

Integrative Structure Validation Report ?

February 18, 2025 - 08:38 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

ATSAS Version 3.2.1 (r14885)

PyMOL Version 2.5.0

PDB ID	9A44
PDB-Dev ID	PDBDEV_00000225
Structure Title	Man5 fully-glycosylated model of mouse N-cadherin EC1-EC5
Structure Authors	Tsai, Y.-X.; Chang, H.-T.; Wang, Y.-S.; Hsu, M.-F.; Hanus, C.; Sikora, M.; Hsu, S.-T.D.
Deposited on	2023-12-03

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

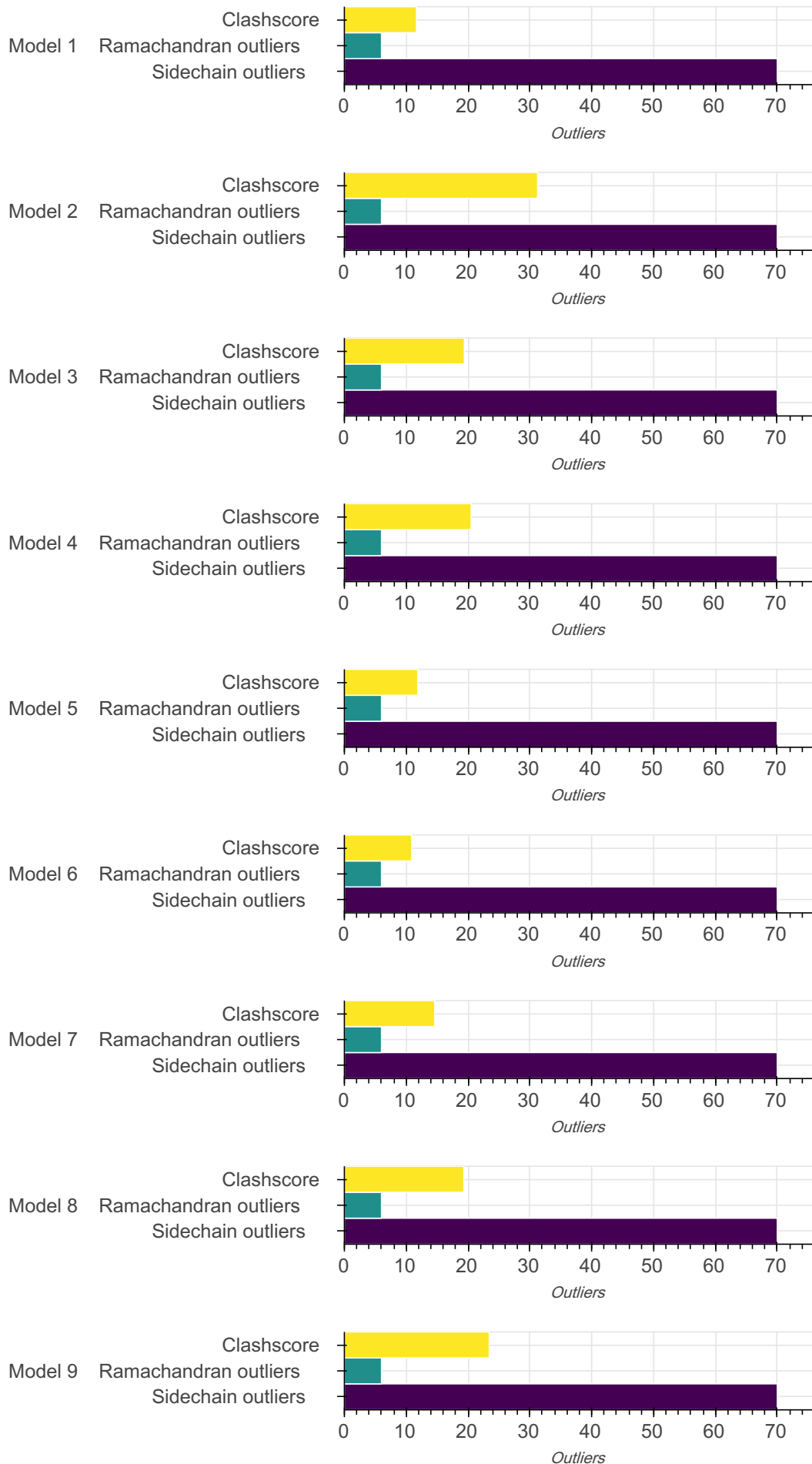
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

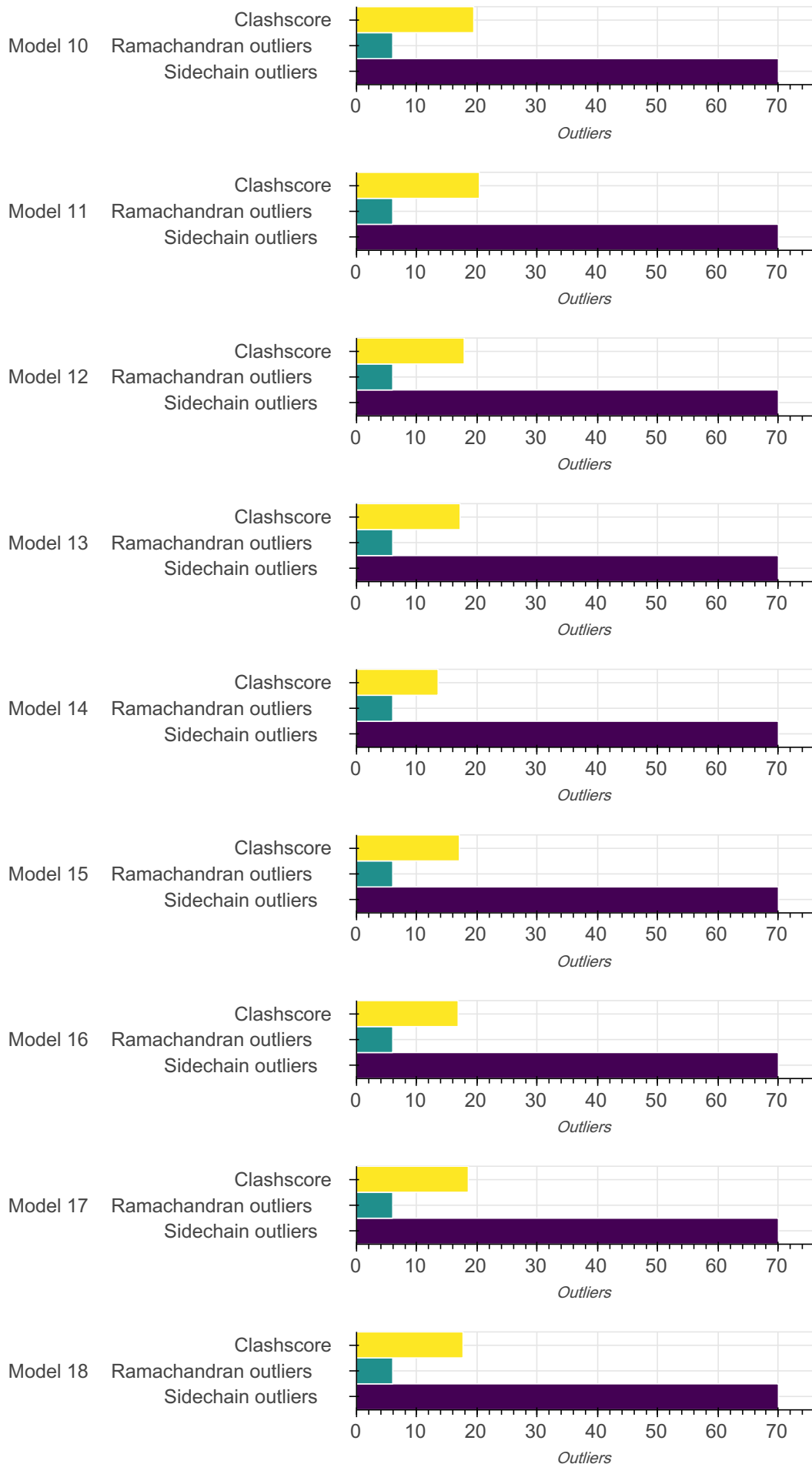
List of references used to build this report is available [here](#).

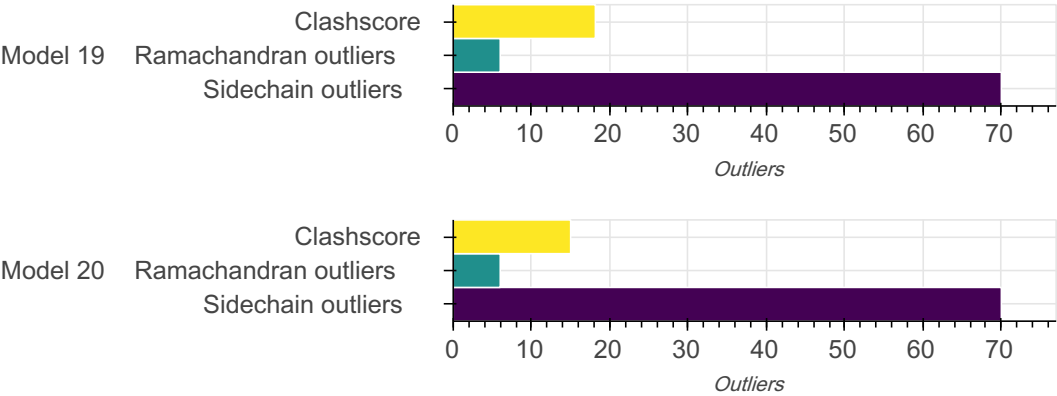
Overall quality ?

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 1 distinct ensemble(s).

Summary ?

This entry consists of 20 model(s). A total of 2 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	1-20	1	Cadherin-2	A	541	-	1-541	100.00 / 100.00	Atomic
				B					
		2	alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	C	Non-polymeric	-	-	Not available / Not available	Atomic
				D					
				E					
				F					
				G					
				H					
				I					
				J					
				K					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				L					
				M					
				N					
				O					
				P					
				Q					
				R					

Datasets used for modeling ?

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	SAS data	SASBDB	SASDT35
2	Experimental model	PDB	3Q2W

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	None	Use GlycoSHIELD, the tool we have developed, to graft MD-simulated glycan ensemble onto the x-ray protein structure (PDB ID: 3Q2W).	None	20	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	GlycoSHIELD	Not available	model building	https://github.com/GlycoSHIELD-MD/GlycoSHIELD-MD
2	GASBOR	Not available	model building	https://www.embl-hamburg.de/biosaxs/gasbor.html

ID	Software name	Software version	Software classification	Software location
3	FoXSDock	Not available	data analysis	https://modbase.compbio.ucsf.edu/foxsdock/

Data quality ?

SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

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 570 bond length outliers in this entry (0.29% of 196822 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)
J	4	MAN	C1-C2	6.65	1.39	1.53	14	1
R	4	MAN	C1-C2	6.65	1.39	1.53	14	1
A	23	ARG	NE-CZ	6.46	1.25	1.33	1	1
G	4	MAN	C3-C4	6.22	1.65	1.52	16	2
O	4	MAN	C3-C4	6.22	1.65	1.52	16	2
H	4	MAN	C3-C4	6.20	1.65	1.52	15	2
P	4	MAN	C3-C4	6.20	1.65	1.52	15	2
C	5	MAN	C5-O5	6.11	1.54	1.42	19	1
K	5	MAN	C5-O5	6.11	1.54	1.42	19	1
L	5	MAN	C5-O5	6.02	1.54	1.42	17	1
D	5	MAN	C5-O5	6.02	1.54	1.42	17	1
E	3	BMA	C4-C5	5.97	1.41	1.53	5	1
M	3	BMA	C4-C5	5.97	1.41	1.53	5	1
A	66	LEU	C-N	5.96	1.41	1.33	1	1
G	7	MAN	C1-C2	5.95	1.41	1.53	13	1
O	7	MAN	C1-C2	5.95	1.41	1.53	13	1
J	1	NAG	C4-C5	5.88	1.41	1.53	9	2
R	1	NAG	C4-C5	5.88	1.41	1.53	9	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
G	5	MAN	C1-O5	5.88	1.52	1.40	12	2
O	5	MAN	C1-O5	5.88	1.52	1.40	12	2
J	7	MAN	C5-O5	5.85	1.53	1.42	18	1
R	7	MAN	C5-O5	5.85	1.53	1.42	18	1
J	4	MAN	C3-C4	5.78	1.41	1.52	4	2
R	4	MAN	C3-C4	5.78	1.41	1.52	4	2
F	3	BMA	C5-C6	5.75	1.41	1.53	10	1
N	3	BMA	C5-C6	5.75	1.41	1.53	10	1
J	1	NAG	C5-C6	5.65	1.63	1.51	2	1
R	1	NAG	C5-C6	5.65	1.63	1.51	2	1
H	7	MAN	C1-C2	5.64	1.41	1.53	12	1
P	7	MAN	C1-C2	5.64	1.41	1.53	12	1
R	3	BMA	C2-C3	5.53	1.43	1.54	7	3
J	3	BMA	C2-C3	5.53	1.43	1.54	7	3
L	6	MAN	C6-O6	5.53	1.52	1.41	18	1
D	6	MAN	C6-O6	5.53	1.52	1.41	18	1
I	7	MAN	C1-C2	5.49	1.42	1.53	10	2
Q	7	MAN	C1-C2	5.49	1.42	1.53	10	2
D	1	NAG	C5-O5	5.49	1.52	1.41	17	1
L	1	NAG	C5-O5	5.49	1.52	1.41	17	1
C	6	MAN	C6-O6	5.41	1.52	1.41	20	1
K	6	MAN	C6-O6	5.41	1.52	1.41	20	1
I	6	MAN	C6-O6	5.39	1.51	1.41	13	1
Q	6	MAN	C6-O6	5.39	1.51	1.41	13	1
J	3	BMA	C3-O3	5.35	1.51	1.41	2	2
R	3	BMA	C3-O3	5.35	1.51	1.41	2	2
L	1	NAG	C4-O4	5.33	1.52	1.41	15	1
D	1	NAG	C4-O4	5.33	1.52	1.41	15	1
F	2	NAG	C3-O3	5.32	1.51	1.40	13	1
N	2	NAG	C3-O3	5.32	1.51	1.40	13	1
O	6	MAN	C5-O5	5.26	1.52	1.42	7	2
G	6	MAN	C5-O5	5.26	1.52	1.42	7	2
C	2	NAG	C3-C4	5.25	1.63	1.52	11	1
K	2	NAG	C3-C4	5.25	1.63	1.52	11	1
G	6	MAN	C1-O5	5.25	1.50	1.40	9	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
O	6	MAN	C1-O5	5.25	1.50	1.40	9	1
C	3	BMA	C3-C4	5.25	1.44	1.54	12	2
K	3	BMA	C3-C4	5.25	1.44	1.54	12	2
D	2	NAG	C4-O4	5.24	1.51	1.41	16	1
L	2	NAG	C4-O4	5.24	1.51	1.41	16	1
N	4	MAN	C1-C2	5.23	1.42	1.53	14	1
F	4	MAN	C1-C2	5.23	1.42	1.53	14	1
C	1	NAG	C4-O4	5.23	1.51	1.41	17	1
K	1	NAG	C4-O4	5.23	1.51	1.41	17	1
G	1	NAG	C5-O5	5.22	1.52	1.41	19	1
O	1	NAG	C5-O5	5.22	1.52	1.41	19	1
G	3	BMA	C3-C4	5.21	1.44	1.54	10	1
O	3	BMA	C3-C4	5.21	1.44	1.54	10	1
F	2	NAG	C4-C5	5.20	1.43	1.53	19	1
N	2	NAG	C4-C5	5.20	1.43	1.53	19	1
P	3	BMA	C3-C4	5.19	1.44	1.54	9	3
H	3	BMA	C3-C4	5.19	1.44	1.54	9	3
C	2	NAG	C4-O4	5.15	1.51	1.41	18	1
K	2	NAG	C4-O4	5.15	1.51	1.41	18	1
E	7	MAN	C5-C6	5.11	1.62	1.51	14	2
M	7	MAN	C5-C6	5.11	1.62	1.51	14	2
G	3	BMA	C3-O3	5.10	1.51	1.41	8	2
O	3	BMA	C3-O3	5.10	1.51	1.41	8	2
M	1	NAG	C2-C3	5.09	1.42	1.53	4	1
E	1	NAG	C2-C3	5.09	1.42	1.53	4	1
G	3	BMA	C2-O2	5.07	1.50	1.40	14	1
O	3	BMA	C2-O2	5.07	1.50	1.40	14	1
E	3	BMA	C2-C3	5.06	1.44	1.54	15	1
M	3	BMA	C2-C3	5.06	1.44	1.54	15	1
I	6	MAN	C5-O5	5.06	1.52	1.42	6	1
Q	6	MAN	C5-O5	5.06	1.52	1.42	6	1
F	4	MAN	C6-O6	5.06	1.51	1.41	12	1
N	4	MAN	C6-O6	5.06	1.51	1.41	12	1
R	1	NAG	C5-O5	5.06	1.51	1.41	20	3
J	1	NAG	C5-O5	5.06	1.51	1.41	20	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H	3	BMA	C2-O2	5.04	1.50	1.40	13	1
P	3	BMA	C2-O2	5.04	1.50	1.40	13	1
H	3	BMA	C1-C2	5.04	1.42	1.52	9	1
P	3	BMA	C1-C2	5.04	1.42	1.52	9	1
G	3	BMA	C1-C2	5.03	1.42	1.52	10	1
O	3	BMA	C1-C2	5.03	1.42	1.52	10	1
E	6	MAN	C2-C3	5.00	1.42	1.52	11	1
M	6	MAN	C2-C3	5.00	1.42	1.52	11	1
N	4	MAN	C1-O5	4.99	1.50	1.40	20	2
F	4	MAN	C1-O5	4.99	1.50	1.40	20	2
E	3	BMA	C3-C4	4.98	1.44	1.54	11	1
M	3	BMA	C3-C4	4.98	1.44	1.54	11	1

Standard geometry: angle outliers ?

There are 268 bond angle outliers in this entry (0.10% of 266666 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)
B	501	ASP	N-CA-CB	11.69	90.63	110.50	8	20
A	501	ASP	N-CA-CB	11.69	90.63	110.50	8	20
A	501	ASP	N-CA-C	8.19	133.93	111.00	10	20
B	501	ASP	N-CA-C	8.19	133.93	111.00	10	20
G	1	NAG	C3-C4-O4	5.53	123.88	107.29	10	1
O	1	NAG	C3-C4-O4	5.53	123.88	107.29	10	1
G	1	NAG	C5-C4-O4	5.50	95.21	111.70	4	1
O	1	NAG	C5-C4-O4	5.50	95.21	111.70	4	1
D	1	NAG	C5-C4-O4	5.38	95.55	111.70	4	1
L	1	NAG	C5-C4-O4	5.38	95.55	111.70	4	1
H	1	NAG	C3-C4-O4	5.36	123.38	107.29	9	4
P	1	NAG	C3-C4-O4	5.36	123.38	107.29	9	4
C	1	NAG	C3-C4-O4	5.33	123.28	107.29	12	3
K	1	NAG	C3-C4-O4	5.33	123.28	107.29	12	3
J	2	NAG	C3-C4-O4	5.31	123.22	107.29	20	3
R	2	NAG	C3-C4-O4	5.31	123.22	107.29	20	3
C	3	BMA	C2-C3-O3	5.28	122.51	106.67	19	1
K	3	BMA	C2-C3-O3	5.28	122.51	106.67	19	1
F	4	MAN	C1-C2-O2	5.18	122.34	106.80	12	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
N	4	MAN	C1-C2-O2	5.18	122.34	106.80	12	2
L	3	BMA	C2-C3-O3	5.11	122.01	106.67	17	2
D	3	BMA	C2-C3-O3	5.11	122.01	106.67	17	2
H	7	MAN	C1-C2-O2	5.01	121.82	106.80	7	1
P	7	MAN	C1-C2-O2	5.01	121.82	106.80	7	1
F	2	NAG	C5-C4-O4	5.00	96.70	111.70	9	1
N	2	NAG	C5-C4-O4	5.00	96.70	111.70	9	1
A	23	ARG	CD-NE-CZ	4.99	131.38	124.40	1	1
J	3	BMA	C1-O5-C5	4.94	104.00	118.82	7	1
R	3	BMA	C1-O5-C5	4.94	104.00	118.82	7	1
J	4	MAN	C2-C3-O3	4.84	122.09	107.58	14	1
R	4	MAN	C2-C3-O3	4.84	122.09	107.58	14	1
L	2	NAG	C3-C4-O4	4.71	121.41	107.29	3	2
D	2	NAG	C3-C4-O4	4.71	121.41	107.29	3	2
J	5	MAN	C1-C2-O2	4.69	120.86	106.80	3	1
R	5	MAN	C1-C2-O2	4.69	120.86	106.80	3	1
G	2	NAG	C3-C4-O4	4.67	121.30	107.29	3	1
O	2	NAG	C3-C4-O4	4.67	121.30	107.29	3	1
N	1	NAG	C5-C4-O4	4.62	97.83	111.70	12	1
F	1	NAG	C5-C4-O4	4.62	97.83	111.70	12	1
C	5	MAN	C1-C2-O2	4.52	120.36	106.80	11	2
K	5	MAN	C1-C2-O2	4.52	120.36	106.80	11	2
P	2	NAG	C5-C4-O4	4.44	98.37	111.70	12	1
H	2	NAG	C5-C4-O4	4.44	98.37	111.70	12	1
P	1	NAG	C5-C4-O4	4.42	98.43	111.70	4	1
H	1	NAG	C5-C4-O4	4.42	98.43	111.70	4	1
I	2	NAG	C5-C4-O4	4.40	98.50	111.70	10	1
Q	2	NAG	C5-C4-O4	4.40	98.50	111.70	10	1
O	1	NAG	C3-C4-C5	4.40	122.57	109.38	19	1
G	1	NAG	C3-C4-C5	4.40	122.57	109.38	19	1
E	3	BMA	C1-O5-C5	4.39	105.66	118.82	14	1
M	3	BMA	C1-O5-C5	4.39	105.66	118.82	14	1
N	1	NAG	C3-C4-O4	4.39	120.45	107.29	12	1
F	1	NAG	C3-C4-O4	4.39	120.45	107.29	12	1
D	5	MAN	C1-C2-O2	4.38	119.94	106.80	15	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	5	MAN	C1-C2-O2	4.38	119.94	106.80	15	1
O	2	NAG	C5-C4-O4	4.38	98.56	111.70	13	1
G	2	NAG	C5-C4-O4	4.38	98.56	111.70	13	1
A	44	ASP	N-CA-CB	4.37	117.92	110.50	10	20
B	44	ASP	N-CA-CB	4.37	117.92	110.50	10	20
C	1	NAG	C5-C4-O4	4.37	98.60	111.70	5	1
K	1	NAG	C5-C4-O4	4.37	98.60	111.70	5	1
R	3	BMA	C6-C5-O5	4.34	96.43	109.44	2	1
J	3	BMA	C6-C5-O5	4.34	96.43	109.44	2	1
G	3	BMA	C2-C3-O3	4.31	119.59	106.67	12	1
O	3	BMA	C2-C3-O3	4.31	119.59	106.67	12	1
D	4	MAN	C2-C3-O3	4.30	120.47	107.58	20	1
L	4	MAN	C2-C3-O3	4.30	120.47	107.58	20	1
E	1	NAG	C5-C4-O4	4.30	98.81	111.70	3	1
M	1	NAG	C5-C4-O4	4.30	98.81	111.70	3	1
N	4	MAN	C2-C3-O3	4.29	120.45	107.58	3	1
F	4	MAN	C2-C3-O3	4.29	120.45	107.58	3	1
O	5	MAN	C3-C4-O4	4.29	119.92	107.06	15	1
G	5	MAN	C3-C4-O4	4.29	119.92	107.06	15	1
P	4	MAN	C2-C3-O3	4.27	120.40	107.58	3	1
H	4	MAN	C2-C3-O3	4.27	120.40	107.58	3	1
D	1	NAG	C3-C4-O4	4.27	120.09	107.29	9	1
L	1	NAG	C3-C4-O4	4.27	120.09	107.29	9	1
L	3	BMA	C1-O5-C5	4.26	106.04	118.82	12	1
D	3	BMA	C1-O5-C5	4.26	106.04	118.82	12	1
Q	3	BMA	C1-O5-C5	4.23	106.12	118.82	9	1
I	3	BMA	C1-O5-C5	4.23	106.12	118.82	9	1
E	2	NAG	C5-C4-O4	4.21	99.08	111.70	19	1
M	2	NAG	C5-C4-O4	4.21	99.08	111.70	19	1
C	3	BMA	C1-O5-C5	4.20	106.21	118.82	14	1
K	3	BMA	C1-O5-C5	4.20	106.21	118.82	14	1
G	4	MAN	C1-C2-O2	4.20	119.40	106.80	20	1
O	4	MAN	C1-C2-O2	4.20	119.40	106.80	20	1
D	1	NAG	C6-C5-O5	4.19	96.16	108.73	10	1
L	1	NAG	C6-C5-O5	4.19	96.16	108.73	10	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	3	BMA	C1-C2-O2	4.19	120.97	108.40	8	1
K	3	BMA	C1-C2-O2	4.19	120.97	108.40	8	1
J	6	MAN	C6-C5-O5	4.17	119.80	107.28	16	1
R	6	MAN	C6-C5-O5	4.17	119.80	107.28	16	1
E	1	NAG	C3-C4-O4	4.17	119.79	107.29	3	2
M	1	NAG	C3-C4-O4	4.17	119.79	107.29	3	2
J	2	NAG	C2-C1-O5	4.15	97.60	110.06	7	1
R	2	NAG	C2-C1-O5	4.15	97.60	110.06	7	1
P	1	NAG	C3-C4-C5	4.15	121.83	109.38	18	1
H	1	NAG	C3-C4-C5	4.15	121.83	109.38	18	1
H	5	MAN	C1-C2-O2	4.14	119.23	106.80	6	1

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	11.66	119
2	31.23	318
3	19.40	198
4	20.50	209
5	11.86	121
6	10.87	111
7	14.61	149
8	19.31	197
9	23.42	239
10	19.45	198
11	20.38	208
12	17.86	182
13	17.19	175
14	13.54	138
15	17.06	174
16	16.86	172
17	18.54	189
18	17.67	180
19	18.15	185

Model ID	Clash score	Number of clashes
20	14.99	153

There are 3615 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:504:GLN:CB	H:1:NAG:CT	1.62	12	2
A:488:THR:HB	I:1:NAG:CT	1.60	3	2
B:342:PRO:HG2	O:2:NAG:C6	1.60	17	1
B:488:THR:HB	Q:1:NAG:CT	1.60	3	2
A:458:GLU:HG2	H:2:NAG:CT	1.59	9	1
A:342:PRO:HG2	G:2:NAG:C6	1.59	17	1
B:458:GLU:HG2	P:2:NAG:CT	1.59	9	1
B:532:ASN:HD21	R:1:NAG:C1	1.57	7	5
A:342:PRO:CG	G:2:NAG:H62	1.57	17	1
B:458:GLU:CG	P:2:NAG:CT	1.56	9	1
A:532:ASN:HD21	J:1:NAG:C1	1.56	7	5
B:342:PRO:CG	O:2:NAG:H62	1.56	17	1
A:458:GLU:CG	H:2:NAG:CT	1.56	9	1
A:243:ASN:HD21	F:1:NAG:C1	1.55	20	3
A:460:ASN:CB	H:1:NAG:H61	1.55	4	1
B:243:ASN:HD21	N:1:NAG:C1	1.54	20	3
B:460:ASN:CB	P:1:NAG:H61	1.54	4	1
A:502:PHE:CG	H:1:NAG:CT	1.53	19	2
B:502:PHE:CG	P:1:NAG:CT	1.53	19	2
B:240:ILE:CD1	N:1:NAG:H61	1.52	9	1
A:240:ILE:CD1	F:1:NAG:H61	1.52	9	1
B:502:PHE:CD1	P:1:NAG:CT	1.52	19	2
A:502:PHE:CD1	H:1:NAG:CT	1.52	19	2
A:112:VAL:CG1	D:1:NAG:C	1.51	13	1
B:112:VAL:CG1	L:1:NAG:C	1.51	13	1
A:445:GLN:NE2	J:1:NAG:C	1.51	17	2
B:445:GLN:NE2	R:1:NAG:C	1.51	17	2
A:148:ARG:CB	E:1:NAG:C3	1.50	20	2
B:148:ARG:CB	M:1:NAG:C3	1.50	20	2
A:240:ILE:CD1	F:1:NAG:C4	1.47	17	2
B:460:ASN:CG	P:1:NAG:H61	1.47	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:240:ILE:CD1	N:1:NAG:C4	1.47	17	2
A:460:ASN:CG	H:1:NAG:H61	1.47	4	1
A:445:GLN:HE22	J:1:NAG:C1	1.47	19	5
B:445:GLN:HE22	R:1:NAG:C1	1.47	19	5
B:463:ASN:HD21	P:1:NAG:C1	1.46	3	2
A:413:ASN:ND2	G:1:NAG:C1	1.46	10	5
A:463:ASN:HD21	H:1:NAG:C1	1.46	3	2
B:240:ILE:HD13	N:1:NAG:C4	1.46	17	2
A:112:VAL:HG12	D:1:NAG:C	1.46	13	1
A:433:GLN:CB	G:1:NAG:H61	1.46	17	1
A:240:ILE:HD13	F:1:NAG:C4	1.45	17	2
B:112:VAL:HG12	L:1:NAG:C	1.45	13	1
A:504:GLN:HB3	H:1:NAG:CT	1.45	12	1
B:433:GLN:HB3	O:1:NAG:C6	1.45	17	1
A:166:ASN:HD21	E:1:NAG:C1	1.45	16	6
B:166:ASN:HD21	M:1:NAG:C1	1.45	16	6
B:433:GLN:CB	O:1:NAG:H61	1.45	17	1
B:460:ASN:HB3	P:1:NAG:C6	1.45	4	1
A:433:GLN:HB3	G:1:NAG:C6	1.45	17	1
A:469:TYR:HE2	J:2:NAG:C2	1.44	1	1
A:460:ASN:HB3	H:1:NAG:C6	1.44	4	1
A:435:TYR:OH	G:2:NAG:CT	1.44	17	1
A:433:GLN:CD	G:1:NAG:CT	1.44	13	1
B:530:LYS:CE	R:2:NAG:CT	1.44	16	1
B:433:GLN:CD	O:1:NAG:CT	1.44	13	1
A:530:LYS:CE	J:2:NAG:CT	1.44	16	1
B:435:TYR:OH	O:2:NAG:CT	1.44	17	1
B:469:TYR:HE2	R:2:NAG:C2	1.44	1	1
B:243:ASN:ND2	N:1:NAG:C1	1.42	20	5
B:512:GLU:N	Q:2:NAG:H4	1.42	16	1
A:512:GLU:N	I:2:NAG:H4	1.42	16	1
A:243:ASN:ND2	F:1:NAG:C1	1.42	20	5
A:532:ASN:ND2	J:1:NAG:C1	1.42	7	6
B:532:ASN:ND2	R:1:NAG:C1	1.42	7	6
A:413:ASN:OD1	G:1:NAG:C1	1.41	16	6

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:240:ILE:CG2	F:1:NAG:O	1.41	4	2
B:240:ILE:CG2	N:1:NAG:O	1.41	4	2
A:530:LYS:NZ	J:2:NAG:C	1.41	16	2
B:530:LYS:NZ	R:2:NAG:C	1.41	16	2
A:342:PRO:CG	G:2:NAG:C6	1.41	17	1
A:463:ASN:HD21	H:1:NAG:C2	1.40	10	4
B:342:PRO:CG	O:2:NAG:C6	1.40	17	1
A:510:LYS:H	I:1:NAG:CT	1.40	13	1
B:463:ASN:ND2	P:1:NAG:C1	1.40	3	11
B:463:ASN:HD21	P:1:NAG:C2	1.40	10	4
B:510:LYS:H	Q:1:NAG:CT	1.40	13	1
A:512:GLU:N	I:2:NAG:C4	1.40	16	1
A:463:ASN:ND2	H:1:NAG:C1	1.40	3	11
B:512:GLU:N	Q:2:NAG:C4	1.40	16	1
B:148:ARG:CB	M:1:NAG:H3	1.39	20	2
A:163:THR:CG2	E:1:NAG:CT	1.39	7	1
A:148:ARG:CB	E:1:NAG:H3	1.39	20	2
A:150:LEU:CD2	E:7:MAN:H61	1.39	7	1
A:148:ARG:HA	E:1:NAG:N	1.39	20	2
B:150:LEU:CD2	M:7:MAN:H61	1.39	7	1
A:240:ILE:CD1	F:1:NAG:C6	1.39	9	1
B:148:ARG:HA	M:1:NAG:N	1.38	20	2
B:240:ILE:CD1	N:1:NAG:C6	1.38	9	1
A:112:VAL:CG1	D:1:NAG:O	1.38	13	2
B:112:VAL:CG1	L:1:NAG:O	1.38	13	2
A:504:GLN:HB2	H:1:NAG:CT	1.37	10	2
A:488:THR:CB	I:1:NAG:CT	1.37	3	1
A:413:ASN:HD21	G:1:NAG:C1	1.37	10	3
B:488:THR:CB	Q:1:NAG:CT	1.37	3	1
A:460:ASN:OD1	H:1:NAG:C4	1.37	4	2
B:460:ASN:OD1	P:1:NAG:C4	1.36	4	2
A:278:PRO:HD2	F:7:MAN:O6	1.35	9	1
B:278:PRO:HD2	N:7:MAN:O6	1.34	9	1
B:498:LEU:HD11	P:1:NAG:O	1.34	9	1

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	1074	982	86	6
2	1074	982	86	6
3	1074	982	86	6
4	1074	982	86	6
5	1074	982	86	6
6	1074	982	86	6
7	1074	982	86	6
8	1074	982	86	6
9	1074	982	86	6
10	1074	982	86	6
11	1074	982	86	6
12	1074	982	86	6
13	1074	982	86	6
14	1074	982	86	6
15	1074	982	86	6
16	1074	982	86	6
17	1074	982	86	6
18	1074	982	86	6
19	1074	982	86	6
20	1074	982	86	6

There are 6 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	342	PRO	20
A	500	GLY	20
A	501	ASP	20
B	342	PRO	20
B	500	GLY	20
B	501	ASP	20

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	942	750	122	70
2	942	750	122	70
3	942	750	122	70
4	942	750	122	70
5	942	750	122	70
6	942	750	122	70
7	942	750	122	70
8	942	750	122	70
9	942	750	122	70
10	942	750	122	70
11	942	750	122	70
12	942	750	122	70
13	942	750	122	70
14	942	750	122	70
15	942	750	122	70
16	942	750	122	70
17	942	750	122	70
18	942	750	122	70
19	942	750	122	70
20	942	750	122	70


There are 70 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	4	ILE	20
A	22	VAL	20
A	24	ILE	20
A	28	ARG	20
A	31	ASN	20
A	38	VAL	20
A	60	LEU	20
A	62	VAL	20
A	81	VAL	20
A	83	ILE	20
A	94	ILE	20
A	98	VAL	20

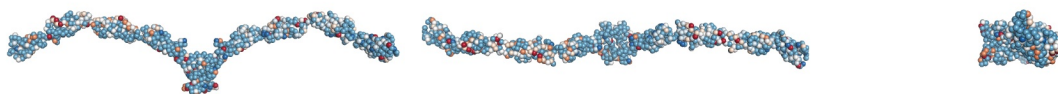
Chain	Res	Type	Models (Total)
A	131	THR	20
A	145	LEU	20
A	180	ARG	20
A	208	THR	20
A	227	THR	20
A	234	GLU	20
A	237	VAL	20
A	269	THR	20
A	271	ARG	20
A	286	THR	20
A	291	ILE	20
A	301	LEU	20
A	325	VAL	20
A	338	PHE	20
A	348	GLU	20
A	373	ILE	20
A	403	GLU	20
A	409	ASN	20
A	465	THR	20
A	482	LEU	20
A	499	ASN	20
A	507	LEU	20
A	515	ILE	20
B	4	ILE	20
B	22	VAL	20
B	24	ILE	20
B	28	ARG	20
B	31	ASN	20
B	38	VAL	20
B	60	LEU	20
B	62	VAL	20
B	81	VAL	20
B	83	ILE	20
B	94	ILE	20
B	98	VAL	20

Chain	Res	Type	Models (Total)
B	131	THR	20
B	145	LEU	20
B	180	ARG	20
B	208	THR	20
B	227	THR	20
B	234	GLU	20
B	237	VAL	20
B	269	THR	20
B	271	ARG	20
B	286	THR	20
B	291	ILE	20
B	301	LEU	20
B	325	VAL	20
B	338	PHE	20
B	348	GLU	20
B	373	ILE	20
B	403	GLU	20
B	409	ASN	20
B	465	THR	20
B	482	LEU	20
B	499	ASN	20
B	507	LEU	20
B	515	ILE	20

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: 20/20).



Fit of model to data used for modeling ?

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

Fit of model to data used for validation ?

Validation for this section is under development.

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