

Integrative Structure Validation Report

July 22, 2024 - 05:24 PM PDT

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

| | |
|-------------------|--|
| PDB ID | 9A3Q |
| PDB-Dev ID | PDBDEV_00000211 |
| Structure Title | Modeling hLINE1 ORF2p |
| Structure Authors | Baldwin, E.T.; van Eeuwen, T.; Hoyos, T.; Zalevsky, A.; Tchesnokov, E.P; Sanchez, R.; DiStefano, L.; Ruiz, F.X; Hancock, M.; Walpole, T.; Nichols, C.; Wan, P.; Riento, K.; Kass, R.-H.; Augustin, M.; Lammens, A.; Jestel, A.; Upla, P.; Xibinaku, K.; Congreve, S.; Hennink, M.; Rogala, K.B.; Schneider, A.M.; Fairman, J.E.; Christensen, S.M.; Miao, W.; Zaller, D.M.; Sali, A.; Weichenrieder, O.; Burns, K.H.; Gotte, M.; Rout, M.P.; Arnold, E.; Greenbaum, B.D.; Romero, D.L.; LaCava, J.; Taylor, M.S. |

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

We welcome your comments at pdb-dev@mail.wwpdb.org

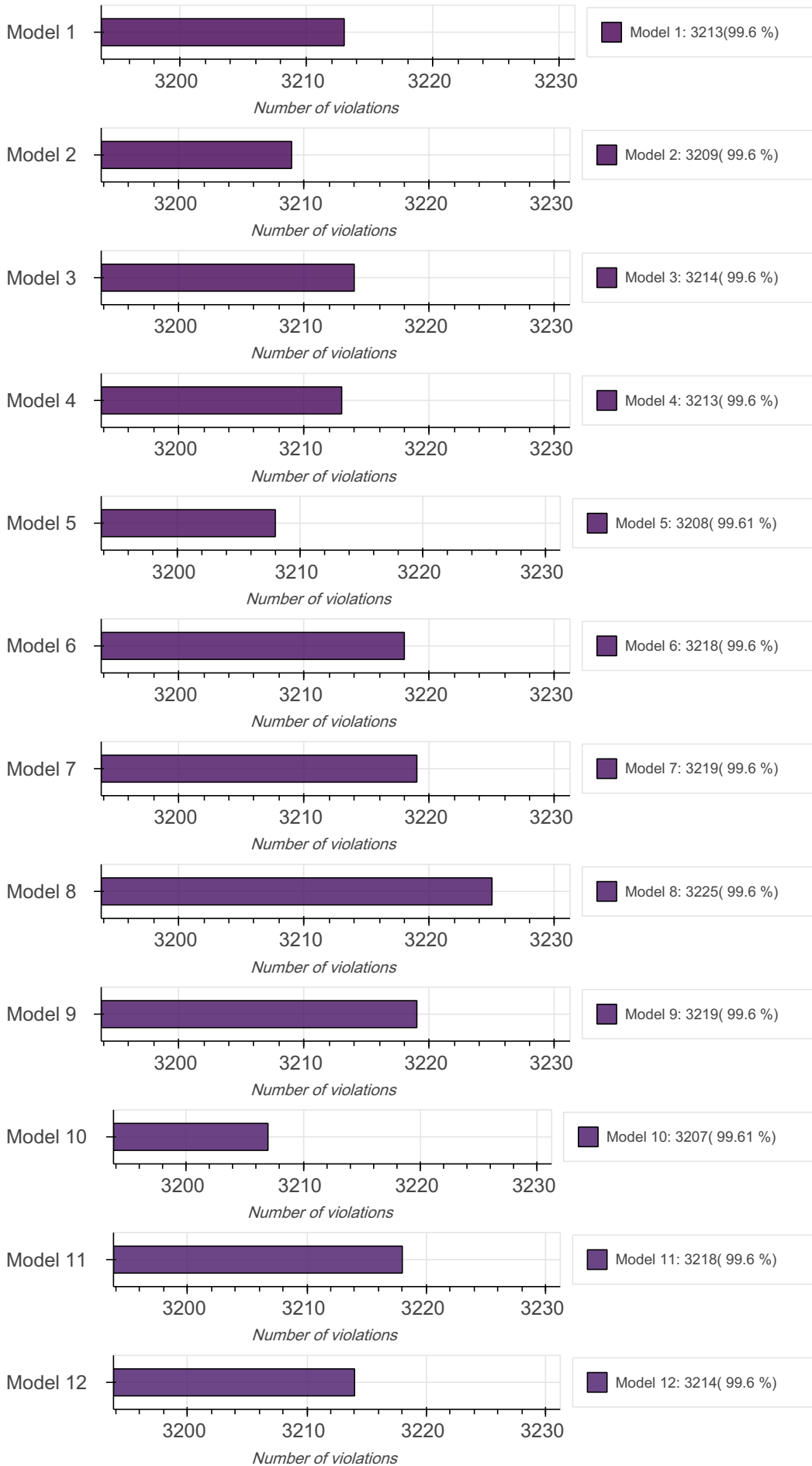
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

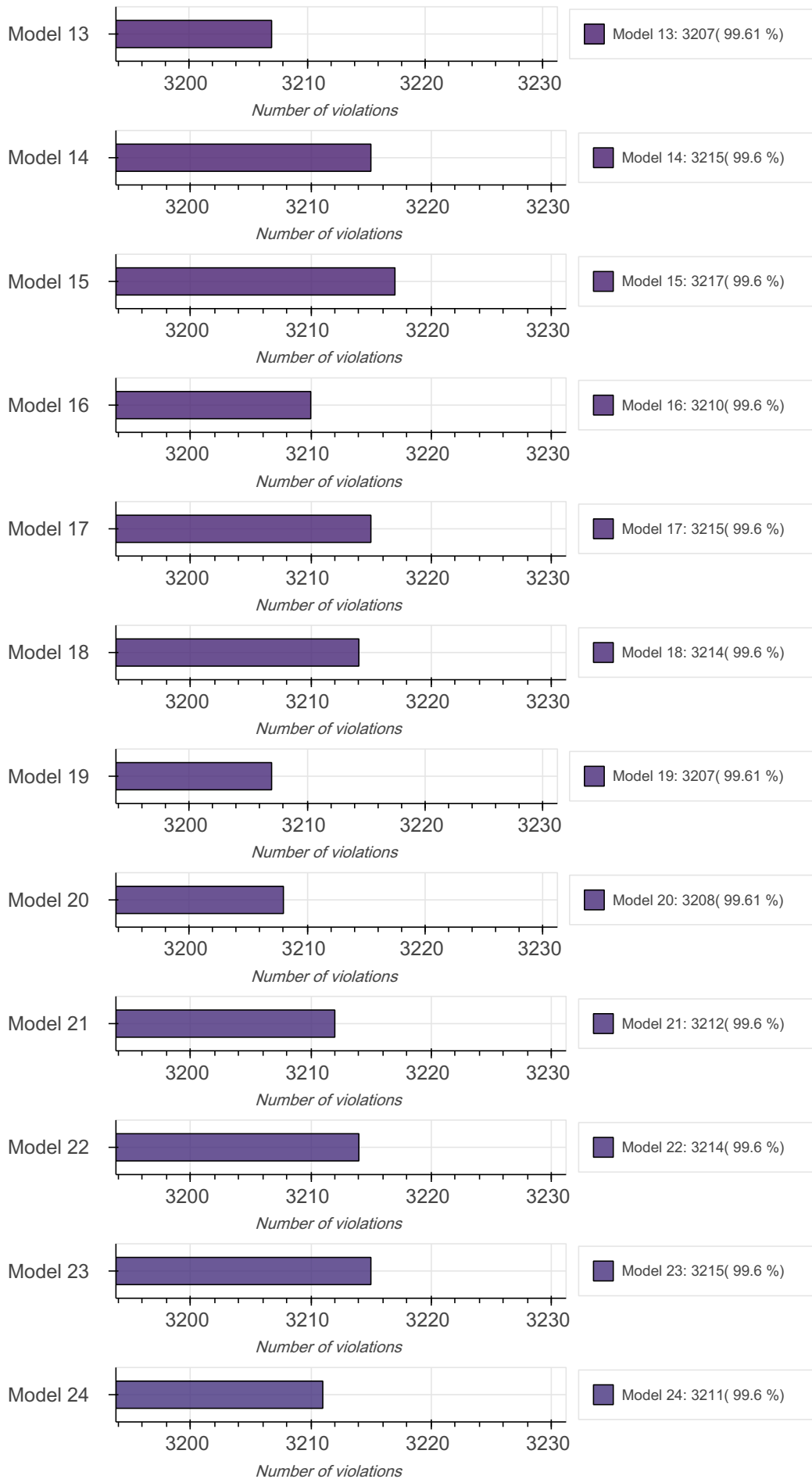
List of references used to build this report is available [here](#).

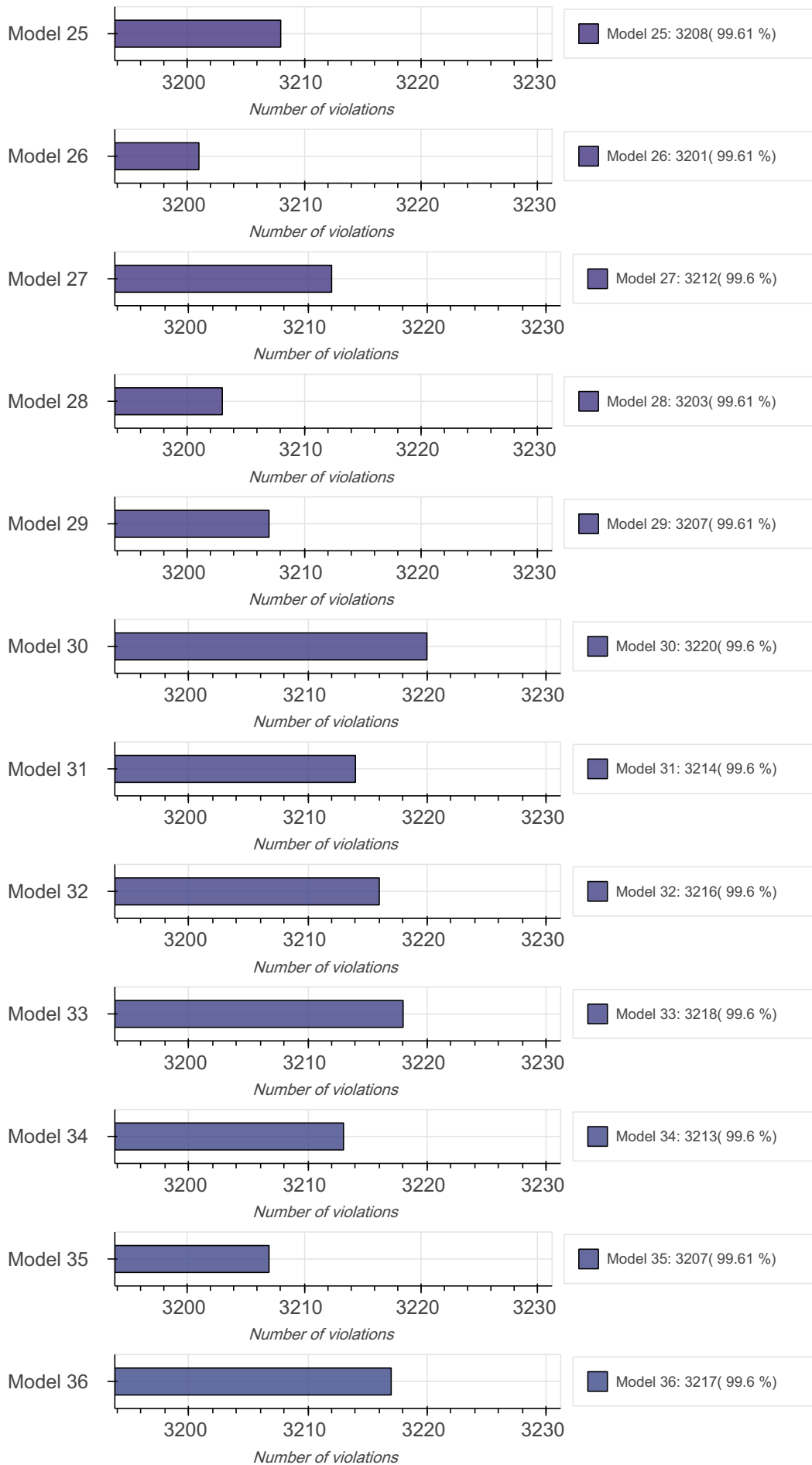
Overall quality

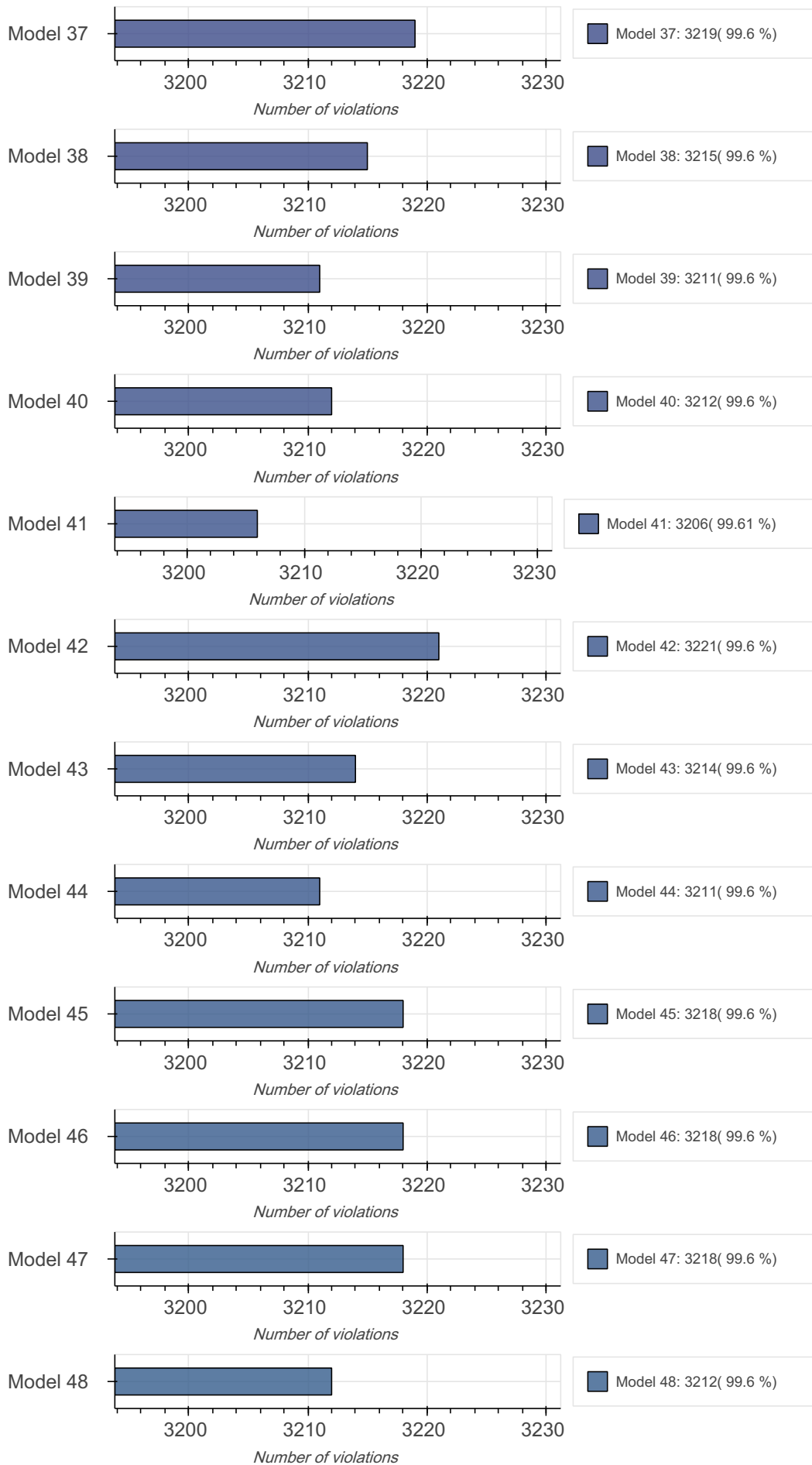
This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to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

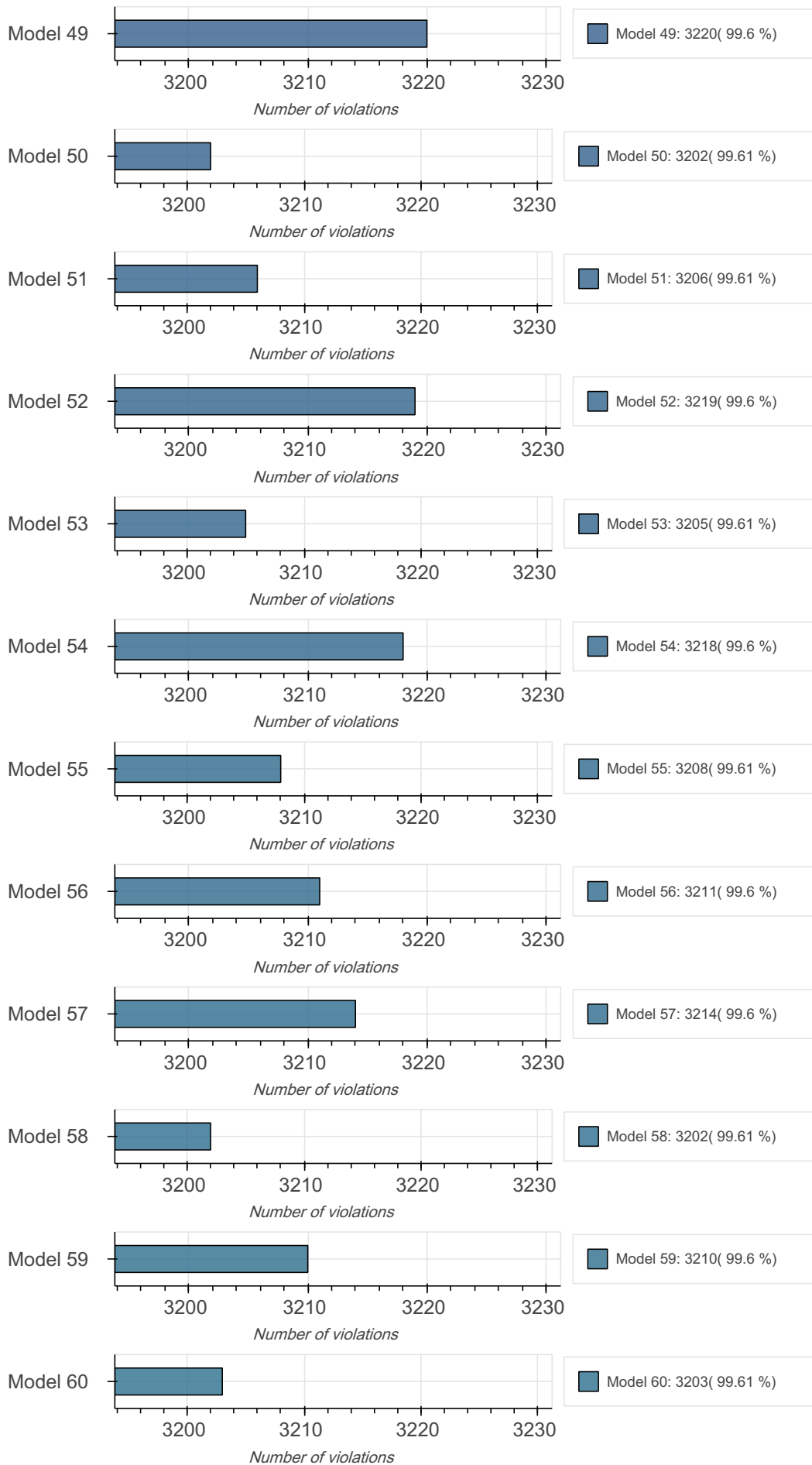
Model Quality: Excluded Volume Analysis

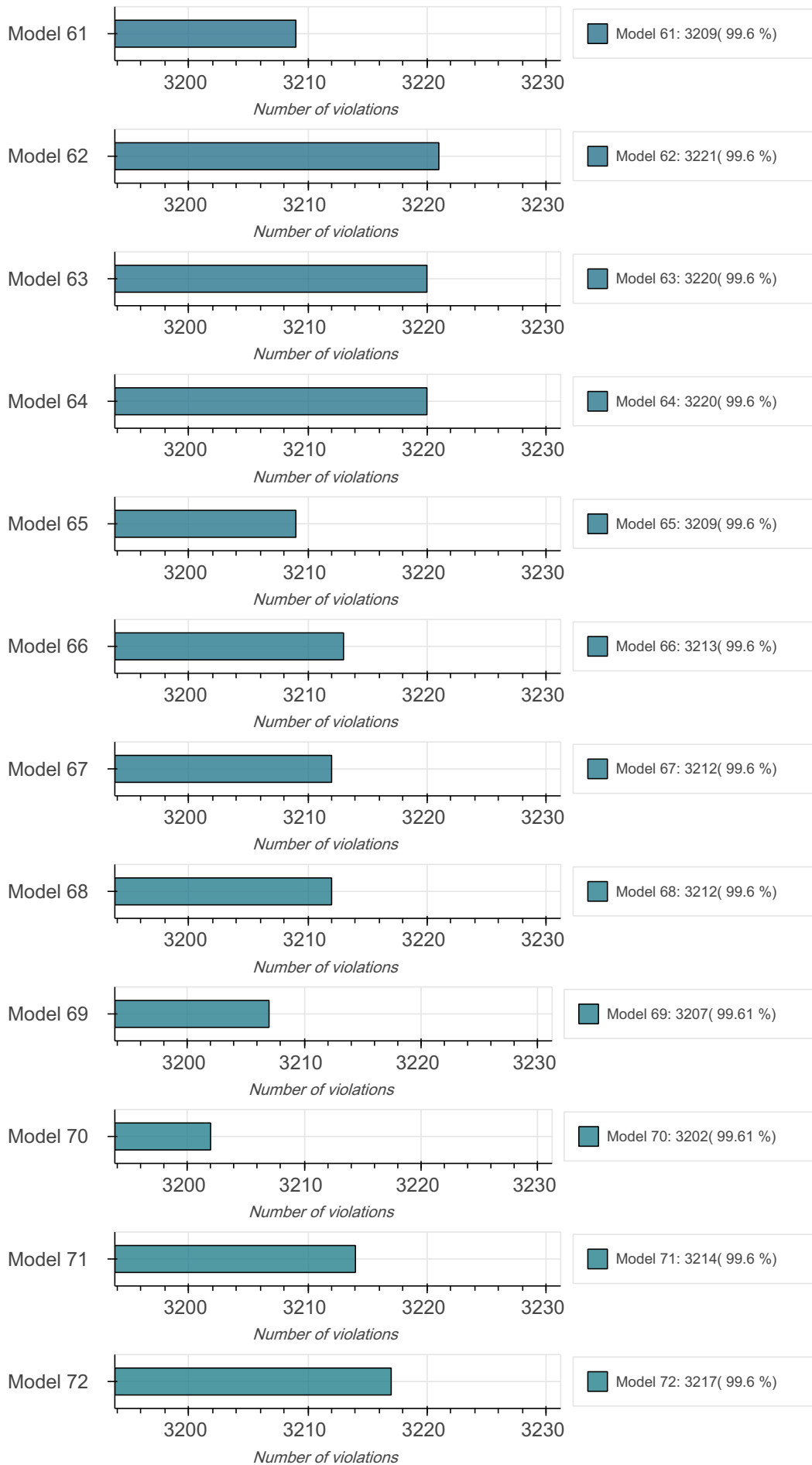


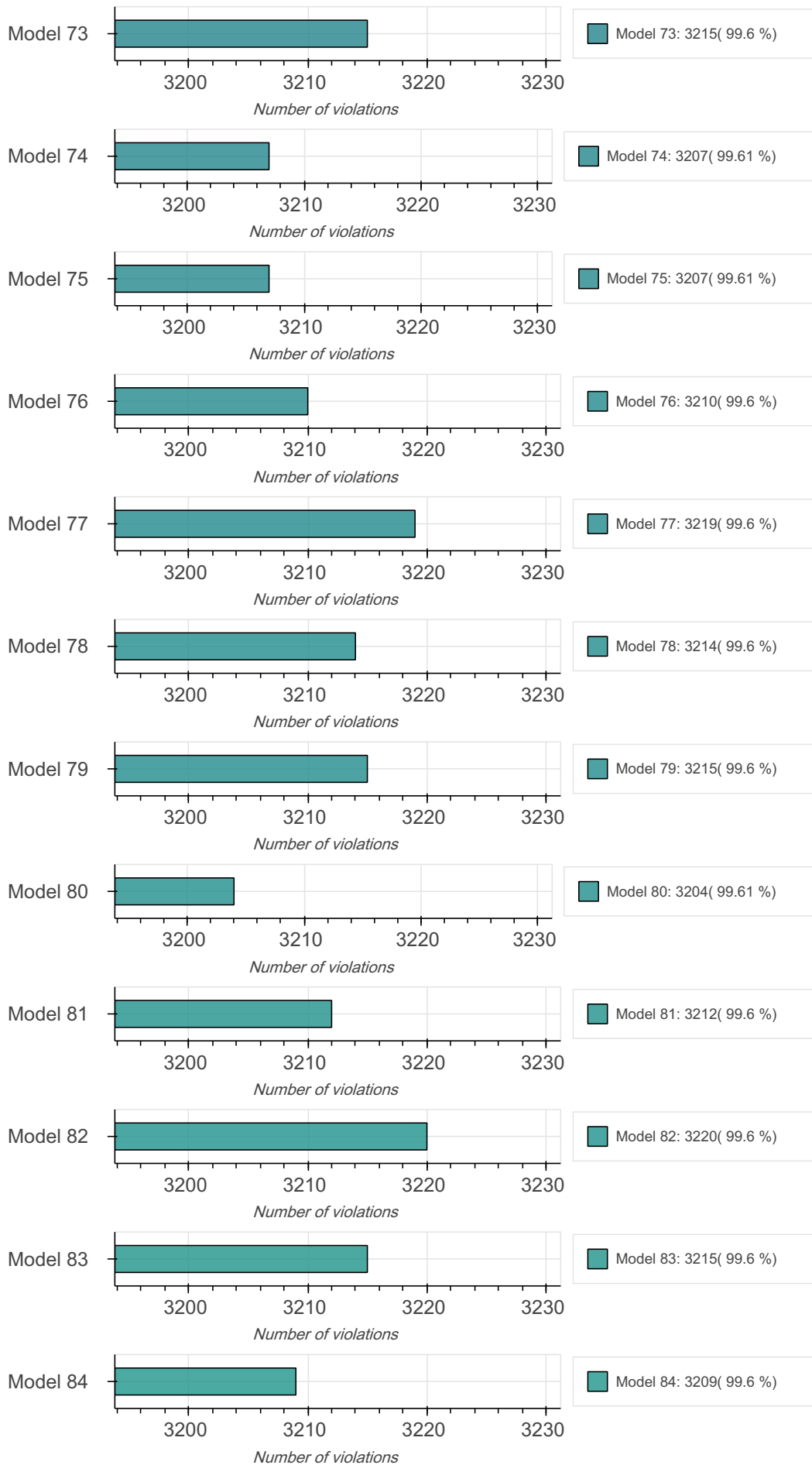


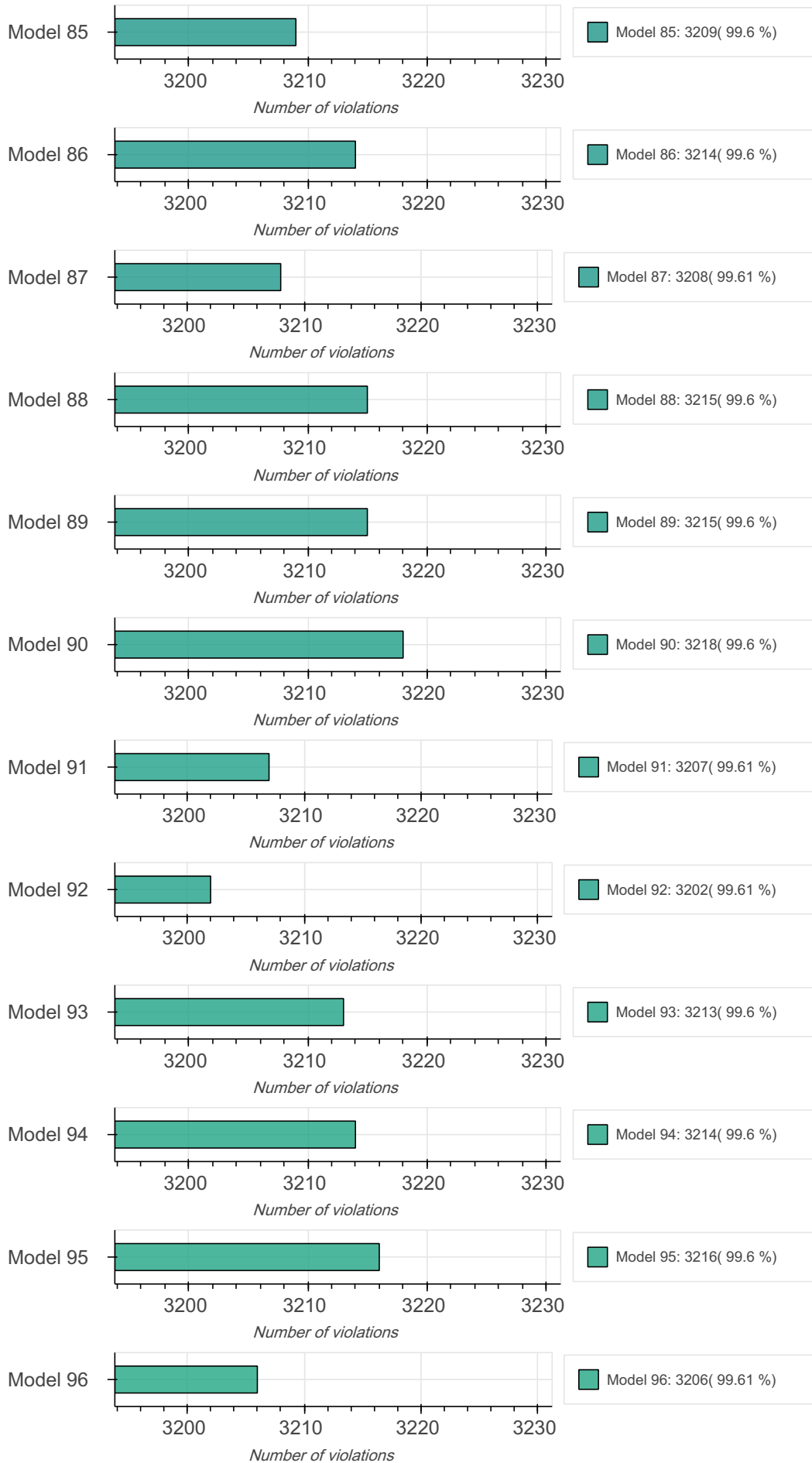


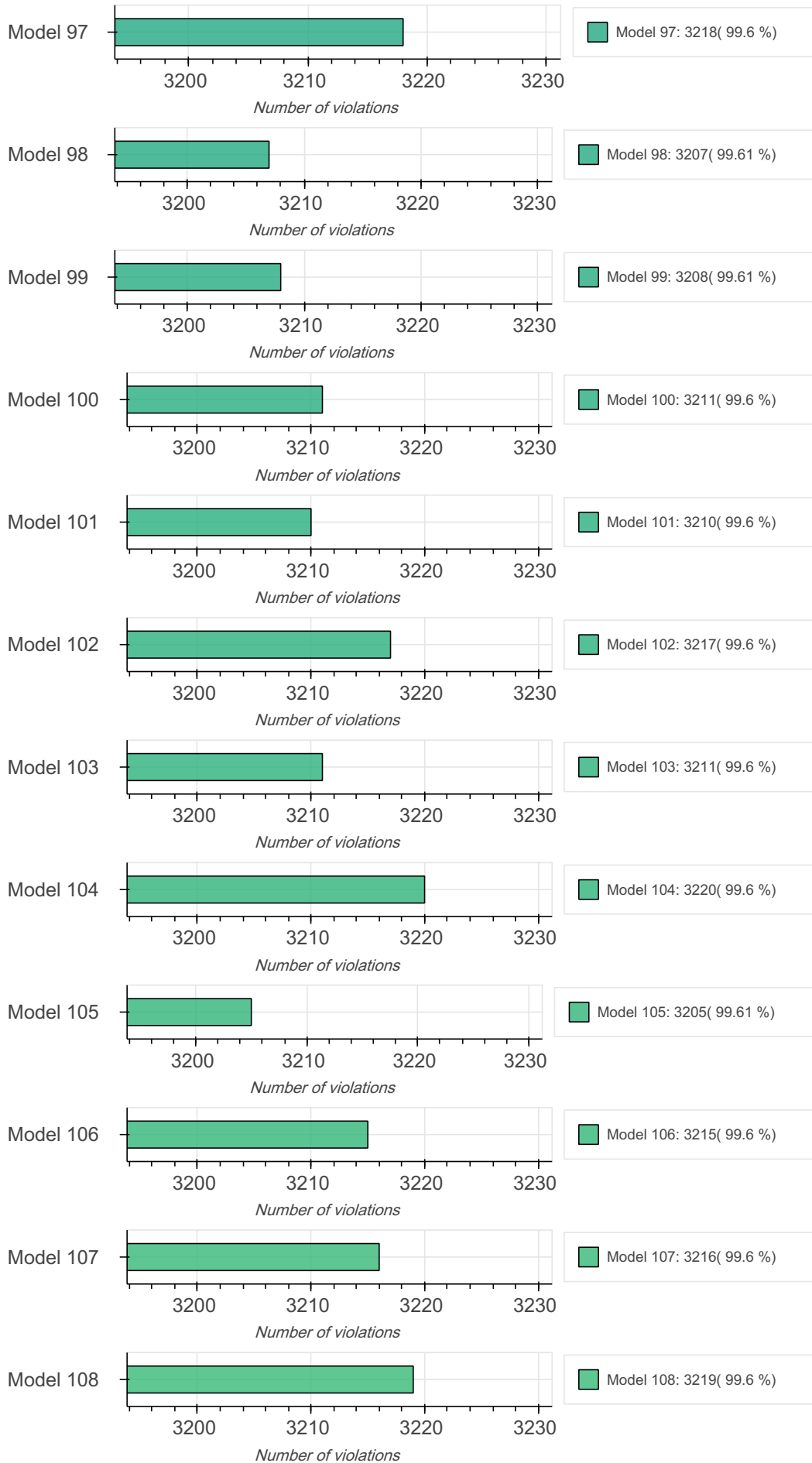








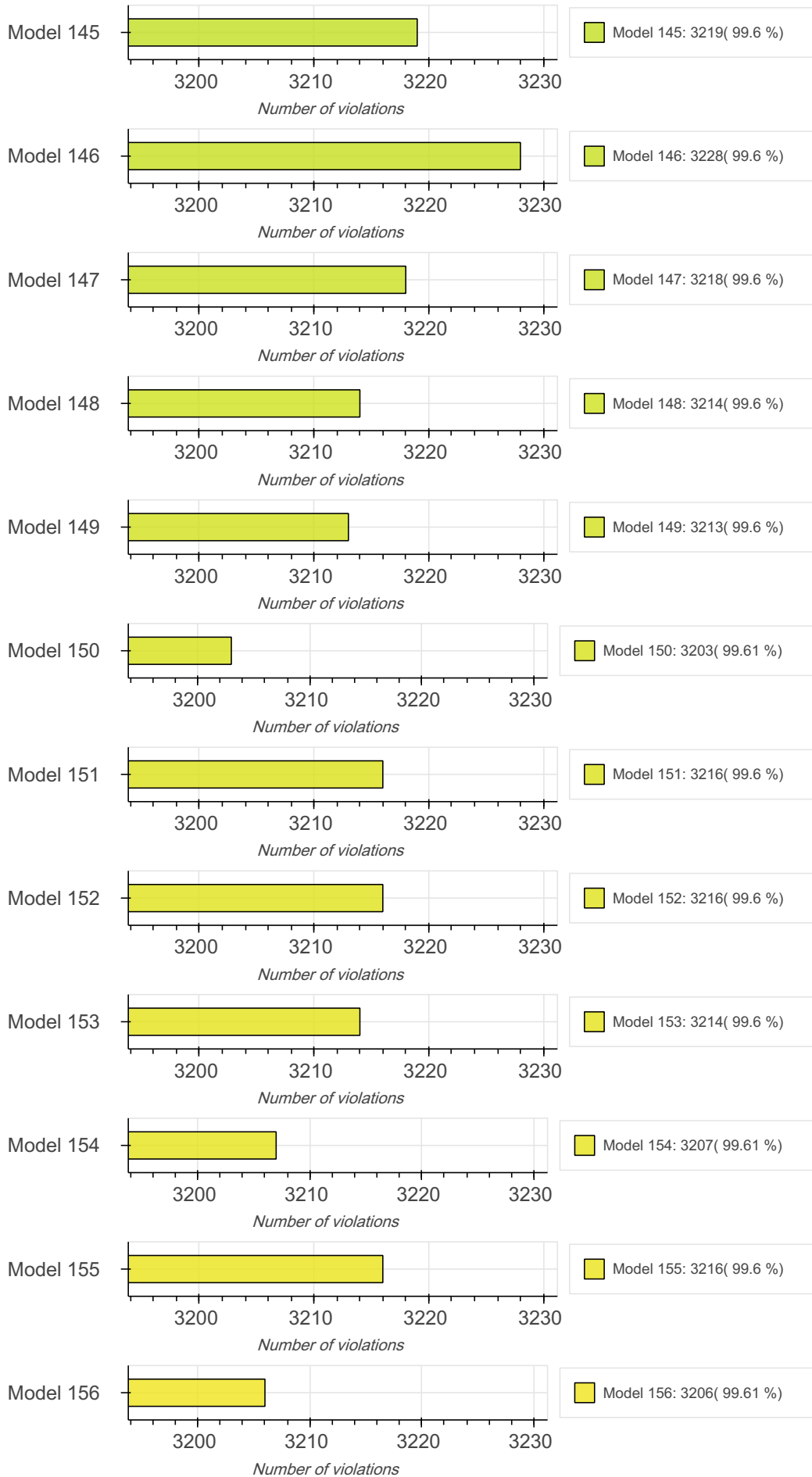


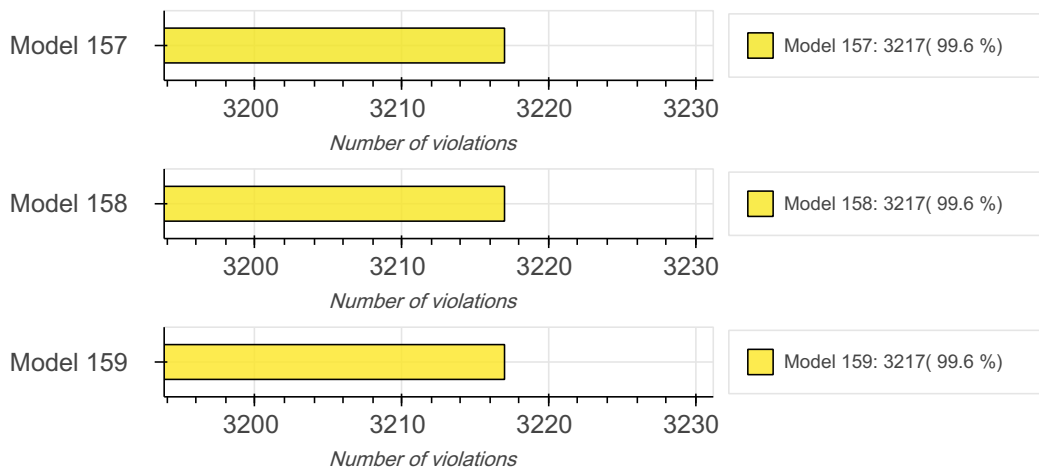












Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 159 unique models, with 1 subunits in each model. A total of 16 datasets or restraints were used to build this entry. Each model is represented by 15 rigid bodies and 14 flexible or non-rigid units.

Entry composition ?

There are 159 unique types of models in this entry. These models are titled Class_001_short_hybrid, Class_002_short_hybrid, Class_003_short_hybrid, Class_004_short_hybrid, Class_005_short_hybrid, Class_006_short_hybrid, Class_007_short_hybrid, Class_008_short_hybrid, Class_009_short_hybrid, Class_010_short_hybrid, Class_011_short_hybrid, Class_012_short_hybrid, Class_013_short_hybrid, Class_014_short_hybrid, Class_015_short_hybrid, Class_016_short_hybrid, Class_017_short_hybrid, Class_018_short_hybrid, Class_019_short_hybrid, Class_020_short_hybrid, Class_021_short_hybrid, Class_022_short_hybrid, Class_023_short_hybrid, Class_024_short_hybrid, Class_025_short_hybrid, Class_026_short_hybrid, Class_027_short_hybrid, Class_028_short_hybrid, Class_029_short_hybrid, Class_030_short_hybrid, Class_031_short_hybrid, Class_032_short_hybrid, Class_033_short_hybrid, Class_034_short_hybrid, Class_035_short_hybrid, Class_036_short_hybrid, Class_037_short_hybrid, Class_038_short_hybrid, Class_039_short_hybrid, Class_040_short_hybrid, Class_041_short_hybrid, Class_042_short_hybrid, Class_043_short_hybrid, Class_044_short_hybrid, Class_045_short_hybrid, Class_046_short_hybrid, Class_047_short_hybrid, Class_048_short_hybrid, Class_049_short_hybrid, Class_050_short_hybrid, Class_051_short_hybrid, Class_052_short_hybrid, Class_053_short_hybrid, Class_054_short_hybrid, Class_055_short_hybrid, Class_056_short_hybrid, Class_057_short_hybrid, Class_058_short_hybrid, Class_059_short_hybrid, Class_060_short_hybrid, Class_061_short_hybrid, Class_062_short_hybrid, Class_063_short_hybrid, Class_064_short_hybrid, Class_065_short_hybrid, Class_066_short_hybrid, Class_067_short_hybrid, Class_068_short_hybrid, Class_069_short_hybrid, Class_070_short_hybrid, Class_071_short_hybrid, Class_072_short_hybrid, Class_073_short_hybrid, Class_074_short_hybrid, Class_075_short_hybrid, Class_076_short_hybrid, Class_077_short_hybrid, Class_078_short_hybrid, Class_079_short_hybrid, Class_080_short_hybrid, Class_081_short_hybrid,

Class_082_short_hybrid, Class_083_short_hybrid, Class_084_short_hybrid, Class_085_short_hybrid, Class_086_short_hybrid, Class_087_short_hybrid, Class_088_short_hybrid, Class_089_short_hybrid, Class_090_short_hybrid, Class_091_L376_RNA, Class_092_L376_RNA, Class_093_L376_RNA, Class_094_L376_RNA, Class_095_L376_RNA, Class_096_L376_RNA, Class_097_L376_RNA, Class_098_L376_RNA, Class_099_L376_RNA, Class_100_L376_RNA, Class_101_L376_RNA, Class_102_L376_RNA, Class_103_L376_RNA, Class_104_L376_RNA, Class_105_L376_RNA, Class_106_L376_RNA, Class_107_L376_RNA, Class_108_L376_RNA, Class_109_L376_RNA, Class_110_L376_RNA, Class_111_L376_RNA, Class_112_L376_RNA, Class_113_L376_RNA, Class_114_L376_RNA, Class_115_L376_RNA, Class_116_L376_RNA, Class_117_L376_RNA, Class_118_L376_RNA, Class_119_L376_RNA, Class_120_L376_RNA, Class_121_L376_RNA, Class_122_L376_RNA, Class_123_L376_RNA, Class_124_L376_RNA, Class_125_L376_RNA, Class_126_L376_RNA, Class_127_L376_RNA, Class_128_L376_RNA, Class_129_L376_RNA, Class_130_L376_RNA, Class_131_L376_RNA, Class_132_L376_RNA, Class_133_L376_RNA, Class_134_L376_RNA, Class_135_L376_RNA, Class_136_L376_RNA, Class_137_L376_RNA, Class_138_L376_RNA, Class_139_L376_RNA, Class_140_L376_RNA, Class_141_L376_RNA, Class_142_L376_RNA, Class_143_L376_RNA, Class_144_L376_RNA, Class_145_L376_RNA, Class_146_L376_RNA, Class_147_L376_RNA, Class_148_L376_RNA, Class_149_L376_RNA, Class_150_L376_RNA, Class_151_L376_RNA, Class_152_L376_RNA, Class_153_L376_RNA, Class_154_L376_RNA, Class_155_L376_RNA, Class_156_L376_RNA, Class_157_L376_RNA, Class_158_L376_RNA, Class_159_L376_RNA respectively.

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 1 | 1 | 1 | ORF2 | A | A | 1275 |
| 2 | 1 | 1 | ORF2 | A | A | 1275 |
| 3 | 1 | 1 | ORF2 | A | A | 1275 |
| 4 | 1 | 1 | ORF2 | A | A | 1275 |
| 5 | 1 | 1 | ORF2 | A | A | 1275 |
| 6 | 1 | 1 | ORF2 | A | A | 1275 |
| 7 | 1 | 1 | ORF2 | A | A | 1275 |
| 8 | 1 | 1 | ORF2 | A | A | 1275 |
| 9 | 1 | 1 | ORF2 | A | A | 1275 |
| 10 | 1 | 1 | ORF2 | A | A | 1275 |
| 11 | 1 | 1 | ORF2 | A | A | 1275 |
| 12 | 1 | 1 | ORF2 | A | A | 1275 |
| 13 | 1 | 1 | ORF2 | A | A | 1275 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 14 | 1 | 1 | ORF2 | A | A | 1275 |
| 15 | 1 | 1 | ORF2 | A | A | 1275 |
| 16 | 1 | 1 | ORF2 | A | A | 1275 |
| 17 | 1 | 1 | ORF2 | A | A | 1275 |
| 18 | 1 | 1 | ORF2 | A | A | 1275 |
| 19 | 1 | 1 | ORF2 | A | A | 1275 |
| 20 | 1 | 1 | ORF2 | A | A | 1275 |
| 21 | 1 | 1 | ORF2 | A | A | 1275 |
| 22 | 1 | 1 | ORF2 | A | A | 1275 |
| 23 | 1 | 1 | ORF2 | A | A | 1275 |
| 24 | 1 | 1 | ORF2 | A | A | 1275 |
| 25 | 1 | 1 | ORF2 | A | A | 1275 |
| 26 | 1 | 1 | ORF2 | A | A | 1275 |
| 27 | 1 | 1 | ORF2 | A | A | 1275 |
| 28 | 1 | 1 | ORF2 | A | A | 1275 |
| 29 | 1 | 1 | ORF2 | A | A | 1275 |
| 30 | 1 | 1 | ORF2 | A | A | 1275 |
| 31 | 1 | 1 | ORF2 | A | A | 1275 |
| 32 | 1 | 1 | ORF2 | A | A | 1275 |
| 33 | 1 | 1 | ORF2 | A | A | 1275 |
| 34 | 1 | 1 | ORF2 | A | A | 1275 |
| 35 | 1 | 1 | ORF2 | A | A | 1275 |
| 36 | 1 | 1 | ORF2 | A | A | 1275 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 37 | 1 | 1 | ORF2 | A | A | 1275 |
| 38 | 1 | 1 | ORF2 | A | A | 1275 |
| 39 | 1 | 1 | ORF2 | A | A | 1275 |
| 40 | 1 | 1 | ORF2 | A | A | 1275 |
| 41 | 1 | 1 | ORF2 | A | A | 1275 |
| 42 | 1 | 1 | ORF2 | A | A | 1275 |
| 43 | 1 | 1 | ORF2 | A | A | 1275 |
| 44 | 1 | 1 | ORF2 | A | A | 1275 |
| 45 | 1 | 1 | ORF2 | A | A | 1275 |
| 46 | 1 | 1 | ORF2 | A | A | 1275 |
| 47 | 1 | 1 | ORF2 | A | A | 1275 |
| 48 | 1 | 1 | ORF2 | A | A | 1275 |
| 49 | 1 | 1 | ORF2 | A | A | 1275 |
| 50 | 1 | 1 | ORF2 | A | A | 1275 |
| 51 | 1 | 1 | ORF2 | A | A | 1275 |
| 52 | 1 | 1 | ORF2 | A | A | 1275 |
| 53 | 1 | 1 | ORF2 | A | A | 1275 |
| 54 | 1 | 1 | ORF2 | A | A | 1275 |
| 55 | 1 | 1 | ORF2 | A | A | 1275 |
| 56 | 1 | 1 | ORF2 | A | A | 1275 |
| 57 | 1 | 1 | ORF2 | A | A | 1275 |
| 58 | 1 | 1 | ORF2 | A | A | 1275 |
| 59 | 1 | 1 | ORF2 | A | A | 1275 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 60 | 1 | 1 | ORF2 | A | A | 1275 |
| 61 | 1 | 1 | ORF2 | A | A | 1275 |
| 62 | 1 | 1 | ORF2 | A | A | 1275 |
| 63 | 1 | 1 | ORF2 | A | A | 1275 |
| 64 | 1 | 1 | ORF2 | A | A | 1275 |
| 65 | 1 | 1 | ORF2 | A | A | 1275 |
| 66 | 1 | 1 | ORF2 | A | A | 1275 |
| 67 | 1 | 1 | ORF2 | A | A | 1275 |
| 68 | 1 | 1 | ORF2 | A | A | 1275 |
| 69 | 1 | 1 | ORF2 | A | A | 1275 |
| 70 | 1 | 1 | ORF2 | A | A | 1275 |
| 71 | 1 | 1 | ORF2 | A | A | 1275 |
| 72 | 1 | 1 | ORF2 | A | A | 1275 |
| 73 | 1 | 1 | ORF2 | A | A | 1275 |
| 74 | 1 | 1 | ORF2 | A | A | 1275 |
| 75 | 1 | 1 | ORF2 | A | A | 1275 |
| 76 | 1 | 1 | ORF2 | A | A | 1275 |
| 77 | 1 | 1 | ORF2 | A | A | 1275 |
| 78 | 1 | 1 | ORF2 | A | A | 1275 |
| 79 | 1 | 1 | ORF2 | A | A | 1275 |
| 80 | 1 | 1 | ORF2 | A | A | 1275 |
| 81 | 1 | 1 | ORF2 | A | A | 1275 |
| 82 | 1 | 1 | ORF2 | A | A | 1275 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 83 | 1 | 1 | ORF2 | A | A | 1275 |
| 84 | 1 | 1 | ORF2 | A | A | 1275 |
| 85 | 1 | 1 | ORF2 | A | A | 1275 |
| 86 | 1 | 1 | ORF2 | A | A | 1275 |
| 87 | 1 | 1 | ORF2 | A | A | 1275 |
| 88 | 1 | 1 | ORF2 | A | A | 1275 |
| 89 | 1 | 1 | ORF2 | A | A | 1275 |
| 90 | 1 | 1 | ORF2 | A | A | 1275 |
| 91 | 1 | 1 | ORF2 | A | A | 1275 |
| 92 | 1 | 1 | ORF2 | A | A | 1275 |
| 93 | 1 | 1 | ORF2 | A | A | 1275 |
| 94 | 1 | 1 | ORF2 | A | A | 1275 |
| 95 | 1 | 1 | ORF2 | A | A | 1275 |
| 96 | 1 | 1 | ORF2 | A | A | 1275 |
| 97 | 1 | 1 | ORF2 | A | A | 1275 |
| 98 | 1 | 1 | ORF2 | A | A | 1275 |
| 99 | 1 | 1 | ORF2 | A | A | 1275 |
| 100 | 1 | 1 | ORF2 | A | A | 1275 |
| 101 | 1 | 1 | ORF2 | A | A | 1275 |
| 102 | 1 | 1 | ORF2 | A | A | 1275 |
| 103 | 1 | 1 | ORF2 | A | A | 1275 |
| 104 | 1 | 1 | ORF2 | A | A | 1275 |
| 105 | 1 | 1 | ORF2 | A | A | 1275 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 106 | 1 | 1 | ORF2 | A | A | 1275 |
| 107 | 1 | 1 | ORF2 | A | A | 1275 |
| 108 | 1 | 1 | ORF2 | A | A | 1275 |
| 109 | 1 | 1 | ORF2 | A | A | 1275 |
| 110 | 1 | 1 | ORF2 | A | A | 1275 |
| 111 | 1 | 1 | ORF2 | A | A | 1275 |
| 112 | 1 | 1 | ORF2 | A | A | 1275 |
| 113 | 1 | 1 | ORF2 | A | A | 1275 |
| 114 | 1 | 1 | ORF2 | A | A | 1275 |
| 115 | 1 | 1 | ORF2 | A | A | 1275 |
| 116 | 1 | 1 | ORF2 | A | A | 1275 |
| 117 | 1 | 1 | ORF2 | A | A | 1275 |
| 118 | 1 | 1 | ORF2 | A | A | 1275 |
| 119 | 1 | 1 | ORF2 | A | A | 1275 |
| 120 | 1 | 1 | ORF2 | A | A | 1275 |
| 121 | 1 | 1 | ORF2 | A | A | 1275 |
| 122 | 1 | 1 | ORF2 | A | A | 1275 |
| 123 | 1 | 1 | ORF2 | A | A | 1275 |
| 124 | 1 | 1 | ORF2 | A | A | 1275 |
| 125 | 1 | 1 | ORF2 | A | A | 1275 |
| 126 | 1 | 1 | ORF2 | A | A | 1275 |
| 127 | 1 | 1 | ORF2 | A | A | 1275 |
| 128 | 1 | 1 | ORF2 | A | A | 1275 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 129 | 1 | 1 | ORF2 | A | A | 1275 |
| 130 | 1 | 1 | ORF2 | A | A | 1275 |
| 131 | 1 | 1 | ORF2 | A | A | 1275 |
| 132 | 1 | 1 | ORF2 | A | A | 1275 |
| 133 | 1 | 1 | ORF2 | A | A | 1275 |
| 134 | 1 | 1 | ORF2 | A | A | 1275 |
| 135 | 1 | 1 | ORF2 | A | A | 1275 |
| 136 | 1 | 1 | ORF2 | A | A | 1275 |
| 137 | 1 | 1 | ORF2 | A | A | 1275 |
| 138 | 1 | 1 | ORF2 | A | A | 1275 |
| 139 | 1 | 1 | ORF2 | A | A | 1275 |
| 140 | 1 | 1 | ORF2 | A | A | 1275 |
| 141 | 1 | 1 | ORF2 | A | A | 1275 |
| 142 | 1 | 1 | ORF2 | A | A | 1275 |
| 143 | 1 | 1 | ORF2 | A | A | 1275 |
| 144 | 1 | 1 | ORF2 | A | A | 1275 |
| 145 | 1 | 1 | ORF2 | A | A | 1275 |
| 146 | 1 | 1 | ORF2 | A | A | 1275 |
| 147 | 1 | 1 | ORF2 | A | A | 1275 |
| 148 | 1 | 1 | ORF2 | A | A | 1275 |
| 149 | 1 | 1 | ORF2 | A | A | 1275 |
| 150 | 1 | 1 | ORF2 | A | A | 1275 |
| 151 | 1 | 1 | ORF2 | A | A | 1275 |

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|----------|----------------|------------|--------------|----------|-----------------|----------------|
| 152 | 1 | 1 | ORF2 | A | A | 1275 |
| 153 | 1 | 1 | ORF2 | A | A | 1275 |
| 154 | 1 | 1 | ORF2 | A | A | 1275 |
| 155 | 1 | 1 | ORF2 | A | A | 1275 |
| 156 | 1 | 1 | ORF2 | A | A | 1275 |
| 157 | 1 | 1 | ORF2 | A | A | 1275 |
| 158 | 1 | 1 | ORF2 | A | A | 1275 |
| 159 | 1 | 1 | ORF2 | A | A | 1275 |

Datasets used for modeling

There are 16 unique datasets used to build the models in this entry.

| ID | Dataset type | Database name | Data access code |
|----|----------------------|---------------|-------------------------|
| 12 | 3DEM volume | File | 10.5281/zenodo.10377421 |
| 7 | Crosslinking-MS data | File | 10.5281/zenodo.10377421 |
| 8 | Crosslinking-MS data | File | 10.5281/zenodo.10377421 |
| 9 | Crosslinking-MS data | File | 10.5281/zenodo.10377421 |
| 14 | 2DEM class average | File | 10.5281/zenodo.10377421 |
| 15 | 2DEM class average | File | 10.5281/zenodo.10377421 |
| 16 | 2DEM class average | File | 10.5281/zenodo.10377421 |
| 1 | De Novo model | AlphaFoldDB | O00370 |
| 2 | De Novo model | MODEL ARCHIVE | ma-fejd6 |
| 3 | De Novo model | MODEL ARCHIVE | ma-joo4d |
| 4 | De Novo model | MODEL ARCHIVE | ma-lzyrq |

| ID | Dataset type | Database name | Data access code |
|----|------------------------|---------------|------------------|
| 5 | De Novo model | MODEL ARCHIVE | ma-xlzzy |
| 13 | De Novo model | MODEL ARCHIVE | ma-9wovj |
| 6 | Mass Spectrometry data | PRIDE | PXD038615 |
| 10 | EM raw micrographs | EMPIAR | EMPIAR-11556 |
| 11 | 3DEM volume | EMDB | 40856 |

Representation ?

This entry has only one representation and includes 15 rigid bodies and 14 flexible units

| Chain ID | Rigid bodies | Non-rigid segments |
|----------|--|--|
| A | 8-237, 250-258, 260-277, 284-310, 313-352, 353-359, 362-370, 375-381, 393-849, 857-862, 864-868, 873-955, 960-1030, 1033-1061, 1068-1275 | 1-7, 238-249, 259-259, 278-283, 311-312, 360-361, 371-374, 382-392, 850-856, 863-863, 869-872, 956-959, 1031-1032, 1062-1067 |

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 | AlphaFold2 | Sampling | Modeling of full-length ORF2p with AlphaFold2 using varying alignment depth. Details of the simulations are available in the ModelArchive entry ma-fejd6 | None | False | False |

| Step number | Protocol ID | Method name | Method type | Method description | Number of computed models | Multi state modeling | Multi scale modeling |
|-------------|-------------|--|-------------|---|---------------------------|----------------------|----------------------|
| 2 | 1 | Molecular Dynamics simulations | Sampling | Details of molecular dynamics simulations are available ModelArchive entries | None | False | False |
| 3 | 1 | Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo | Sampling | 20 replicas; 3 runs; 10000 models per run | 30000 | False | True |
| 4 | 1 | Steepest descent | Refinement | Conversion of a Ca-model to a full backbone model | 159 | False | False |
| 5 | 1 | SCWRL | Refinement | Conversion of a backbone model to a full-atom model | 159 | False | False |
| 6 | 1 | Geometry optimization | Refinement | Conversion of a backbone model to a full-atom model | 159 | False | False |

There are 7 software packages reported in this entry.

| ID | Software name | Software version | Software classification | Software location |
|----|--|------------------|----------------------------|---|
| 7 | Sampcon | 2.18.0 | validation | https://github.com/salilab/imp-sampcon |
| 3 | ColabFold | 1.3.0 | model building | https://github.com/sokrypton/ColabFold |
| 4 | GROMACS | 2022.3 | model building | https://www.gromacs.org/ |
| 1 | IMP PMI module | 2.19.0 | integrative model building | https://integrativemodeling.org |

| ID | Software name | Software version | Software classification | Software location |
|----|-------------------------------------|------------------|----------------------------|---|
| 5 | PULCHRA | 3.04 | model building | https://sites.gatech.edu/cssb/pulchra/ |
| 6 | SCWRL4.0 | 4.0 | model building | http://dunbrack.fccc.edu/lab/scwrl |
| 2 | Integrative Modeling Platform (IMP) | 2.19.0 | integrative model building | https://integrativemodeling.org |

Data quality ?

EM raw micrographs

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

2DEM class average

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality ?

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

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below.

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|--------|----------------------------------|----------------------|
| 1 | 99.6 | 3213.0 |
| 2 | 99.6 | 3209.0 |
| 3 | 99.6 | 3214.0 |
| 4 | 99.6 | 3213.0 |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|---------------|---|-----------------------------|
| 5 | 99.61 | 3208.0 |
| 6 | 99.6 | 3218.0 |
| 7 | 99.6 | 3219.0 |
| 8 | 99.6 | 3225.0 |
| 9 | 99.6 | 3219.0 |
| 10 | 99.61 | 3207.0 |
| 11 | 99.6 | 3218.0 |
| 12 | 99.6 | 3214.0 |
| 13 | 99.61 | 3207.0 |
| 14 | 99.6 | 3215.0 |
| 15 | 99.6 | 3217.0 |
| 16 | 99.6 | 3210.0 |
| 17 | 99.6 | 3215.0 |
| 18 | 99.6 | 3214.0 |
| 19 | 99.61 | 3207.0 |
| 20 | 99.61 | 3208.0 |
| 21 | 99.6 | 3212.0 |
| 22 | 99.6 | 3214.0 |
| 23 | 99.6 | 3215.0 |
| 24 | 99.6 | 3211.0 |
| 25 | 99.61 | 3208.0 |
| 26 | 99.61 | 3201.0 |
| 27 | 99.6 | 3212.0 |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|---------------|---|-----------------------------|
| 28 | 99.61 | 3203.0 |
| 29 | 99.61 | 3207.0 |
| 30 | 99.6 | 3220.0 |
| 31 | 99.6 | 3214.0 |
| 32 | 99.6 | 3216.0 |
| 33 | 99.6 | 3218.0 |
| 34 | 99.6 | 3213.0 |
| 35 | 99.61 | 3207.0 |
| 36 | 99.6 | 3217.0 |
| 37 | 99.6 | 3219.0 |
| 38 | 99.6 | 3215.0 |
| 39 | 99.6 | 3211.0 |
| 40 | 99.6 | 3212.0 |
| 41 | 99.61 | 3206.0 |
| 42 | 99.6 | 3221.0 |
| 43 | 99.6 | 3214.0 |
| 44 | 99.6 | 3211.0 |
| 45 | 99.6 | 3218.0 |
| 46 | 99.6 | 3218.0 |
| 47 | 99.6 | 3218.0 |
| 48 | 99.6 | 3212.0 |
| 49 | 99.6 | 3220.0 |
| 50 | 99.61 | 3202.0 |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|---------------|---|-----------------------------|
| 51 | 99.61 | 3206.0 |
| 52 | 99.6 | 3219.0 |
| 53 | 99.61 | 3205.0 |
| 54 | 99.6 | 3218.0 |
| 55 | 99.61 | 3208.0 |
| 56 | 99.6 | 3211.0 |
| 57 | 99.6 | 3214.0 |
| 58 | 99.61 | 3202.0 |
| 59 | 99.6 | 3210.0 |
| 60 | 99.61 | 3203.0 |
| 61 | 99.6 | 3209.0 |
| 62 | 99.6 | 3221.0 |
| 63 | 99.6 | 3220.0 |
| 64 | 99.6 | 3220.0 |
| 65 | 99.6 | 3209.0 |
| 66 | 99.6 | 3213.0 |
| 67 | 99.6 | 3212.0 |
| 68 | 99.6 | 3212.0 |
| 69 | 99.61 | 3207.0 |
| 70 | 99.61 | 3202.0 |
| 71 | 99.6 | 3214.0 |
| 72 | 99.6 | 3217.0 |
| 73 | 99.6 | 3215.0 |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|---------------|---|-----------------------------|
| 74 | 99.61 | 3207.0 |
| 75 | 99.61 | 3207.0 |
| 76 | 99.6 | 3210.0 |
| 77 | 99.6 | 3219.0 |
| 78 | 99.6 | 3214.0 |
| 79 | 99.6 | 3215.0 |
| 80 | 99.61 | 3204.0 |
| 81 | 99.6 | 3212.0 |
| 82 | 99.6 | 3220.0 |
| 83 | 99.6 | 3215.0 |
| 84 | 99.6 | 3209.0 |
| 85 | 99.6 | 3209.0 |
| 86 | 99.6 | 3214.0 |
| 87 | 99.61 | 3208.0 |
| 88 | 99.6 | 3215.0 |
| 89 | 99.6 | 3215.0 |
| 90 | 99.6 | 3218.0 |
| 91 | 99.61 | 3207.0 |
| 92 | 99.61 | 3202.0 |
| 93 | 99.6 | 3213.0 |
| 94 | 99.6 | 3214.0 |
| 95 | 99.6 | 3216.0 |
| 96 | 99.61 | 3206.0 |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|---------------|---|-----------------------------|
| 97 | 99.6 | 3218.0 |
| 98 | 99.61 | 3207.0 |
| 99 | 99.61 | 3208.0 |
| 100 | 99.6 | 3211.0 |
| 101 | 99.6 | 3210.0 |
| 102 | 99.6 | 3217.0 |
| 103 | 99.6 | 3211.0 |
| 104 | 99.6 | 3220.0 |
| 105 | 99.61 | 3205.0 |
| 106 | 99.6 | 3215.0 |
| 107 | 99.6 | 3216.0 |
| 108 | 99.6 | 3219.0 |
| 109 | 99.6 | 3210.0 |
| 110 | 99.6 | 3213.0 |
| 111 | 99.6 | 3212.0 |
| 112 | 99.61 | 3197.0 |
| 113 | 99.6 | 3212.0 |
| 114 | 99.6 | 3214.0 |
| 115 | 99.6 | 3224.0 |
| 116 | 99.6 | 3214.0 |
| 117 | 99.61 | 3207.0 |
| 118 | 99.6 | 3211.0 |
| 119 | 99.6 | 3209.0 |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|---------------|---|-----------------------------|
| 120 | 99.6 | 3211.0 |
| 121 | 99.6 | 3210.0 |
| 122 | 99.61 | 3206.0 |
| 123 | 99.6 | 3216.0 |
| 124 | 99.6 | 3216.0 |
| 125 | 99.6 | 3213.0 |
| 126 | 99.6 | 3221.0 |
| 127 | 99.6 | 3211.0 |
| 128 | 99.6 | 3212.0 |
| 129 | 99.6 | 3218.0 |
| 130 | 99.61 | 3207.0 |
| 131 | 99.6 | 3217.0 |
| 132 | 99.6 | 3213.0 |
| 133 | 99.61 | 3207.0 |
| 134 | 99.6 | 3217.0 |
| 135 | 99.6 | 3214.0 |
| 136 | 99.6 | 3217.0 |
| 137 | 99.6 | 3219.0 |
| 138 | 99.61 | 3206.0 |
| 139 | 99.61 | 3205.0 |
| 140 | 99.6 | 3214.0 |
| 141 | 99.6 | 3214.0 |
| 142 | 99.6 | 3209.0 |

| Models | Excluded Volume Satisfaction (%) | Number of violations |
|--------|----------------------------------|----------------------|
| 143 | 99.6 | 3211.0 |
| 144 | 99.61 | 3205.0 |
| 145 | 99.6 | 3219.0 |
| 146 | 99.6 | 3228.0 |
| 147 | 99.6 | 3218.0 |
| 148 | 99.6 | 3214.0 |
| 149 | 99.6 | 3213.0 |
| 150 | 99.61 | 3203.0 |
| 151 | 99.6 | 3216.0 |
| 152 | 99.6 | 3216.0 |
| 153 | 99.6 | 3214.0 |
| 154 | 99.61 | 3207.0 |
| 155 | 99.6 | 3216.0 |
| 156 | 99.61 | 3206.0 |
| 157 | 99.6 | 3217.0 |
| 158 | 99.6 | 3217.0 |
| 159 | 99.6 | 3217.0 |

Fit of model to data used for modeling ?

EM raw micrographs

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

3DEM volume

Validation for this section is under development.

2DEM class average

Validation for this section is under development.

Crosslinking-MS

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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