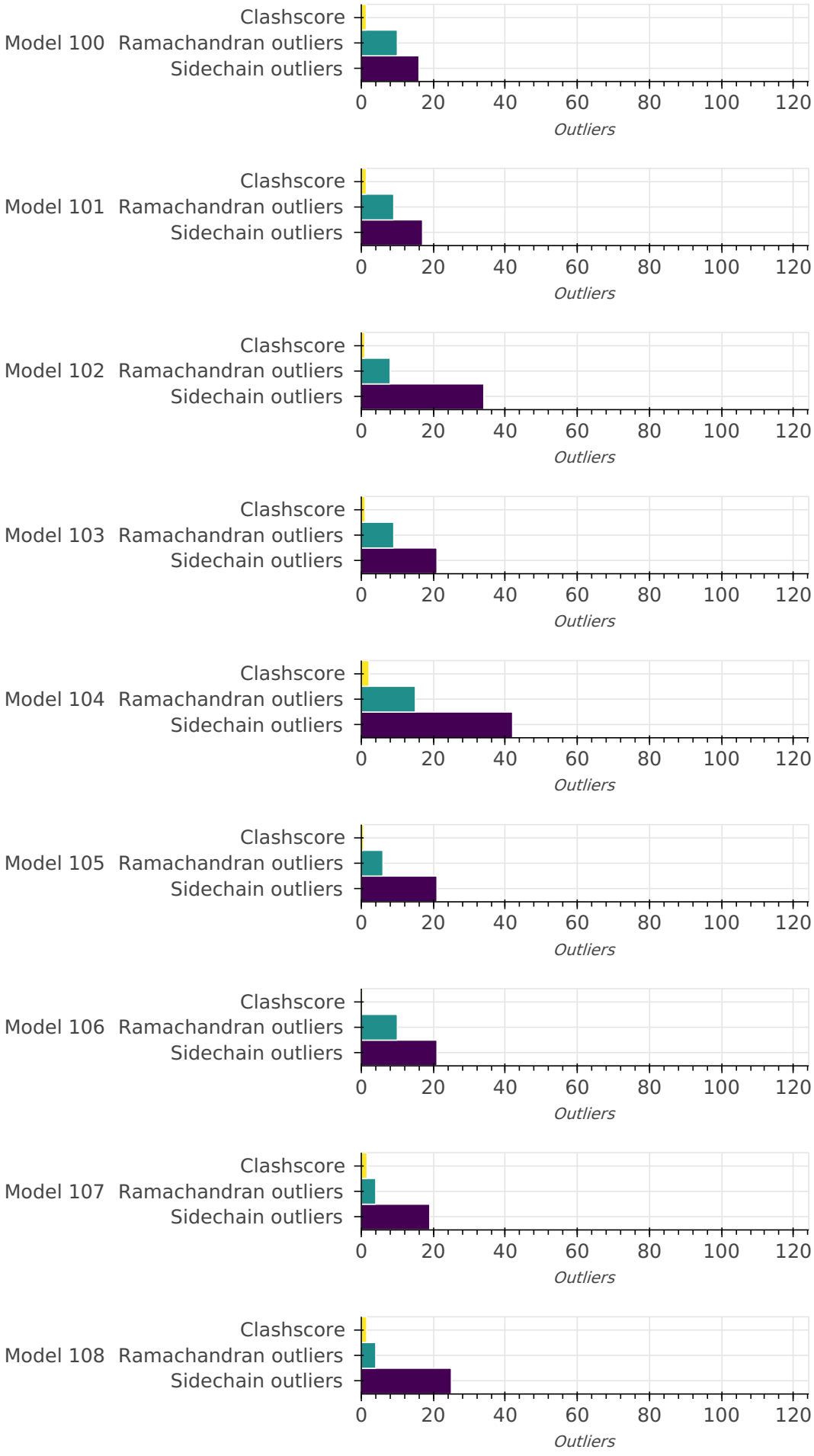
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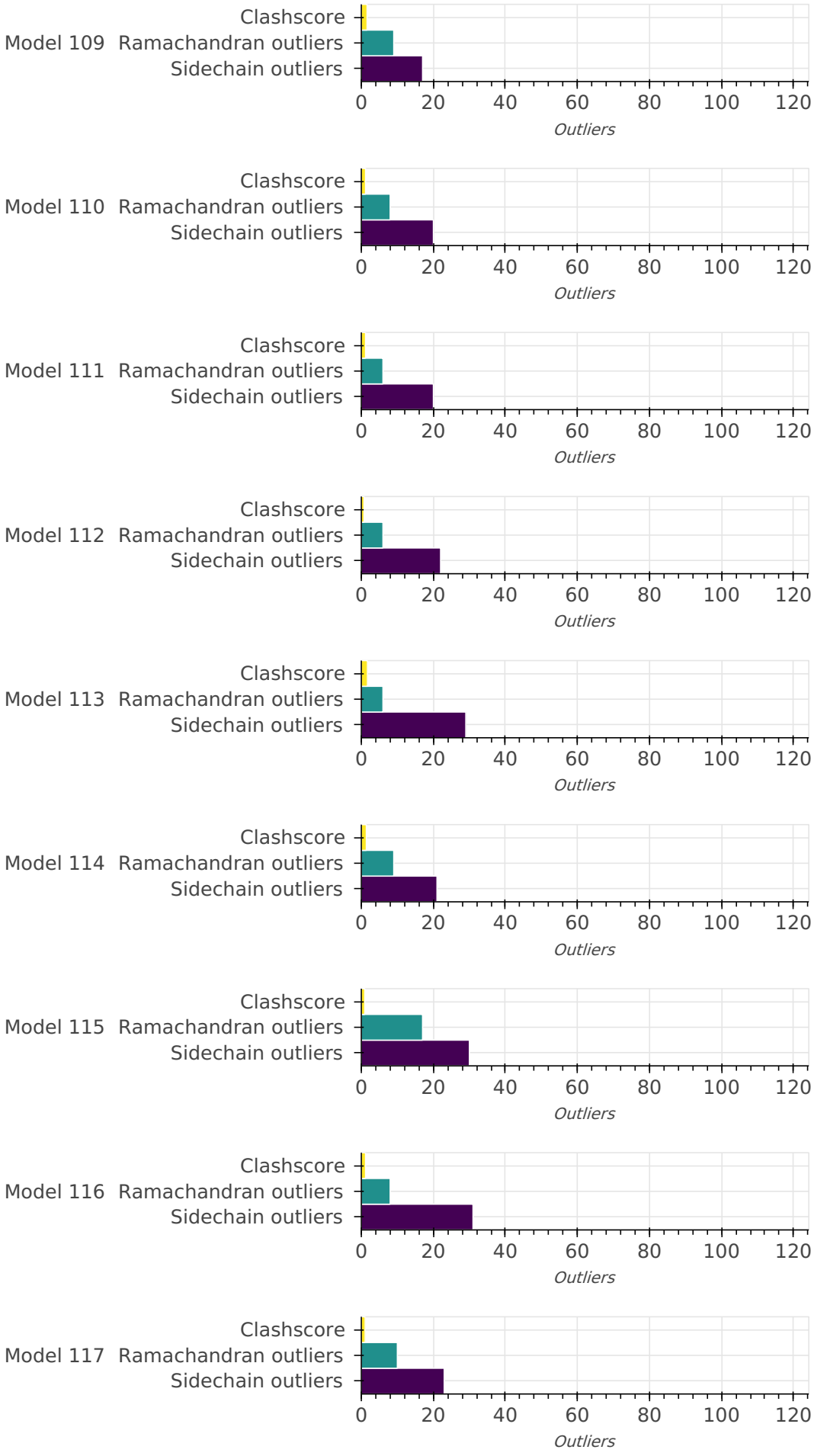
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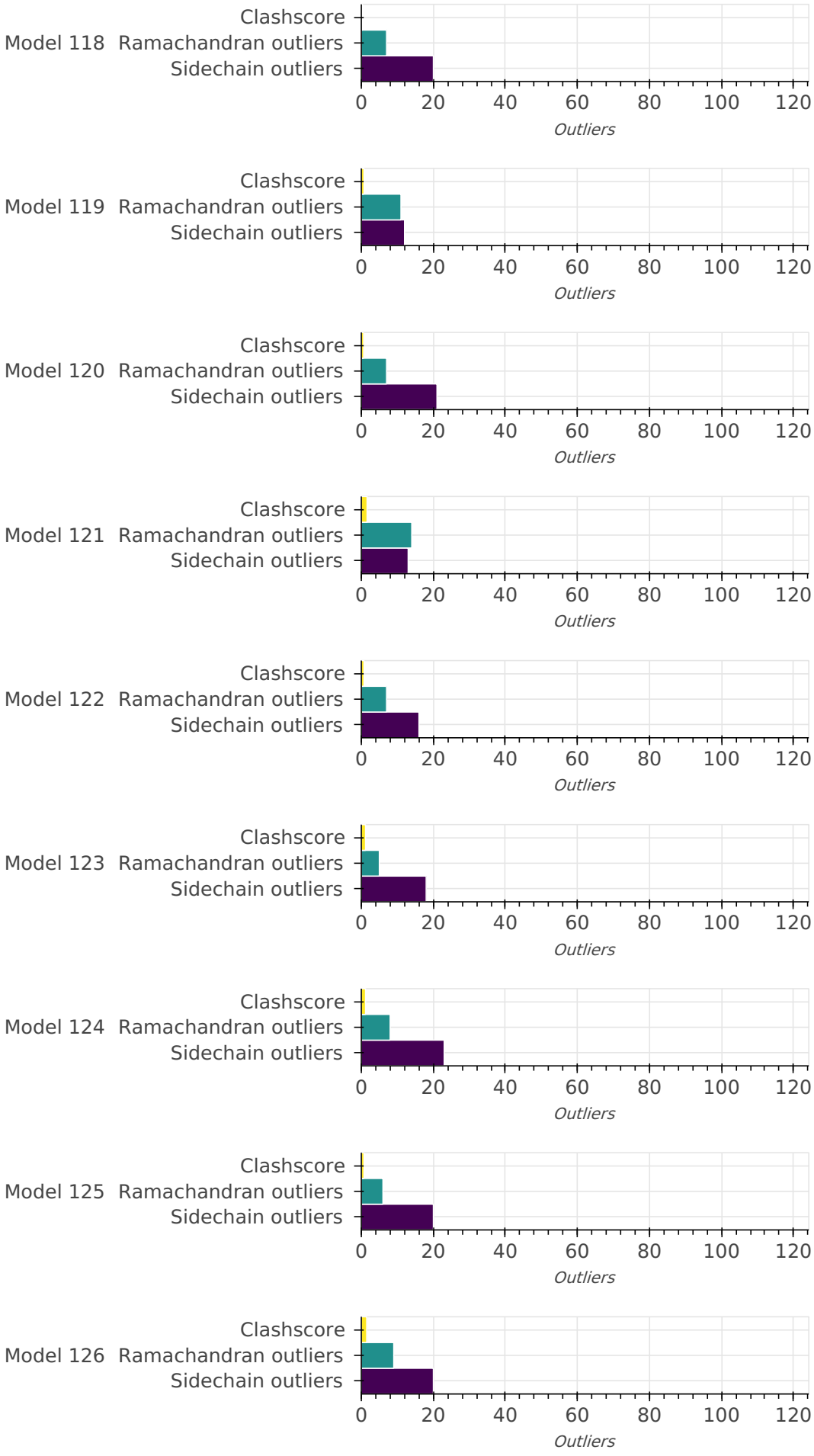
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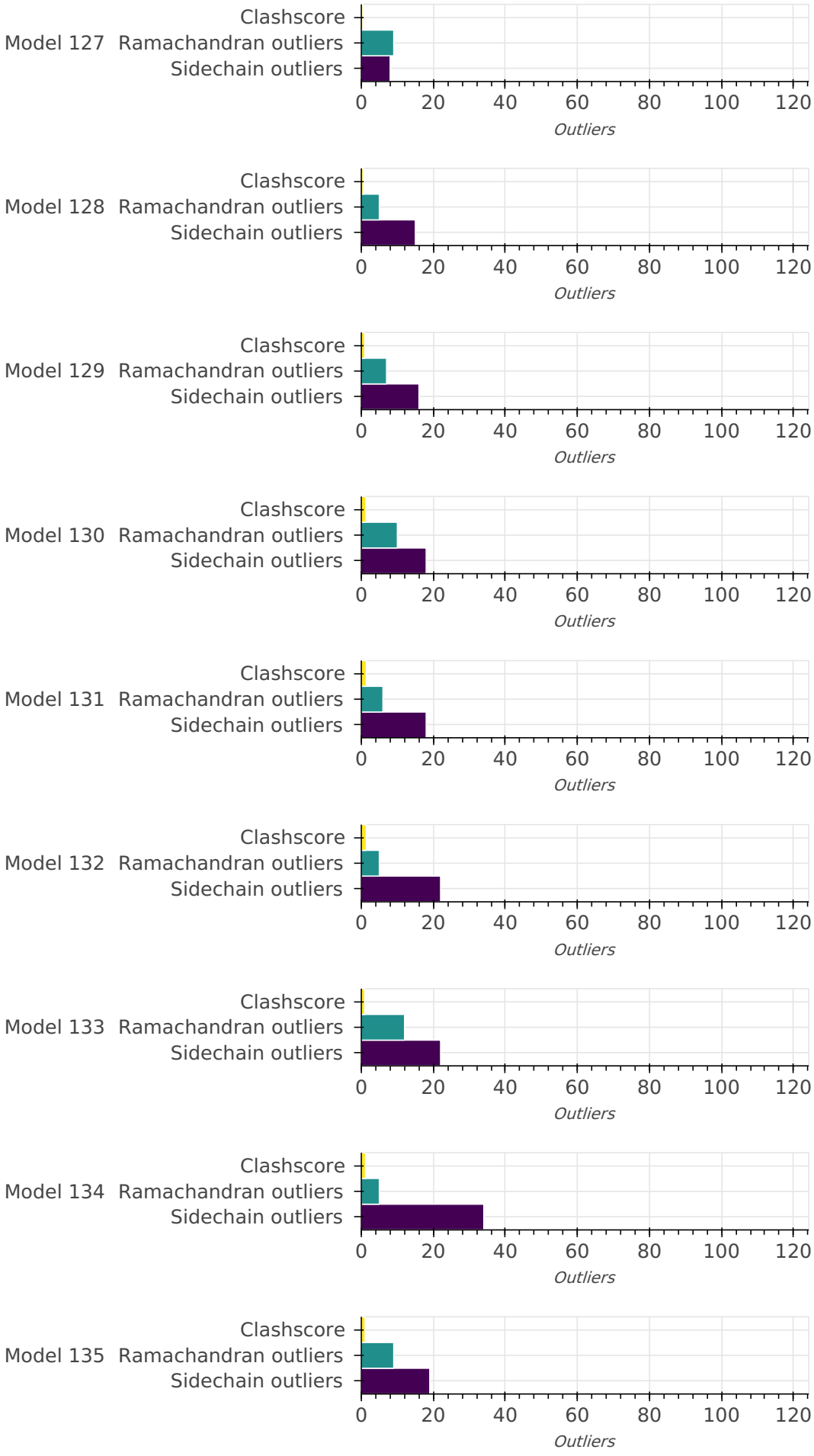
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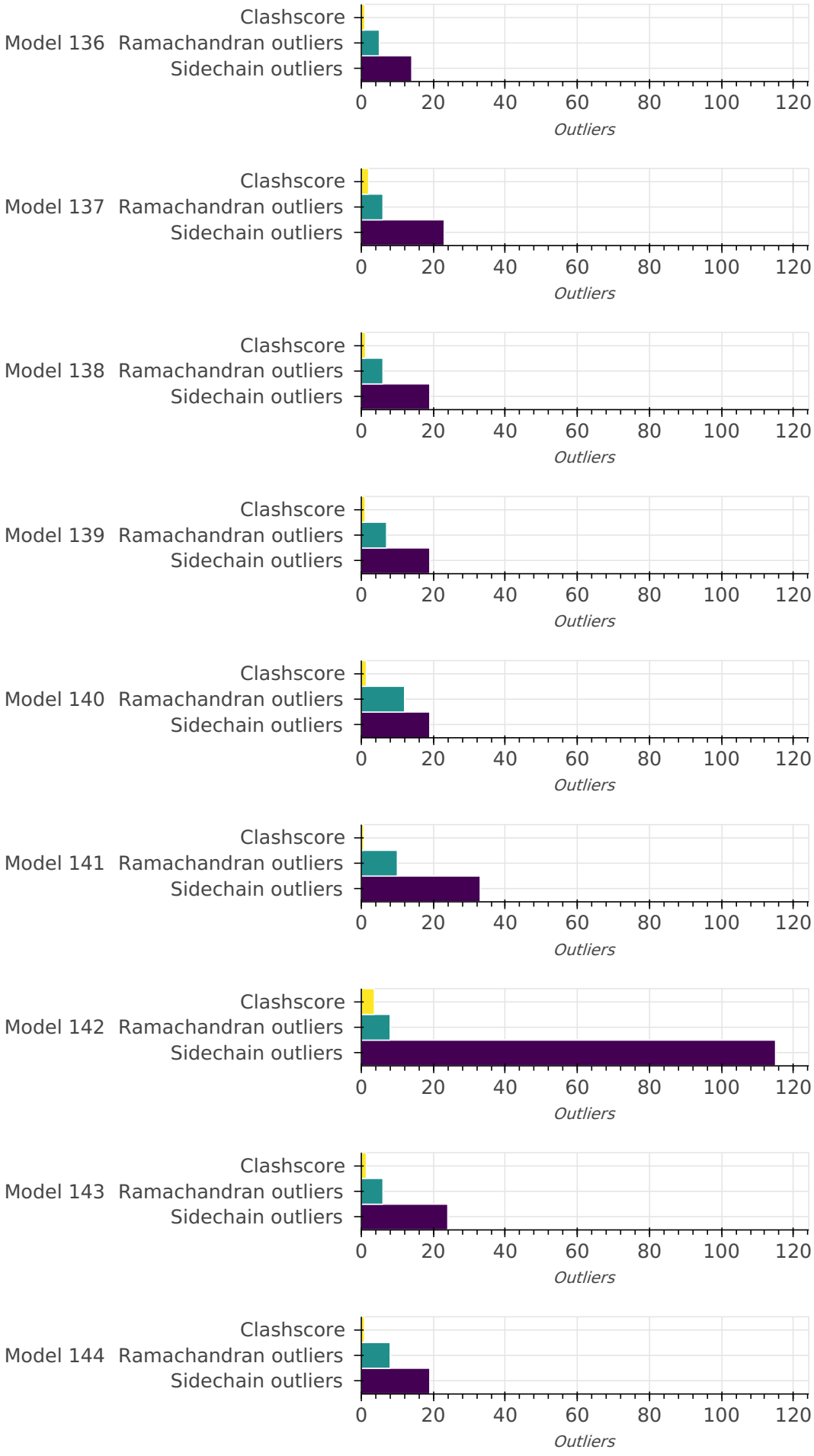
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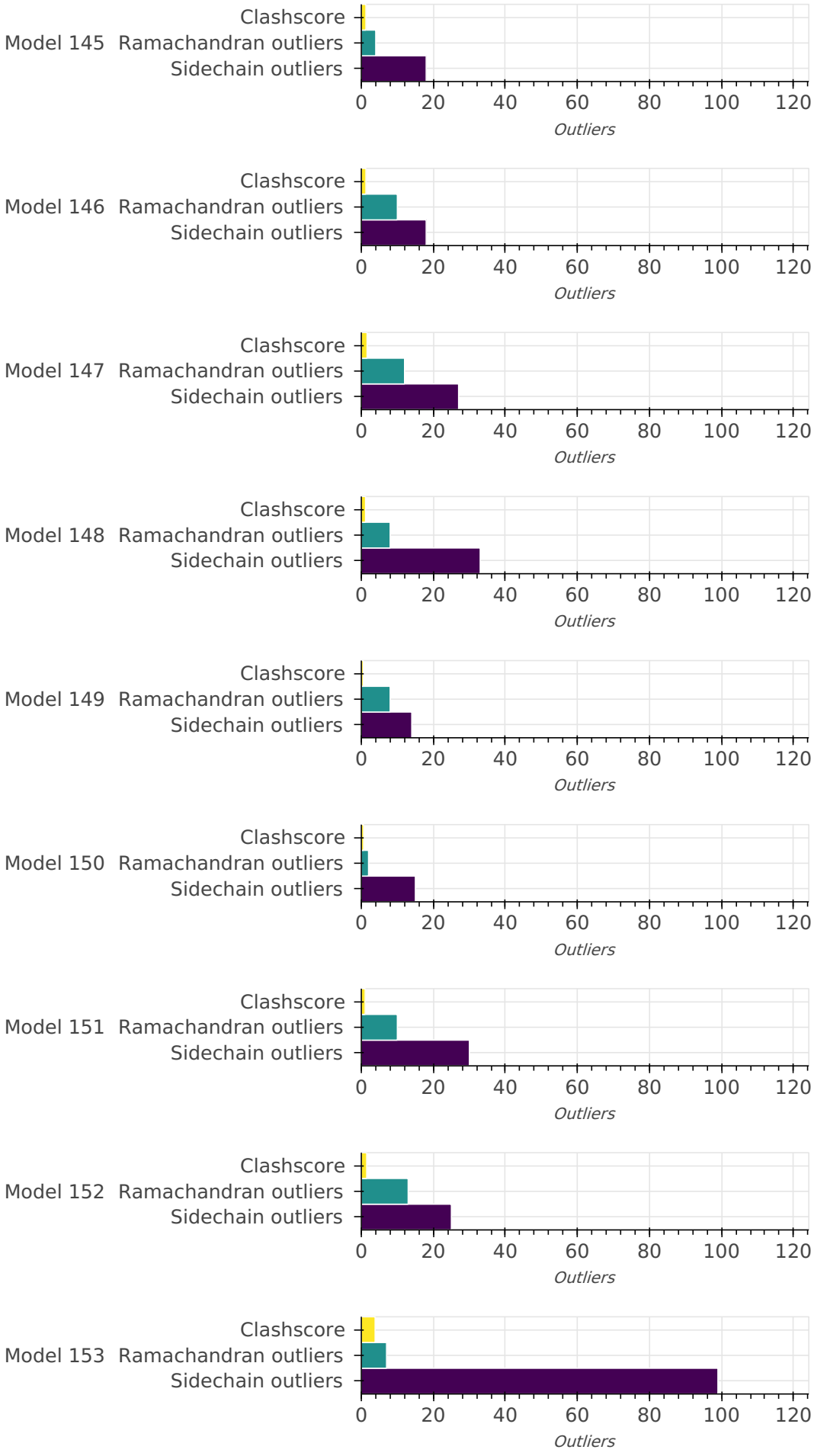
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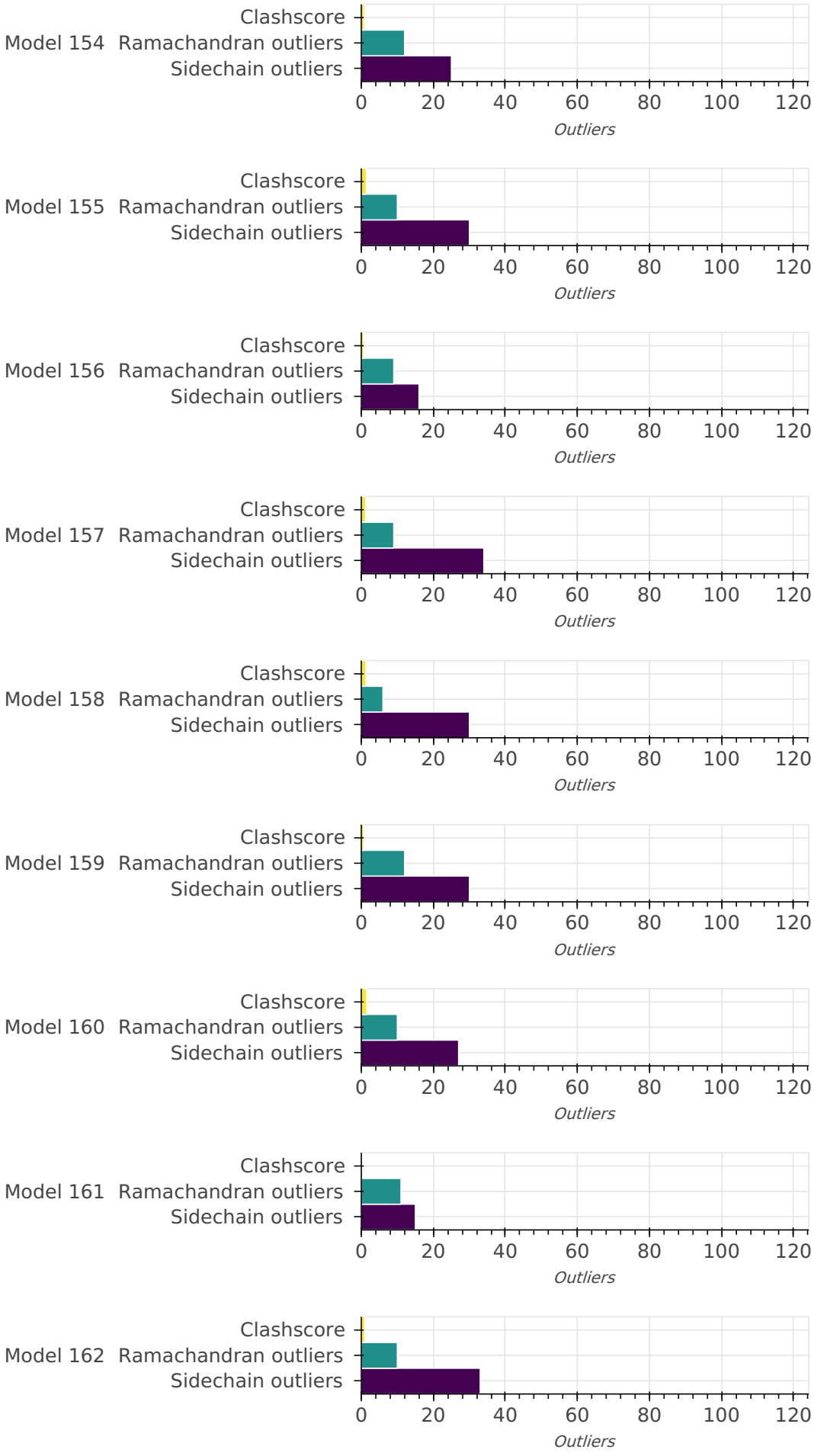
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Model 157 Ramachandran outliers
Sidechain outliers
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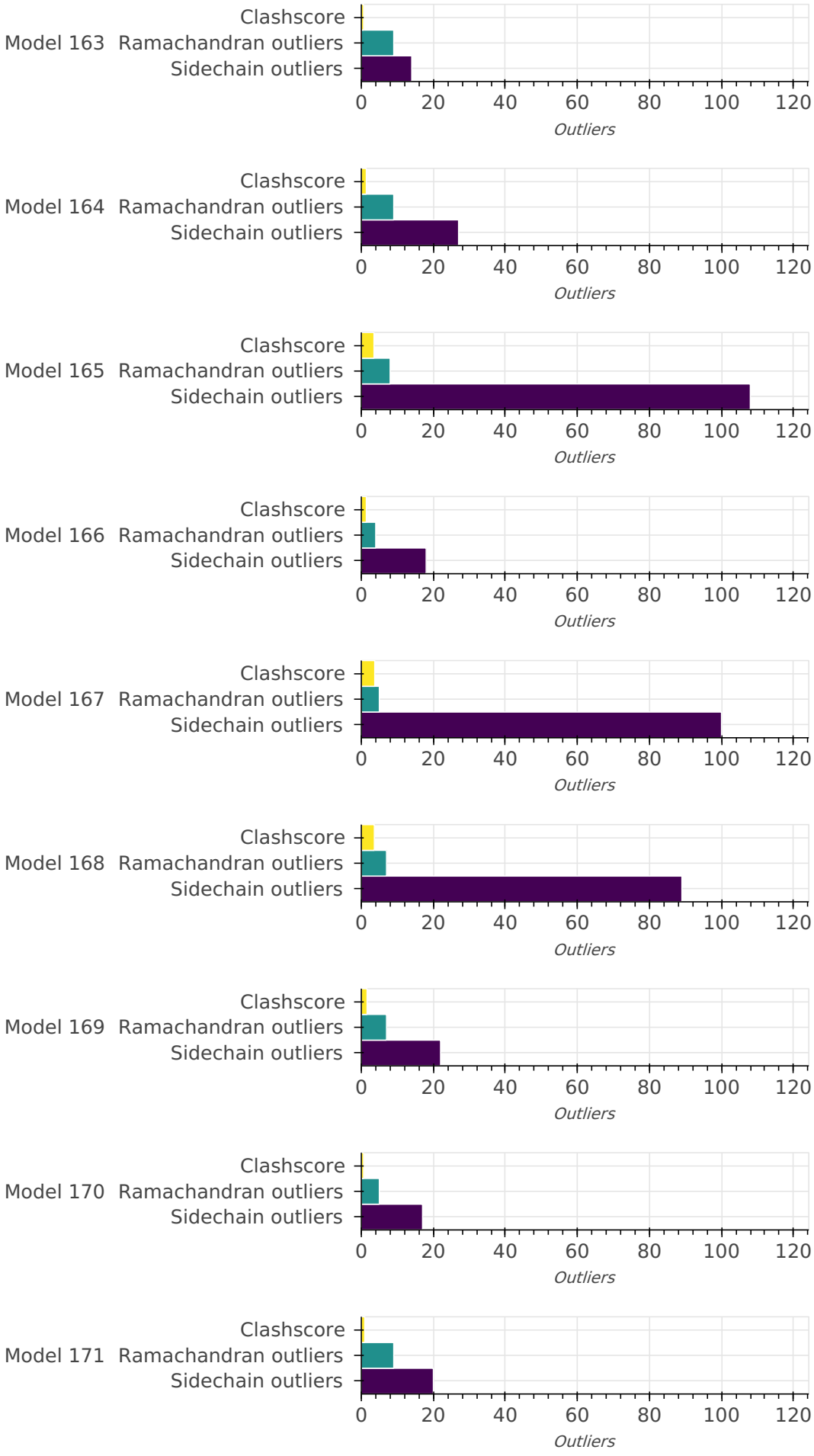
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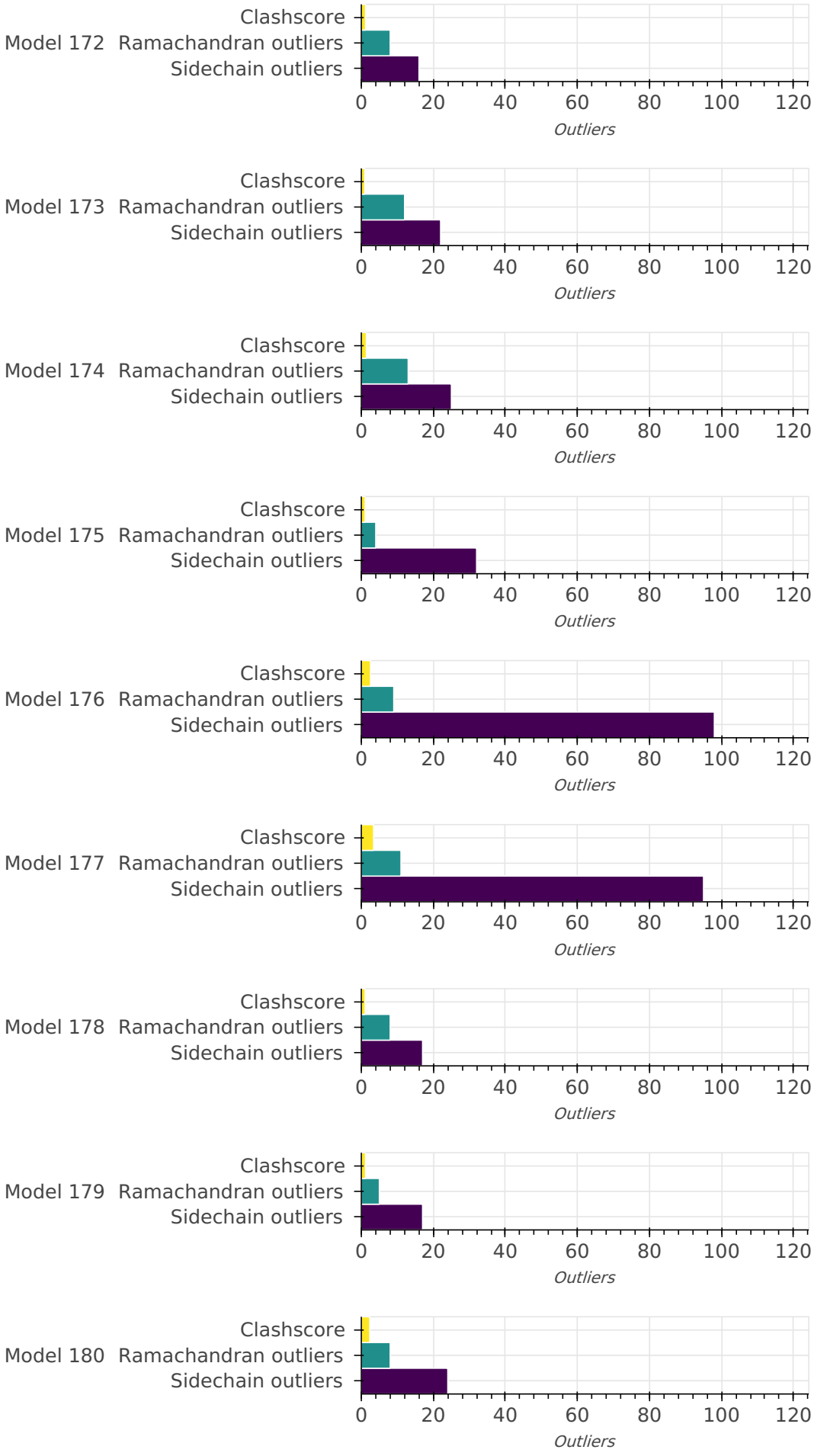
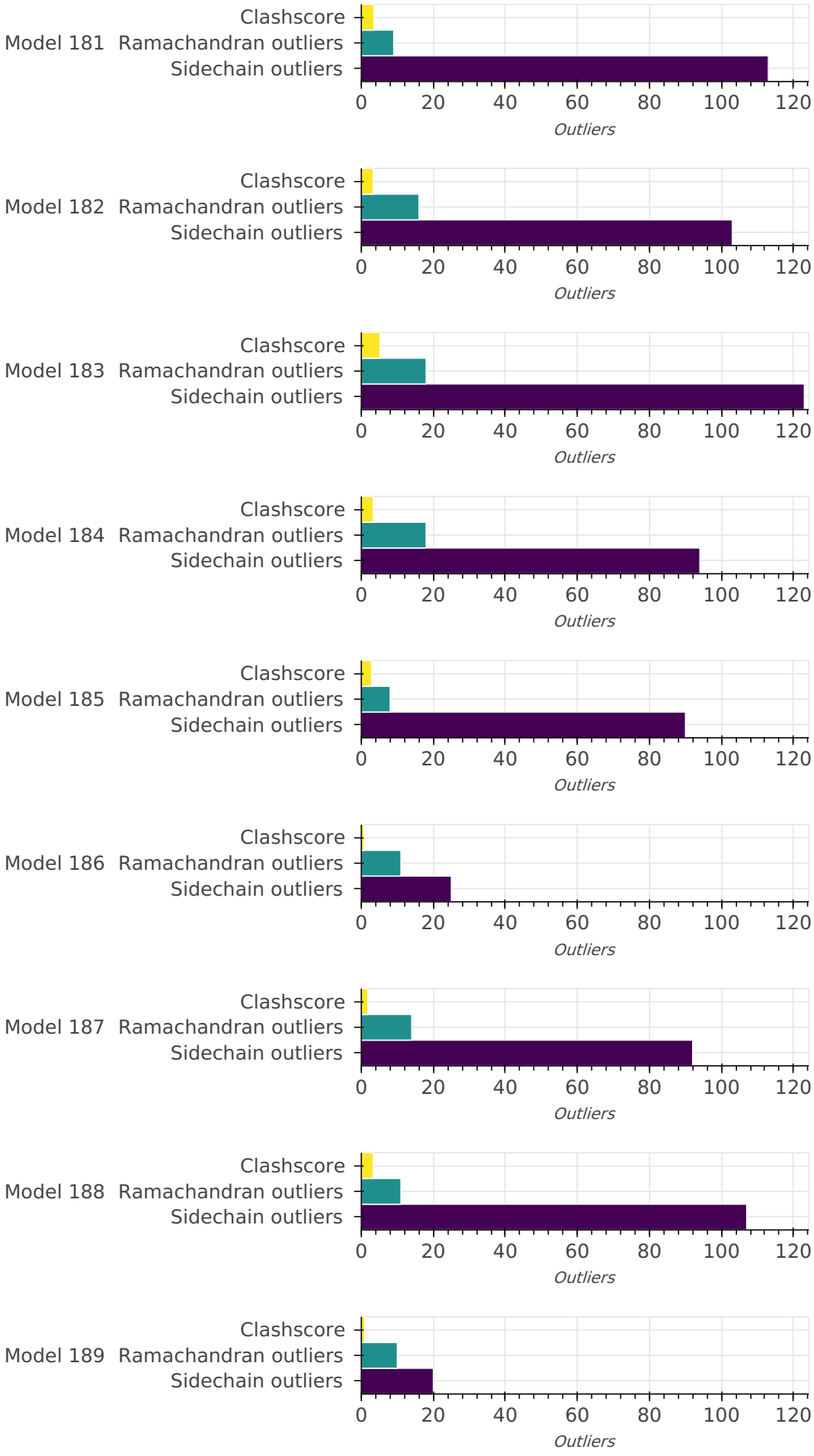
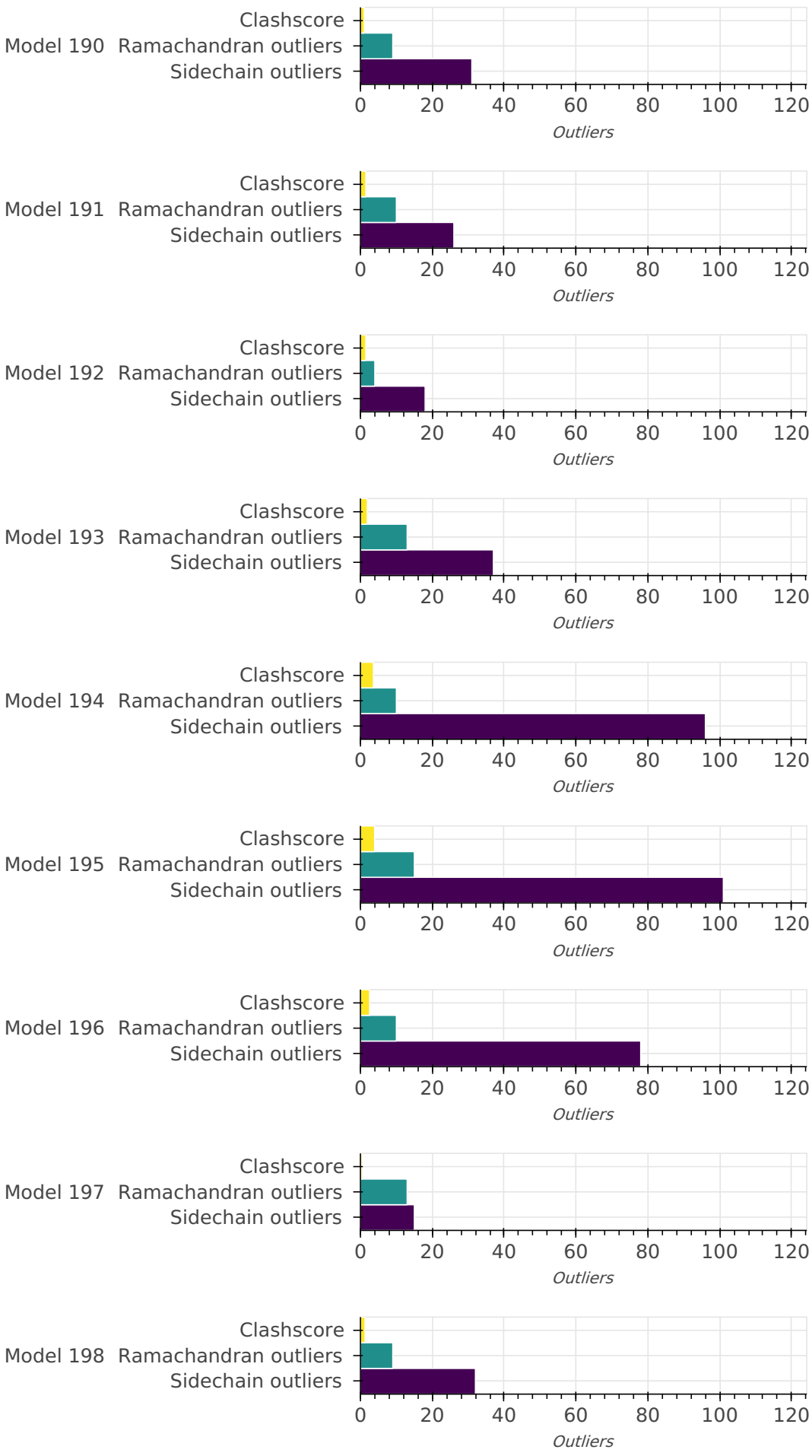
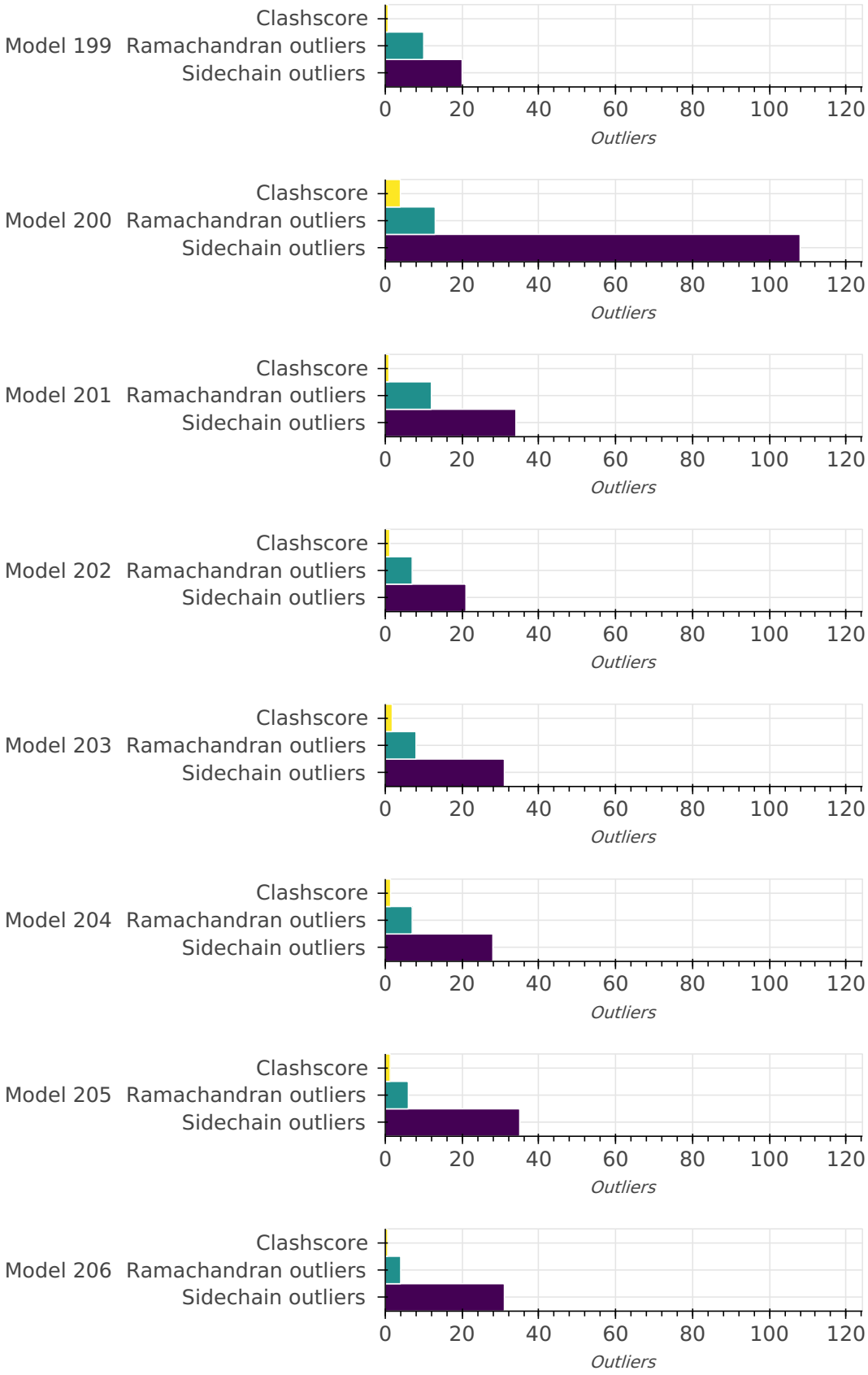
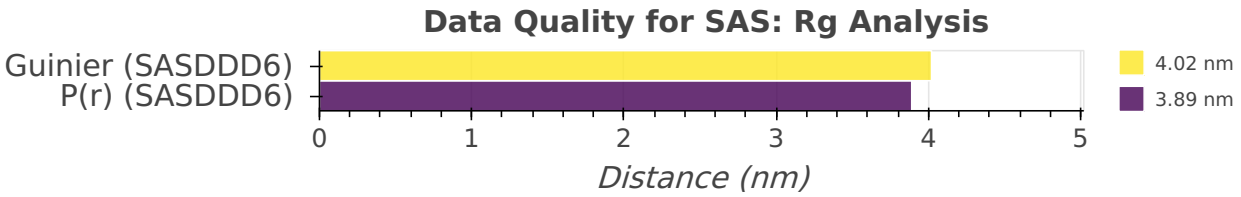
0 20 40 60 80 100 120
Outliers

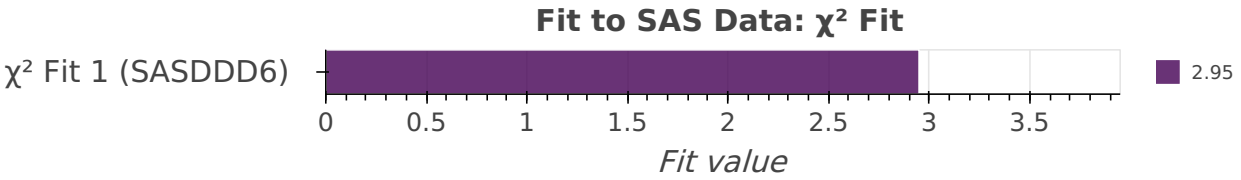

Model 172
Model 173
Model 174
Model 175
Model 176
Model 177
Model 178
Model 179
Model 180
Clashscore
Ramachandran outliers
Sidechain outliers
0
20
40
60
80
100
120
Outliers


Clashscore
Model 181 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 182 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 183 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 184 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 185 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 186 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 187 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 188 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 189 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers


Clashscore
Model 190 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 191 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 192 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 193 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 194 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 195 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 196 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 197 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 198 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers


Clashscore
Model 199 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 200 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 201 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 202 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 203 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 204 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 205 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers
Clashscore
Model 206 Ramachandran outliers
Sidechain outliers
0 20 40 60 80 100 120
Outliers





Ensemble information

This entry consists of 2 distinct ensemble(s).

Summary

This entry consists of 206 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	1-206	1	hGBP1 wildtype	A	583	-	1-583	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	Experimental model	PDB	1DG3
2	SAS data	SASBDB	SASDDD6

ID	Dataset type	Database name	Data access code
3	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
4	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
5	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
6	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
7	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
8	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
9	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
10	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
11	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
12	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
13	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
14	Ensemble FRET data	Zenodo	10.5281/zenodo.6534557
15	EPR data	Zenodo	10.5281/zenodo.6534557
16	EPR data	Zenodo	10.5281/zenodo.6534557
17	EPR data	Zenodo	10.5281/zenodo.6534557
18	EPR data	Zenodo	10.5281/zenodo.6534557
19	EPR data	Zenodo	10.5281/zenodo.6534557
20	EPR data	Zenodo	10.5281/zenodo.6534557
21	EPR data	Zenodo	10.5281/zenodo.6534557
22	EPR data	Zenodo	10.5281/zenodo.6534557
23	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
24	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
25	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
26	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
27	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
28	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
29	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
30	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
31	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
32	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
33	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557
34	Single molecule FRET data	Zenodo	10.5281/zenodo.6534557

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	Rigid body docking	None	None	None	True	False
2	1	Targeted NMSim	None	None	None	True	False
3	1	MD simulation	None	None	None	True	False

There are 4 software packages reported in this entry.

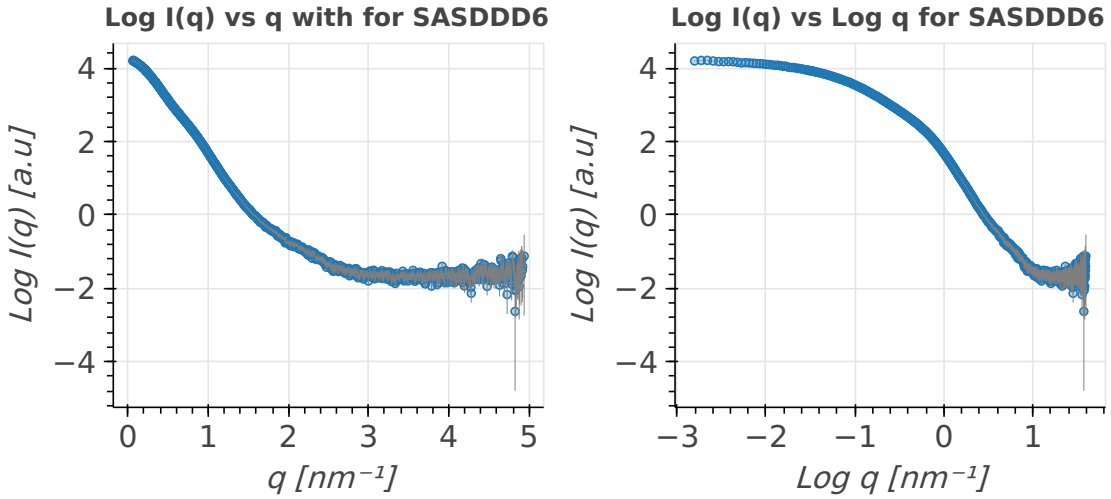
ID	Software name	Software version	Software classification	Software location
1	FPS	Not available	Model building	https://github.com/Fluorescence-Tools/FPS
2	NMSim	Not available	Model building	http://www.nmsim.de
3	Amber 14	Not available	Model building	https://ambermd.org/
4	DeerAnalysis2006	Not available	Data analysis	https://epr.ethz.ch/software/older-versions/old_deeranalysis.html

Data quality

Scattering profile

SAS data used in this integrative model was obtained from 1 deposited SASBDB entry (entries).

Scattering profile for SASDDD6: data from solutions of biological macromolecules are presented as both log I(q) vs q and log I(q) vs log (q) based on SAS validation task force (SASvtf) recommendations. I(q) is the intensity (in arbitrary units) and q is the modulus of the scattering vector.



Key experimental estimates

Molecular weight (MW) estimates from experiments and analysis: true molecular weight can be compared to the Porod estimate from scattering profiles.

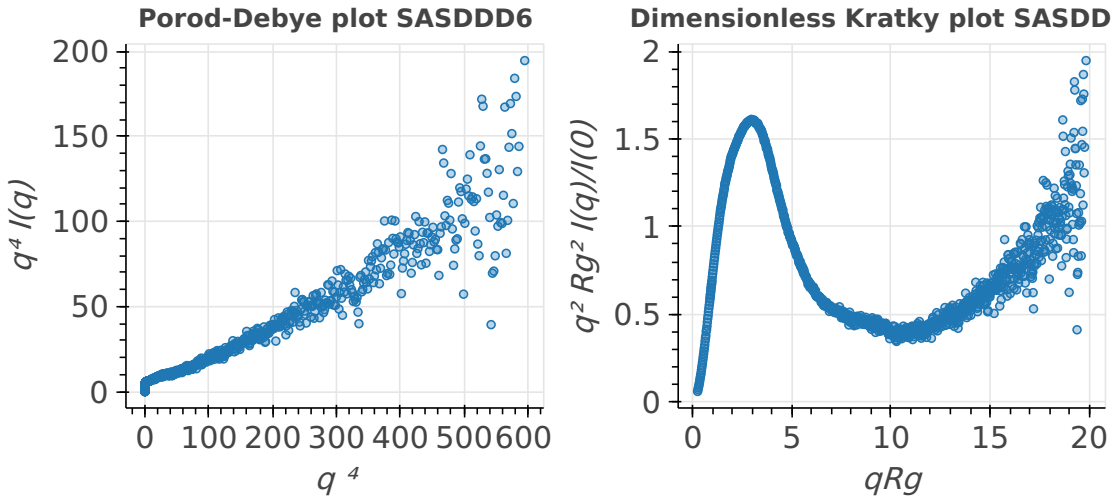
SASDB ID	Chemical composition MW	Standard MW	Porod Volume/MW
SASDDD6	65.3 kDa	Not available	1.59 nm³/kDa

Volume estimates from experiments and analysis: estimated volume can be compared to Porod volume obtained from scattering profiles.

SASDB ID	Estimated Volume	Porod Volume	Specific Volume	Sample Contrast	Sample Concentration
SASDDD6	Not available	104.90 nm³	Not available	Not available	16.10 mg/mL

Flexibility analysis

Flexibility analysis for SASDDD6: In a Porod-Debye plot, a clear plateau is observed for globular (partial or fully folded) domains, whereas, fully unfolded domains are devoid of any discernable plateau. For details, refer to Figure 5 in Rambo and Tainer, 2011. In a Kratky plot, a parabolic shape is observed for globular (partial or fully folded) domains and a hyperbolic shape is observed for fully unfolded domains.

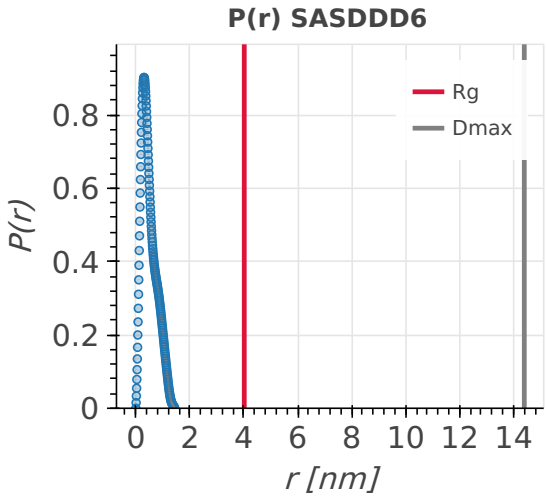


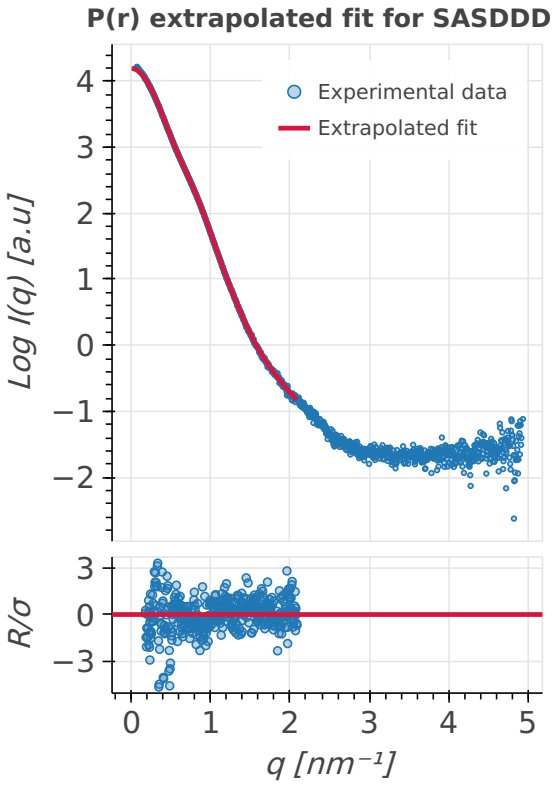
Pair-distance distribution analysis

P(r) analysis: P(r) represents the distribution of distances between all pairs of atoms within the particle weighted by the respective electron densities. P(r) is the Fourier transform of I(s) (and vice versa). R_g can be estimated from integrating the P(r) function. Agreement between the P(r) and Guinier-determined R_g (table below) is a good measure of the self-consistency of the SAS profile. R_g is a measure for the overall size of a macromolecule; e.g. a protein with a smaller R_g is more compact than a protein with a larger R_g, provided both have the same molecular weight (MW). The point where P(r) is decaying to zero is called D_{max} and represents the maximum size of the particle.

SASDB ID	Software used	D_{max}	D_{max} error	R_g	R_g error
SASDDD6	GNOM 5.0	14.400 nm	Not available	4.018 nm	Not available

P(r) for SASDDD6: The value of P(r) should be zero beyond r=D_{max}.



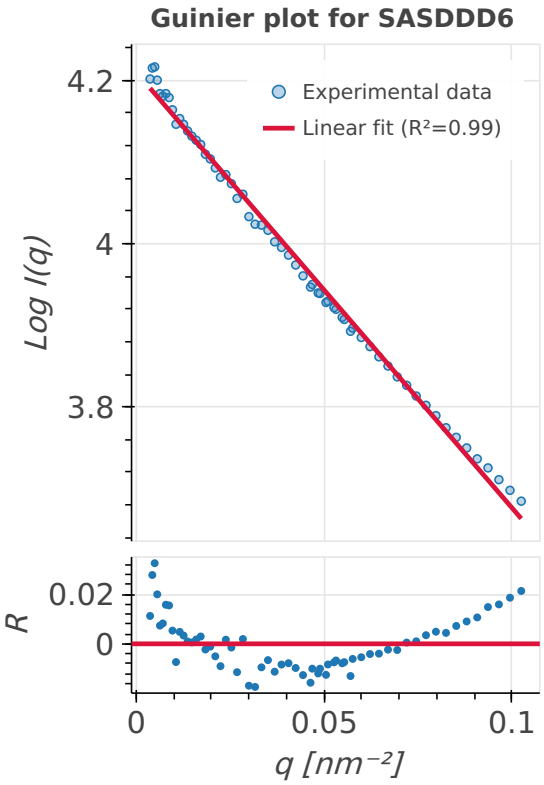


Guinier analysis

Guinier analysis: agreement between the P(r) and Guinier-determined R_g (table below) is a good measure of the self-consistency of the SAS profile. Molecular weight estimates can also be compared to Porod and sample molecular weights for consistency.

SASDB ID	R_g	R_g error	MW	MW error
SASDDD6	3.89 nm	0.06 nm	Not available	Not available

Guinier analysis: the linearity of the Guinier plot is a sensitive indicator of the quality of the experimental SAS data; a linear Guinier plot is a necessary but not sufficient demonstration that a solution contains monodisperse particles of the same size. Deviations from linearity usually point to strong interference effects, polydispersity of the samples or improper background subtraction. Residual value plot and coefficient of determination (R^2) are measures to assess linear fit to the data. A perfect fit has an R^2 value of 1. Residual values should be equally and randomly spaced around the horizontal axis.



Single molecule FRET

Validation for this section is under development.

Ensemble FRET

Validation for this section is under development.

EPR

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 19400 bond length outliers in this entry (1.98% of 982002 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	74	HIS	ND1-CE1	11.60	1.44	1.32	146	47
A	507	HIS	ND1-CE1	10.66	1.43	1.32	47	57
A	6	HIS	ND1-CE1	10.47	1.43	1.32	200	44
A	358	ARG	CZ-NH2	10.26	1.20	1.33	92	53

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	74	HIS	CE1-NE2	9.98	1.42	1.32	37	44
A	507	HIS	CE1-NE2	9.90	1.42	1.32	112	48
A	85	HIS	ND1-CE1	9.83	1.42	1.32	92	43
A	91	HIS	ND1-CE1	9.71	1.42	1.32	129	52
A	243	HIS	ND1-CE1	9.58	1.42	1.32	159	53
A	74	HIS	CG-ND1	9.58	1.48	1.38	100	34
A	334	HIS	CG-CD2	9.56	1.46	1.35	105	22
A	378	HIS	CE1-NE2	9.51	1.42	1.32	105	42
A	6	HIS	CE1-NE2	9.49	1.42	1.32	23	46
A	406	ARG	CD-NE	9.47	1.59	1.46	106	22
A	378	HIS	CD2-NE2	9.42	1.48	1.37	189	23
A	243	HIS	CE1-NE2	9.35	1.41	1.32	157	56
A	150	HIS	CE1-NE2	9.30	1.41	1.32	175	51
A	527	HIS	CE1-NE2	9.26	1.41	1.32	90	52
A	527	HIS	ND1-CE1	9.13	1.41	1.32	206	45
A	527	HIS	CG-ND1	9.13	1.48	1.38	25	44
A	292	ARG	CZ-NH2	9.10	1.21	1.33	103	48
A	291	PRO	N-CD	9.10	1.35	1.47	55	16
A	378	HIS	ND1-CE1	9.07	1.41	1.32	97	47
A	151	ARG	CZ-NH2	9.04	1.21	1.33	14	47
A	91	HIS	CE1-NE2	8.98	1.41	1.32	115	50
A	357	HIS	ND1-CE1	8.87	1.41	1.32	64	58
A	334	HIS	CE1-NE2	8.84	1.41	1.32	161	45
A	81	TRP	NE1-CE2	8.84	1.47	1.37	177	26
A	434	ARG	CD-NE	8.84	1.58	1.46	104	21
A	507	HIS	CG-ND1	8.78	1.47	1.38	76	42
A	417	PRO	N-CD	8.77	1.35	1.47	169	19
A	378	HIS	CG-ND1	8.73	1.47	1.38	50	55
A	392	ARG	CZ-NH2	8.72	1.22	1.33	173	51
A	48	ARG	CZ-NH2	8.68	1.22	1.33	145	43
A	85	HIS	CE1-NE2	8.66	1.41	1.32	2	45
A	452	ARG	CZ-NH2	8.64	1.22	1.33	151	44
A	35	THR	CB-OG1	8.64	1.29	1.43	151	17
A	481	THR	C-N	8.63	1.45	1.33	137	12
A	7	MET	C-N	8.62	1.45	1.33	41	13

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	539	ARG	CZ-NH2	8.61	1.22	1.33	39	62
A	357	HIS	CE1-NE2	8.61	1.41	1.32	4	53
A	243	HIS	CG-ND1	8.59	1.47	1.38	34	37
A	150	HIS	ND1-CE1	8.58	1.41	1.32	61	55
A	507	HIS	CB-CG	8.58	1.62	1.50	116	23
A	373	PHE	C-N	8.58	1.45	1.33	90	11
A	223	ARG	N-CA	8.58	1.62	1.46	118	15
A	6	HIS	CG-ND1	8.55	1.47	1.38	27	36
A	409	GLY	CA-C	8.52	1.67	1.52	116	9
A	153	ARG	CZ-NH2	8.51	1.22	1.33	160	60
A	227	ARG	CZ-NH2	8.49	1.22	1.33	35	41
A	357	HIS	CG-ND1	8.48	1.47	1.38	116	30
A	271	SER	C-N	8.45	1.45	1.33	192	9
A	227	ARG	NE-CZ	8.39	1.23	1.33	119	24
A	334	HIS	ND1-CE1	8.38	1.40	1.32	54	51
A	433	TYR	C-N	8.35	1.45	1.33	92	14
A	91	HIS	CG-ND1	8.35	1.47	1.38	13	31
A	392	ARG	CD-NE	8.33	1.57	1.46	38	20
A	370	ARG	CD-NE	8.31	1.57	1.46	155	18
A	358	ARG	CD-NE	8.20	1.57	1.46	178	22
A	244	ARG	CZ-NH1	8.20	1.21	1.32	123	17
A	570	ARG	CZ-NH2	8.19	1.22	1.33	154	38
A	452	ARG	CD-NE	8.18	1.57	1.46	80	14
A	570	ARG	CD-NE	8.16	1.57	1.46	108	26
A	150	HIS	CG-CD2	8.14	1.44	1.35	128	20
A	334	HIS	CG-ND1	8.13	1.47	1.38	129	35
A	493	ARG	CZ-NH2	8.13	1.22	1.33	164	56
A	548	ARG	CZ-NH2	8.08	1.22	1.33	6	44
A	347	THR	CB-OG1	8.06	1.30	1.43	76	22
A	434	ARG	C-N	8.04	1.44	1.33	90	7
A	183	ARG	CZ-NH2	8.03	1.23	1.33	88	56
A	95	LEU	N-CA	8.03	1.61	1.46	143	4
A	212	THR	CB-OG1	7.99	1.31	1.43	109	13
A	6	HIS	CD2-NE2	7.97	1.46	1.37	175	21
A	268	ASP	C-N	7.96	1.44	1.33	60	9

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	392	ARG	CZ-NH1	7.94	1.21	1.32	183	21
A	362	ARG	CZ-NH1	7.94	1.21	1.32	158	18
A	411	LEU	C-N	7.94	1.44	1.33	125	8
A	362	ARG	CZ-NH2	7.94	1.23	1.33	151	48
A	581	THR	CB-OG1	7.93	1.31	1.43	136	21
A	151	ARG	NE-CZ	7.91	1.24	1.33	123	17
A	240	ARG	CZ-NH1	7.90	1.21	1.32	193	28
A	152	ILE	C-N	7.89	1.44	1.33	193	14
A	183	ARG	CD-NE	7.88	1.57	1.46	91	23
A	260	PRO	N-CA	7.88	1.58	1.47	56	10
A	114	TRP	NE1-CE2	7.83	1.46	1.37	48	27
A	79	TRP	NE1-CE2	7.82	1.46	1.37	29	31
A	522	ARG	CZ-NH2	7.81	1.23	1.33	42	51
A	357	HIS	CD2-NE2	7.77	1.46	1.37	191	17
A	341	GLN	C-N	7.75	1.44	1.33	27	13
A	244	ARG	CZ-NH2	7.75	1.23	1.33	17	42
A	223	ARG	CZ-NH2	7.73	1.23	1.33	153	51
A	20	ARG	CZ-NH2	7.71	1.23	1.33	82	60
A	299	THR	N-CA	7.71	1.60	1.46	68	8
A	358	ARG	CZ-NH1	7.69	1.22	1.32	10	29
A	243	HIS	CD2-NE2	7.68	1.29	1.37	193	22
A	383	GLU	C-N	7.68	1.44	1.33	138	10
A	227	ARG	CD-NE	7.64	1.56	1.46	60	14
A	440	LEU	CA-C	7.62	1.69	1.52	8	2
A	48	ARG	NE-CZ	7.59	1.41	1.33	82	18
A	6	HIS	CG-CD2	7.57	1.44	1.35	60	22

Standard geometry: angle outliers

There are 64907 bond angle outliers in this entry (4.91% of 1320872 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	229	PHE	CA-CB-CG	16.33	130.13	113.80	19	96
A	574	ASN	OD1-CG-ND2	16.06	106.54	122.60	14	82
A	541	GLN	OE1-CD-NE2	14.75	107.85	122.60	60	88

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	175	PHE	CA-CB-CG	14.72	128.52	113.80	187	52
A	150	HIS	CA-CB-CG	14.53	128.33	113.80	155	58
A	559	GLN	OE1-CD-NE2	14.46	108.14	122.60	202	112
A	274	PHE	CA-CB-CG	14.35	128.15	113.80	152	95
A	362	ARG	NE-CZ-NH2	14.19	131.97	119.20	73	59
A	220	ASN	OD1-CG-ND2	14.04	108.56	122.60	145	87
A	507	HIS	CA-CB-CG	13.90	127.70	113.80	69	55
A	412	GLN	OE1-CD-NE2	13.87	108.73	122.60	136	94
A	480	GLN	OE1-CD-NE2	13.73	108.87	122.60	134	117
A	387	GLN	OE1-CD-NE2	13.68	108.92	122.60	52	110
A	289	ASN	CA-CB-CG	13.68	126.28	112.60	144	70
A	546	GLN	OE1-CD-NE2	13.67	108.93	122.60	109	101
A	184	ASP	CA-CB-CG	13.61	126.21	112.60	198	68
A	177	ASP	CA-CB-CG	13.55	126.15	112.60	92	81
A	249	GLN	OE1-CD-NE2	13.48	109.12	122.60	92	92
A	522	ARG	NE-CZ-NH1	13.37	134.87	121.50	135	52
A	359	ASP	CA-CB-CG	13.33	125.93	112.60	92	55
A	351	GLN	OE1-CD-NE2	13.26	109.34	122.60	57	102
A	580	GLN	OE1-CD-NE2	13.25	109.35	122.60	179	110
A	20	ARG	NE-CZ-NH2	13.18	131.06	119.20	147	53
A	341	GLN	OE1-CD-NE2	13.18	109.42	122.60	43	103
A	174	PHE	CA-CB-CG	13.17	126.97	113.80	13	57
A	141	GLN	OE1-CD-NE2	13.14	109.46	122.60	83	97
A	441	GLN	OE1-CD-NE2	13.12	109.48	122.60	35	104
A	566	GLN	OE1-CD-NE2	13.07	109.53	122.60	38	118
A	344	GLN	OE1-CD-NE2	13.04	109.56	122.60	100	116
A	519	GLN	OE1-CD-NE2	13.03	109.57	122.60	155	108
A	394	ASP	CA-CB-CG	12.95	125.55	112.60	34	54
A	500	GLN	OE1-CD-NE2	12.95	109.65	122.60	100	96
A	321	GLN	OE1-CD-NE2	12.91	109.69	122.60	184	114
A	153	ARG	NE-CZ-NH2	12.91	130.82	119.20	183	61
A	392	ARG	NE-CZ-NH1	12.89	134.39	121.50	162	61
A	329	GLN	OE1-CD-NE2	12.85	109.75	122.60	110	106

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	135	ASN	OD1-CG-ND2	12.83	109.77	122.60	171	83
A	334	HIS	CA-CB-CG	12.78	126.58	113.80	43	51
A	276	ASN	OD1-CG-ND2	12.78	109.82	122.60	33	82
A	392	ARG	NE-CZ-NH2	12.74	107.74	119.20	40	55
A	137	GLN	OE1-CD-NE2	12.71	109.89	122.60	48	100
A	375	ASP	CA-CB-CG	12.70	125.30	112.60	71	72
A	72	GLN	OE1-CD-NE2	12.56	110.04	122.60	87	103
A	185	PHE	CA-CB-CG	12.51	126.31	113.80	168	72
A	265	GLN	OE1-CD-NE2	12.41	110.19	122.60	112	100
A	151	ARG	NE-CZ-NH2	12.40	130.36	119.20	160	45
A	178	PHE	CA-CB-CG	12.40	126.20	113.80	16	77
A	287	GLN	OE1-CD-NE2	12.38	110.22	122.60	83	97
A	399	ASN	OD1-CG-ND2	12.34	110.26	122.60	10	76
A	462	GLN	OE1-CD-NE2	12.28	110.32	122.60	72	107
A	557	GLN	OE1-CD-NE2	12.25	110.35	122.60	149	99
A	171	PHE	CA-CB-CG	12.20	126.00	113.80	102	72
A	230	PHE	CA-CB-CG	12.19	125.99	113.80	58	52
A	214	GLN	OE1-CD-NE2	12.17	110.43	122.60	111	103
A	302	ASN	OD1-CG-ND2	12.17	110.43	122.60	141	86
A	358	ARG	NE-CZ-NH2	12.14	130.12	119.20	202	67
A	289	ASN	OD1-CG-ND2	12.13	110.47	122.60	49	91
A	565	PHE	CA-CB-CG	12.07	125.87	113.80	146	78
A	493	ARG	NE-CZ-NH1	12.06	133.56	121.50	46	55
A	574	ASN	CA-CB-CG	12.04	124.64	112.60	149	53
A	398	GLN	OE1-CD-NE2	12.02	110.58	122.60	119	100
A	140	ASP	CA-CB-CG	11.99	124.59	112.60	202	79
A	530	GLN	OE1-CD-NE2	11.98	110.62	122.60	125	108
A	109	ASN	OD1-CG-ND2	11.97	110.63	122.60	173	81
A	20	ARG	NH1-CZ-NH2	11.97	103.74	119.30	147	50
A	338	GLN	OE1-CD-NE2	11.92	110.68	122.60	35	103

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	129	ASN	OD1-CG-ND2	11.90	110.70	122.60	52	97
A	378	HIS	CA-CB-CG	11.90	125.70	113.80	7	60
A	194	GLN	OE1-CD-NE2	11.89	110.71	122.60	155	105
A	276	ASN	CA-CB-CG	11.83	124.43	112.60	32	56
A	357	HIS	CA-CB-CG	11.81	101.99	113.80	97	66
A	264	GLN	OE1-CD-NE2	11.77	110.83	122.60	26	100
A	308	ASP	CA-CB-CG	11.75	124.35	112.60	42	66
A	116	PHE	CA-CB-CG	11.74	125.54	113.80	55	86
A	400	GLN	OE1-CD-NE2	11.74	110.86	122.60	138	103
A	456	GLN	OE1-CD-NE2	11.70	110.90	122.60	82	108
A	188	ASP	CA-CB-CG	11.66	124.26	112.60	135	67
A	368	PHE	CA-CB-CG	11.64	125.44	113.80	168	72
A	36	GLN	OE1-CD-NE2	11.62	110.98	122.60	125	112
A	314	ASN	OD1-CG-ND2	11.60	111.00	122.60	164	72
A	525	GLN	OE1-CD-NE2	11.60	111.00	122.60	92	106
A	438	GLN	OE1-CD-NE2	11.56	111.04	122.60	36	95
A	129	ASN	CA-CB-CG	11.55	124.15	112.60	113	56
A	240	ARG	NH1-CZ-NH2	11.53	104.31	119.30	159	40
A	515	GLN	OE1-CD-NE2	11.50	111.10	122.60	158	98
A	110	GLN	OE1-CD-NE2	11.47	111.13	122.60	22	104
A	527	HIS	CA-CB-CG	11.42	125.22	113.80	122	55
A	324	ASN	OD1-CG-ND2	11.42	111.18	122.60	191	77
A	126	PHE	CA-CB-CG	11.39	125.19	113.80	31	77
A	170	ASP	CA-CB-CG	11.38	123.98	112.60	122	60
A	103	ASP	CA-CB-CG	11.37	123.97	112.60	148	67
A	65	PHE	CA-CB-CG	11.36	125.16	113.80	88	62
A	238	PHE	CA-CB-CG	11.34	125.14	113.80	122	101
A	539	ARG	NE-CZ-NH2	11.33	129.40	119.20	198	48
A	477	GLN	OE1-CD-NE2	11.32	111.28	122.60	116	109
A	199	ASP	CA-CB-CG	11.28	123.88	112.60	196	77
A	405	ASP	CA-CB-CG	11.24	123.84	112.60	47	59
A	216	ASP	CA-CB-CG	11.23	123.83	112.60	201	57

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	537	ASN	OD1-CG-ND2	11.22	111.38	122.60	19	85
A	236	PHE	CA-CB-CG	11.22	125.02	113.80	98	72

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	2.87	27
2	2.76	26
3	3.72	35
4	2.98	28
5	3.51	33
6	1.06	10
7	0.64	6
8	0.85	8
9	3.19	30
10	1.17	11
11	1.06	10
12	1.38	13
13	2.98	28
14	0.96	9
15	1.60	15
16	0.53	5
17	1.70	16
18	0.53	5
19	3.30	31
20	4.04	38
21	3.72	35
22	3.30	31
23	1.28	12
24	2.87	27
25	1.81	17
26	1.49	14

Model ID	Clash score	Number of clashes
27	1.28	12
28	1.49	14
29	0.96	9
30	2.02	19
31	1.49	14
32	1.49	14
33	1.06	10
34	1.06	10
35	1.06	10
36	0.74	7
37	1.06	10
38	1.17	11
39	0.85	8
40	1.28	12
41	2.87	27
42	1.06	10
43	1.38	13
44	2.23	21
45	1.60	15
46	1.06	10
47	1.06	10
48	1.06	10
49	0.64	6
50	3.72	35
51	1.06	10
52	0.74	7
53	2.98	28
54	4.36	41
55	4.15	39
56	3.72	35
57	0.85	8
58	0.64	6
59	1.38	13
60	1.49	14
61	0.96	9

Model ID	Clash score	Number of clashes
62	0.64	6
63	0.96	9
64	0.85	8
65	0.96	9
66	1.06	10
67	2.87	27
68	2.13	20
69	4.36	41
70	1.06	10
71	0.85	8
72	0.53	5
73	1.06	10
74	2.02	19
75	4.04	38
76	1.49	14
77	0.74	7
78	0.64	6
79	1.60	15
80	0.85	8
81	0.96	9
82	0.85	8
83	1.17	11
84	4.68	44
85	1.28	12
86	0.96	9
87	2.34	22
88	3.40	32
89	2.98	28
90	1.28	12
91	2.76	26
92	0.85	8
93	1.06	10
94	3.51	33
95	1.49	14
96	3.30	31

Model ID	Clash score	Number of clashes
97	0.64	6
98	3.72	35
99	1.49	14
100	1.38	13
101	1.38	13
102	0.96	9
103	1.06	10
104	2.13	20
105	0.64	6
106	0.21	2
107	1.60	15
108	1.49	14
109	1.60	15
110	1.17	11
111	1.17	11
112	0.74	7
113	1.70	16
114	1.38	13
115	0.96	9
116	1.17	11
117	1.06	10
118	0.32	3
119	0.74	7
120	0.64	6
121	1.60	15
122	0.74	7
123	1.17	11
124	1.17	11
125	0.74	7
126	1.49	14
127	0.43	4
128	0.53	5
129	0.96	9
130	1.28	12
131	1.38	13

Model ID	Clash score	Number of clashes
132	1.38	13
133	0.96	9
134	1.17	11
135	1.06	10
136	0.96	9
137	2.02	19
138	1.17	11
139	1.06	10
140	1.38	13
141	0.64	6
142	3.62	34
143	1.38	13
144	0.85	8
145	1.28	12
146	1.28	12
147	1.60	15
148	1.17	11
149	0.53	5
150	0.64	6
151	1.06	10
152	1.49	14
153	3.83	36
154	0.85	8
155	1.38	13
156	0.64	6
157	1.17	11
158	1.28	12
159	0.64	6
160	1.49	14
161	0.21	2
162	0.96	9
163	0.64	6
164	1.38	13
165	3.51	33
166	1.38	13

Model ID	Clash score	Number of clashes
167	3.72	35
168	3.62	34
169	1.60	15
170	0.64	6
171	0.96	9
172	1.17	11
173	0.96	9
174	1.38	13
175	1.06	10
176	2.55	24
177	3.40	32
178	1.06	10
179	1.17	11
180	2.34	22
181	3.51	33
182	3.30	31
183	5.21	49
184	3.30	31
185	2.87	27
186	0.74	7
187	1.81	17
188	3.30	31
189	0.96	9
190	1.06	10
191	1.49	14
192	1.49	14
193	1.91	18
194	3.62	34
195	3.93	37
196	2.55	24
197	0.43	4
198	1.28	12
199	0.74	7
200	3.93	37
201	0.96	9

Model ID	Clash score	Number of clashes
202	1.17	11
203	1.81	17
204	1.38	13
205	1.28	12
206	0.64	6

There are 3198 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:296:LEU:HD12	A:315:ALA:HB1	0.90	200	2
A:353:LEU:HD11	A:395:PHE:CZ	0.89	22	6
A:14:ILE:HD13	A:21:LEU:HD21	0.83	50	8
A:44:VAL:HG22	A:45:GLY:H	0.81	180	18
A:38:MET:HE2	A:293:LEU:HD21	0.79	41	3
A:55:MET:HE2	A:95:LEU:HG	0.78	176	3
A:339:MET:HE1	A:356:LEU:HD21	0.77	139	1
A:247:LEU:H	A:247:LEU:HD23	0.77	189	1
A:14:ILE:HD12	A:21:LEU:HD11	0.77	196	2
A:80:MET:SD	A:94:VAL:HG21	0.77	182	6
A:38:MET:HE1	A:293:LEU:HD22	0.76	19	8
A:38:MET:HE1	A:293:LEU:HD21	0.76	181	8
A:422:VAL:HG21	A:471:MET:HE1	0.75	137	1
A:282:LEU:HD12	A:283:SER:H	0.74	44	2
A:414:ILE:H	A:414:ILE:HD12	0.73	27	1
A:180:TRP:HE1	A:182:LEU:HD22	0.72	89	1
A:7:MET:HE2	A:61:LYS:HE3	0.72	41	1
A:57:LYS:HE3	A:266:VAL:HG21	0.71	120	1
A:152:ILE:HG21	A:171:PHE:HE2	0.70	50	1
A:407:CYS:HB3	A:460:ILE:HG21	0.70	168	6
A:57:LYS:HA	A:57:LYS:HE3	0.70	159	1
A:122:LEU:HD13	A:296:LEU:HD22	0.70	94	2
A:336:GLU:HA	A:391:LYS:HE2	0.69	2	1
A:122:LEU:HD11	A:293:LEU:HD12	0.69	94	3
A:13:LEU:HD13	A:14:ILE:HG23	0.69	172	2
A:114:TRP:CZ2	A:304:ILE:HG21	0.69	89	16
A:80:MET:HE3	A:94:VAL:HG21	0.69	2	11

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:46:LEU:H	A:46:LEU:HD13	0.68	157	1
A:410:LEU:HD11	A:414:ILE:HD12	0.68	139	1
A:55:MET:HE2	A:95:LEU:HB3	0.68	3	1
A:353:LEU:HD11	A:395:PHE:CE1	0.68	20	4
A:174:PHE:CE2	A:312:MET:HE2	0.68	93	1
A:14:ILE:HD11	A:78:ILE:HB	0.68	67	6
A:258:LEU:HD21	A:262:PHE:CD2	0.68	53	7
A:330:LYS:HE2	A:334:HIS:CE1	0.68	176	1
A:31:LEU:HD11	A:80:MET:HE3	0.68	183	1
A:122:LEU:HD13	A:296:LEU:HD12	0.68	193	1
A:40:VAL:HG23	A:94:VAL:HG13	0.67	141	6
A:152:ILE:HG21	A:171:PHE:CE2	0.67	50	7
A:317:LEU:HD22	A:376:VAL:HB	0.67	53	1
A:79:TRP:CG	A:80:MET:H	0.67	194	10
A:121:LEU:HD13	A:312:MET:HG2	0.67	4	1
A:552:LEU:C	A:552:LEU:HD13	0.67	169	6
A:291:PRO:HB2	A:322:ILE:HD12	0.67	134	1
A:120:VAL:HG11	A:175:PHE:CE2	0.66	101	1
A:180:TRP:CD1	A:235:CYS:HG	0.66	45	2
A:342:LYS:HD2	A:356:LEU:HD13	0.66	155	1
A:135:ASN:CG	A:136:GLN:H	0.66	48	1
A:38:MET:HE3	A:40:VAL:HB	0.65	54	5
A:426:ILE:H	A:426:ILE:HD12	0.65	7	1
A:46:LEU:H	A:46:LEU:HD12	0.65	15	2
A:185:PHE:CD2	A:237:VAL:HG23	0.64	24	16
A:177:ASP:HA	A:230:PHE:CE1	0.64	177	12
A:114:TRP:CD1	A:300:TYR:HH	0.64	28	1
A:373:PHE:CZ	A:374:LYS:HE3	0.64	129	1
A:1:MET:HE3	A:2:ALA:H	0.64	153	1
A:316:VAL:HG13	A:317:LEU:HD22	0.64	3	2
A:153:ARG:HH21	A:167:ASP:HB2	0.64	183	1
A:139:MET:HE1	A:219:PHE:CZ	0.64	91	1
A:202:LEU:HD22	A:235:CYS:HB2	0.64	167	3
A:68:GLY:H	A:74:HIS:CE1	0.63	112	6
A:208:LEU:N	A:208:LEU:HD22	0.63	110	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:425:GLY:HA2	A:478:THR:HG23	0.63	22	1
A:67:LEU:H	A:67:LEU:HD22	0.63	45	2
A:178:PHE:CZ	A:226:ILE:HD11	0.63	9	1
A:288:VAL:HG23	A:292:ARG:HD2	0.63	176	2
A:146:THR:HG22	A:225:CYS:HB2	0.63	195	3
A:59:ALA:HB2	A:81:TRP:HE1	0.63	168	5
A:77:GLY:HA2	A:115:ILE:HD13	0.63	197	1
A:404:SER:HB3	A:460:ILE:HD13	0.63	67	1
A:295:SER:O	A:299:THR:HG23	0.63	110	2
A:88:LYS:HE3	A:91:HIS:CD2	0.63	114	1
A:82:CYS:HB2	A:94:VAL:HG23	0.63	124	1
A:269:PHE:CE1	A:273:ILE:HD11	0.63	146	1
A:80:MET:HE2	A:94:VAL:HG11	0.63	195	2
A:557:GLN:CD	A:562:LYS:HE2	0.63	203	1
A:253:LEU:HD13	A:257:GLU:HG2	0.63	5	1
A:7:MET:HE1	A:61:LYS:HG3	0.63	153	1
A:567:LYS:HE3	A:571:ILE:HD11	0.63	156	1
A:414:ILE:HG21	A:447:TYR:CD2	0.63	187	1
A:356:LEU:C	A:356:LEU:HD13	0.63	27	5
A:55:MET:HE3	A:97:ASP:HB2	0.63	21	2
A:7:MET:HG3	A:81:TRP:CH2	0.63	33	1
A:300:TYR:CE1	A:310:PRO:HG2	0.63	55	1
A:206:LEU:HD22	A:223:ARG:HG2	0.62	183	1
A:224:LEU:C	A:224:LEU:HD13	0.62	11	15
A:178:PHE:CD2	A:233:LYS:HE2	0.62	58	3
A:410:LEU:O	A:414:ILE:HG22	0.62	165	3
A:208:LEU:HD21	A:220:ASN:HB2	0.62	196	1
A:215:LYS:HA	A:215:LYS:HE2	0.62	92	1
A:250:LEU:HD11	A:258:LEU:HD13	0.62	196	1
A:282:LEU:CD1	A:292:ARG:HH11	0.62	199	1
A:81:TRP:C	A:94:VAL:HG23	0.62	182	12
A:34:ILE:HD11	A:92:ILE:HD13	0.62	44	3
A:87:LYS:HA	A:87:LYS:HE3	0.62	24	2
A:120:VAL:HG23	A:175:PHE:CD2	0.62	188	2
A:121:LEU:HD23	A:300:TYR:CD2	0.62	188	3

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:171:PHE:CE1	A:229:PHE:CE1	0.62	55	3
A:414:ILE:N	A:414:ILE:HD12	0.62	27	1
A:38:MET:HE1	A:293:LEU:HD11	0.62	55	2

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	581	527	40	14
2	581	512	51	18
3	581	510	57	14
4	581	512	59	10
5	581	513	58	10
6	581	520	54	7
7	581	530	42	9
8	581	525	46	10
9	581	514	53	14
10	581	515	61	5
11	581	531	39	11
12	581	533	41	7
13	581	504	60	17
14	581	531	43	7
15	581	531	45	5
16	581	527	46	8
17	581	535	38	8
18	581	524	49	8
19	581	522	52	7
20	581	505	57	19
21	581	505	60	16
22	581	512	53	16
23	581	528	39	14
24	581	521	48	12
25	581	511	57	13
26	581	526	46	9
27	581	524	48	9
28	581	536	38	7

Model ID	Analysed	Favored	Allowed	Outliers
29	581	527	45	9
30	581	518	51	12
31	581	527	44	10
32	581	536	39	6
33	581	513	52	16
34	581	521	49	11
35	581	523	50	8
36	581	524	50	7
37	581	528	46	7
38	581	531	43	7
39	581	519	52	10
40	581	529	45	7
41	581	526	42	13
42	581	520	45	16
43	581	526	45	10
44	581	529	35	17
45	581	529	45	7
46	581	516	56	9
47	581	535	44	2
48	581	529	49	3
49	581	519	54	8
50	581	529	39	13
51	581	528	42	11
52	581	536	42	3
53	581	496	68	17
54	581	499	67	15
55	581	524	45	12
56	581	521	44	16
57	581	529	44	8
58	581	511	63	7
59	581	525	47	9
60	581	506	62	13
61	581	513	57	11
62	581	527	47	7
63	581	526	45	10

Model ID	Analysed	Favored	Allowed	Outliers
64	581	520	56	5
65	581	515	53	13
66	581	530	39	12
67	581	534	35	12
68	581	526	44	11
69	581	515	57	9
70	581	538	36	7
71	581	536	35	10
72	581	528	44	9
73	581	519	50	12
74	581	521	48	12
75	581	526	44	11
76	581	524	46	11
77	581	528	41	12
78	581	532	46	3
79	581	521	46	14
80	581	522	51	8
81	581	527	47	7
82	581	531	45	5
83	581	518	51	12
84	581	513	56	12
85	581	528	49	4
86	581	534	40	7
87	581	502	65	14
88	581	528	44	9
89	581	535	36	10
90	581	535	40	6
91	581	516	52	13
92	581	511	56	14
93	581	530	39	12
94	581	528	46	7
95	581	511	60	10
96	581	524	44	13
97	581	515	56	10
98	581	521	50	10

Model ID	Analysed	Favored	Allowed	Outliers
99	581	535	34	12
100	581	528	43	10
101	581	527	45	9
102	581	527	46	8
103	581	539	33	9
104	581	514	52	15
105	581	528	47	6
106	581	536	35	10
107	581	543	34	4
108	581	539	38	4
109	581	528	44	9
110	581	526	47	8
111	581	530	45	6
112	581	524	51	6
113	581	527	48	6
114	581	520	52	9
115	581	509	55	17
116	581	508	65	8
117	581	506	65	10
118	581	529	45	7
119	581	530	40	11
120	581	524	50	7
121	581	533	34	14
122	581	538	36	7
123	581	527	49	5
124	581	528	45	8
125	581	528	47	6
126	581	544	28	9
127	581	531	41	9
128	581	541	35	5
129	581	537	37	7
130	581	520	51	10
131	581	526	49	6
132	581	537	39	5
133	581	533	36	12

Model ID	Analysed	Favored	Allowed	Outliers
134	581	533	43	5
135	581	531	41	9
136	581	526	50	5
137	581	524	51	6
138	581	519	56	6
139	581	530	44	7
140	581	522	47	12
141	581	517	54	10
142	581	522	51	8
143	581	524	51	6
144	581	538	35	8
145	581	526	51	4
146	581	534	37	10
147	581	530	39	12
148	581	536	37	8
149	581	522	51	8
150	581	542	37	2
151	581	532	39	10
152	581	518	50	13
153	581	533	41	7
154	581	531	38	12
155	581	531	40	10
156	581	530	42	9
157	581	537	35	9
158	581	522	53	6
159	581	529	40	12
160	581	521	50	10
161	581	529	41	11
162	581	527	44	10
163	581	532	40	9
164	581	514	58	9
165	581	499	74	8
166	581	531	46	4
167	581	537	39	5
168	581	534	40	7

Model ID	Analysed	Favored	Allowed	Outliers
169	581	540	34	7
170	581	531	45	5
171	581	536	36	9
172	581	533	40	8
173	581	514	55	12
174	581	528	40	13
175	581	528	49	4
176	581	536	36	9
177	581	507	63	11
178	581	527	46	8
179	581	529	47	5
180	581	522	51	8
181	581	504	68	9
182	581	509	56	16
183	581	505	58	18
184	581	512	51	18
185	581	519	54	8
186	581	518	52	11
187	581	536	31	14
188	581	527	43	11
189	581	529	42	10
190	581	519	53	9
191	581	524	47	10
192	581	533	44	4
193	581	538	30	13
194	581	528	43	10
195	581	503	63	15
196	581	536	35	10
197	581	530	38	13
198	581	526	46	9
199	581	532	39	10
200	581	514	54	13
201	581	506	63	12
202	581	541	33	7
203	581	533	40	8

Model ID	Analysed	Favored	Allowed	Outliers
204	581	532	42	7
205	581	536	39	6
206	581	537	40	4

There are 314 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	165	VAL	121
A	12	CYS	70
A	108	ASP	58
A	565	PHE	50
A	452	ARG	45
A	176	PRO	40
A	80	MET	30
A	109	ASN	30
A	374	LYS	30
A	63	LYS	28
A	64	GLY	27
A	48	ARG	26
A	161	ASN	24
A	71	VAL	23
A	239	ASP	23
A	241	PRO	23
A	285	GLY	22
A	428	SER	22
A	10	PRO	21
A	134	ILE	21
A	564	GLY	21
A	426	ILE	19
A	34	ILE	18
A	193	GLY	17
A	231	PRO	17
A	49	THR	16
A	68	GLY	16
A	242	VAL	16
A	11	MET	15

Chain	Res	Type	Models (Total)
A	255	ASP	14
A	378	HIS	14
A	77	GLY	13
A	189	LEU	13
A	283	SER	13
A	346	PRO	13
A	50	GLY	12
A	232	LYS	12
A	280	LYS	12
A	290	GLY	12
A	373	PHE	12
A	457	ALA	12
A	480	GLN	12
A	5	ILE	11
A	9	GLY	11
A	156	SER	11
A	233	LYS	11
A	372	SER	11
A	425	GLY	11
A	432	GLY	11
A	172	VAL	10
A	186	SER	10
A	375	ASP	10
A	451	PRO	10
A	566	GLN	10
A	18	ASN	9
A	69	SER	9
A	110	GLN	9
A	144	TYR	9
A	279	THR	9
A	318	ALA	9
A	320	ALA	9
A	468	LYS	9
A	35	THR	8
A	99	GLU	8

Chain	Res	Type	Models (Total)
A	152	ILE	8
A	192	ASP	8
A	310	PRO	8
A	377	ASP	8
A	477	GLN	8
A	481	THR	8
A	3	SER	7
A	7	MET	7
A	90	GLY	7
A	102	GLY	7
A	206	LEU	7
A	211	GLY	7
A	277	SER	7
A	284	GLY	7
A	455	ILE	7
A	483	THR	7
A	32	SER	6
A	51	LYS	6
A	60	GLY	6
A	70	THR	6
A	73	SER	6
A	143	TYR	6
A	154	SER	6
A	158	PRO	6
A	185	PHE	6
A	286	ILE	6
A	316	VAL	6
A	322	ILE	6
A	343	VAL	6
A	347	THR	6
A	376	VAL	6
A	413	VAL	6
A	456	GLN	6
A	6	HIS	5
A	66	SER	5

Chain	Res	Type	Models (Total)
A	74	HIS	5

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	524	335	87	102
2	524	341	83	100
3	524	325	95	104
4	524	325	97	102
5	524	325	97	102
6	524	449	46	29
7	524	444	57	23
8	524	437	65	22
9	524	339	83	102
10	524	447	50	27
11	524	459	48	17
12	524	440	61	23
13	524	317	100	107
14	524	437	72	15
15	524	440	60	24
16	524	452	54	18
17	524	457	51	16
18	524	456	48	20
19	524	325	85	114
20	524	307	99	118
21	524	325	93	106
22	524	340	90	94
23	524	461	40	23
24	524	324	96	104
25	524	445	55	24
26	524	451	56	17
27	524	436	54	34
28	524	446	58	20
29	524	462	43	19
30	524	329	93	102

Model ID	Analysed	Favored	Allowed	Outliers
31	524	439	55	30
32	524	460	46	18
33	524	407	87	30
34	524	454	52	18
35	524	450	47	27
36	524	448	53	23
37	524	451	54	19
38	524	451	47	26
39	524	450	51	23
40	524	434	61	29
41	524	325	109	90
42	524	460	42	22
43	524	423	64	37
44	524	334	89	101
45	524	467	38	19
46	524	417	67	40
47	524	441	53	30
48	524	453	55	16
49	524	466	44	14
50	524	343	86	95
51	524	454	49	21
52	524	442	53	29
53	524	331	89	104
54	524	319	95	110
55	524	359	81	84
56	524	326	91	107
57	524	450	54	20
58	524	451	55	18
59	524	449	49	26
60	524	424	61	39
61	524	421	54	49
62	524	448	54	22
63	524	453	47	24
64	524	431	67	26
65	524	433	63	28

Model ID	Analysed	Favored	Allowed	Outliers
66	524	448	53	23
67	524	326	95	103
68	524	414	66	44
69	524	336	79	109
70	524	454	51	19
71	524	465	44	15
72	524	463	50	11
73	524	436	67	21
74	524	350	89	85
75	524	321	102	101
76	524	446	58	20
77	524	463	46	15
78	524	457	50	17
79	524	468	41	15
80	524	457	48	19
81	524	465	38	21
82	524	448	57	19
83	524	459	49	16
84	524	334	99	91
85	524	441	60	23
86	524	468	36	20
87	524	317	87	120
88	524	353	65	106
89	524	337	86	101
90	524	450	54	20
91	524	418	66	40
92	524	428	62	34
93	524	448	52	24
94	524	343	88	93
95	524	460	49	15
96	524	347	80	97
97	524	439	60	25
98	524	350	81	93
99	524	442	61	21
100	524	455	53	16

Model ID	Analysed	Favored	Allowed	Outliers
101	524	456	51	17
102	524	418	72	34
103	524	451	52	21
104	524	417	65	42
105	524	461	42	21
106	524	446	57	21
107	524	457	48	19
108	524	457	42	25
109	524	448	59	17
110	524	457	47	20
111	524	443	61	20
112	524	465	37	22
113	524	438	57	29
114	524	456	47	21
115	524	441	53	30
116	524	440	53	31
117	524	449	52	23
118	524	459	45	20
119	524	465	47	12
120	524	438	65	21
121	524	455	56	13
122	524	470	38	16
123	524	461	45	18
124	524	448	53	23
125	524	456	48	20
126	524	461	43	20
127	524	456	60	8
128	524	468	41	15
129	524	456	52	16
130	524	455	51	18
131	524	455	51	18
132	524	451	51	22
133	524	442	60	22
134	524	445	45	34
135	524	454	51	19

Model ID	Analysed	Favored	Allowed	Outliers
136	524	460	50	14
137	524	454	47	23
138	524	456	49	19
139	524	450	55	19
140	524	452	53	19
141	524	436	55	33
142	524	337	72	115
143	524	430	70	24
144	524	466	39	19
145	524	437	69	18
146	524	455	51	18
147	524	442	55	27
148	524	441	50	33
149	524	450	60	14
150	524	466	43	15
151	524	436	58	30
152	524	451	48	25
153	524	345	80	99
154	524	446	53	25
155	524	427	67	30
156	524	456	52	16
157	524	430	60	34
158	524	437	57	30
159	524	426	68	30
160	524	442	55	27
161	524	458	51	15
162	524	430	61	33
163	524	450	60	14
164	524	431	66	27
165	524	318	98	108
166	524	457	49	18
167	524	346	78	100
168	524	356	79	89
169	524	449	53	22
170	524	447	60	17

Model ID	Analysed	Favored	Allowed	Outliers
171	524	450	54	20
172	524	453	55	16
173	524	459	43	22
174	524	436	63	25
175	524	429	63	32
176	524	336	90	98
177	524	333	96	95
178	524	450	57	17
179	524	461	46	17
180	524	435	65	24
181	524	320	91	113
182	524	327	94	103
183	524	300	101	123
184	524	333	97	94
185	524	347	87	90
186	524	447	52	25
187	524	336	96	92
188	524	331	86	107
189	524	466	38	20
190	524	436	57	31
191	524	453	45	26
192	524	448	58	18
193	524	416	71	37
194	524	332	96	96
195	524	321	102	101
196	524	350	96	78
197	524	463	46	15
198	524	430	62	32
199	524	452	52	20
200	524	318	98	108
201	524	426	64	34
202	524	455	48	21
203	524	429	64	31
204	524	447	49	28
205	524	421	68	35

Model ID	Analysed	Favored	Allowed	Outliers
206	524	430	63	31

There are 515 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

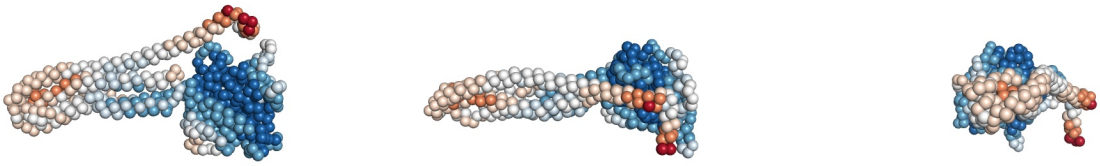
Chain	Res	Type	Models (Total)
A	292	ARG	87
A	294	GLU	81
A	13	LEU	75
A	40	VAL	69
A	528	LEU	69
A	114	TRP	67
A	453	LYS	63
A	127	VAL	60
A	41	VAL	57
A	552	LEU	56
A	233	LYS	55
A	531	LEU	54
A	435	LEU	53
A	78	ILE	52
A	223	ARG	51
A	317	LEU	51
A	350	LEU	51
A	482	LEU	51
A	39	VAL	50
A	229	PHE	50
A	208	LEU	49
A	579	LEU	49
A	46	LEU	47
A	67	LEU	47
A	165	VAL	47
A	379	LEU	47
A	274	PHE	46
A	384	LEU	46
A	95	LEU	45
A	543	LEU	45
A	561	LEU	43

Chain	Res	Type	Models (Total)
A	151	ARG	42
A	183	ARG	42
A	356	LEU	42
A	131	ILE	41
A	506	LEU	41
A	134	ILE	40
A	61	LYS	39
A	265	GLN	39
A	391	LYS	39
A	14	ILE	38
A	406	ARG	38
A	224	LEU	37
A	226	ILE	37
A	298	LEU	37
A	354	LEU	37
A	443	LEU	37
A	293	LEU	36
A	54	LEU	35
A	143	TYR	35
A	309	LEU	35
A	465	LEU	35
A	542	LEU	35
A	101	LEU	34
A	121	LEU	34
A	145	VAL	34
A	92	ILE	33
A	129	ASN	33
A	266	VAL	33
A	282	LEU	33
A	155	LYS	32
A	175	PHE	32
A	237	VAL	32
A	550	LEU	32
A	80	MET	31
A	179	VAL	31

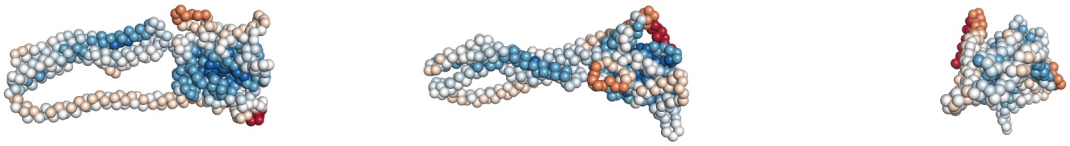
Chain	Res	Type	Models (Total)
A	247	LEU	31
A	554	LEU	31
A	4	GLU	30
A	51	LYS	30
A	55	MET	30
A	120	VAL	30
A	187	LEU	30
A	322	ILE	30
A	330	LYS	30
A	374	LYS	30
A	48	ARG	29
A	115	ILE	29
A	153	ARG	29
A	162	GLU	29
A	288	VAL	29
A	413	VAL	29
A	560	LEU	29
A	5	ILE	28
A	220	ASN	28
A	251	GLU	28
A	367	VAL	28
A	34	ILE	27
A	28	LEU	26
A	56	ASN	26
A	104	VAL	26
A	182	LEU	26
A	286	ILE	26
A	357	HIS	26
A	427	TYR	26
A	475	ILE	26
A	565	PHE	26
A	58	LEU	25
A	180	TRP	25
A	426	ILE	25

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: 100/100).



PrISM analysis for Ensemble 2 (models deposited/total: 106/106).



Fit of model to data used for modeling

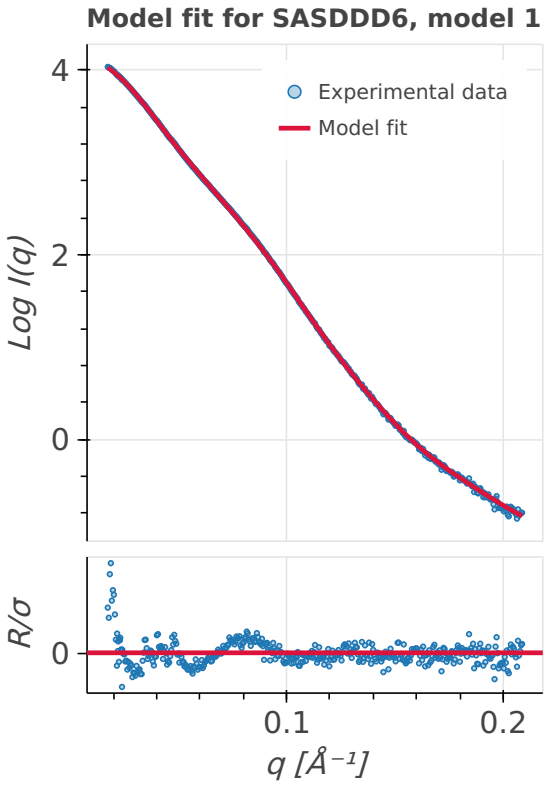
Fit of model(s) to SAS data

χ^2 goodness of fit and cormap analysis

Model and fits displayed below were obtained from SASBDB. χ^2 values are a measure of fit of the model to data. A perfect fit has a χ^2 value of 1.0. ATSAS DATCMP was used for hypothesis testing. All data sets are similar (i.e. the fit and the data collected) is the null hypothesis. p-value is a measure of evidence against the null hypothesis, smaller the value, the stronger the evidence that you should reject the null hypothesis.

SASDB ID	Model	χ^2	p-value
SASDDD6	1	2.95	0.00

Model fit(s): Residual value plot is a measure to assess fit to the data. Residual values should be equally and randomly spaced around the horizontal axis.



Single molecule FRET

Validation for this section is under development.

Ensemble FRET

Validation for this section is under development.

EPR

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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