

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	9A46
PDB-Dev ID	PDBDEV_00000227
Structure Title	F1N6 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	2023-12-05

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

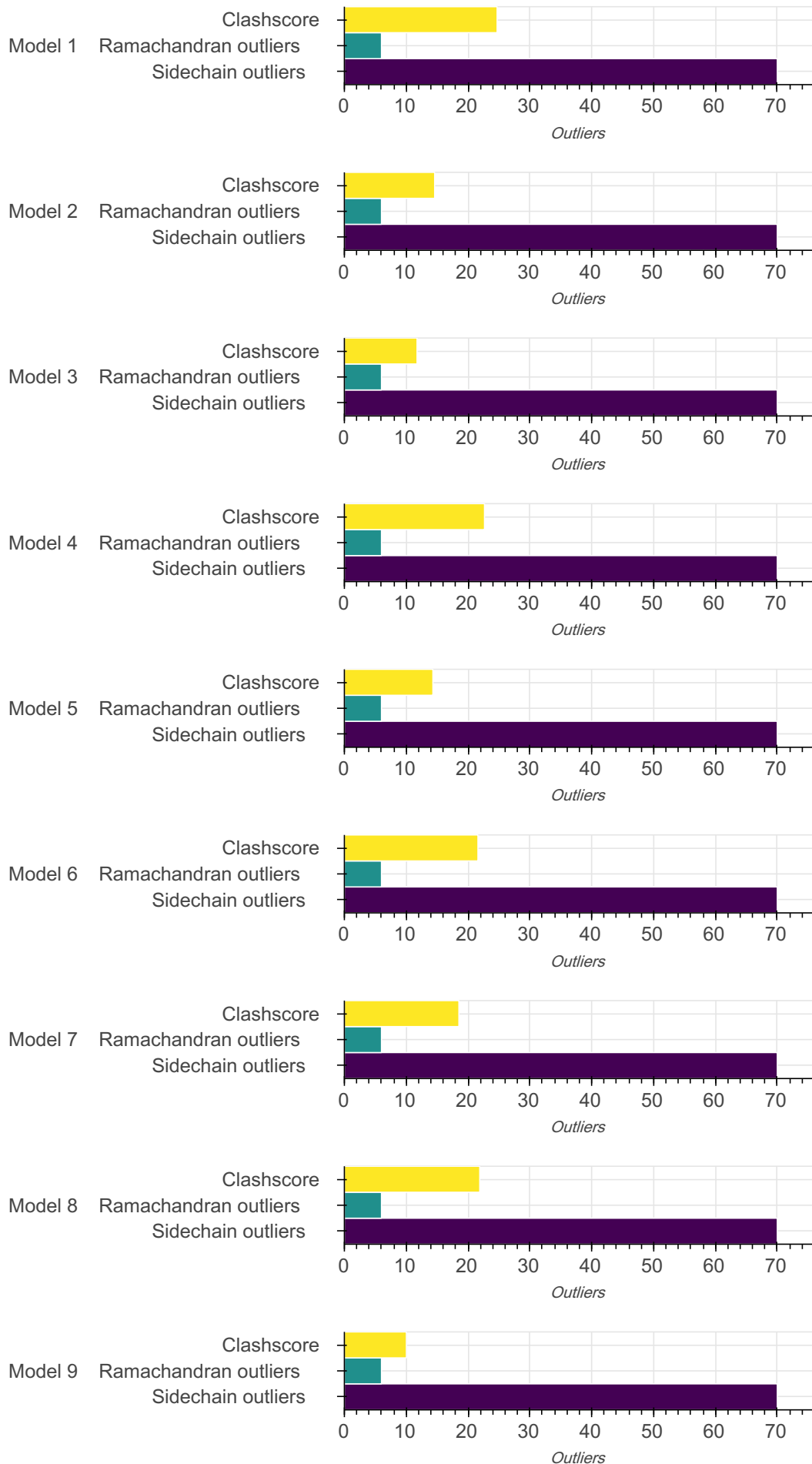
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

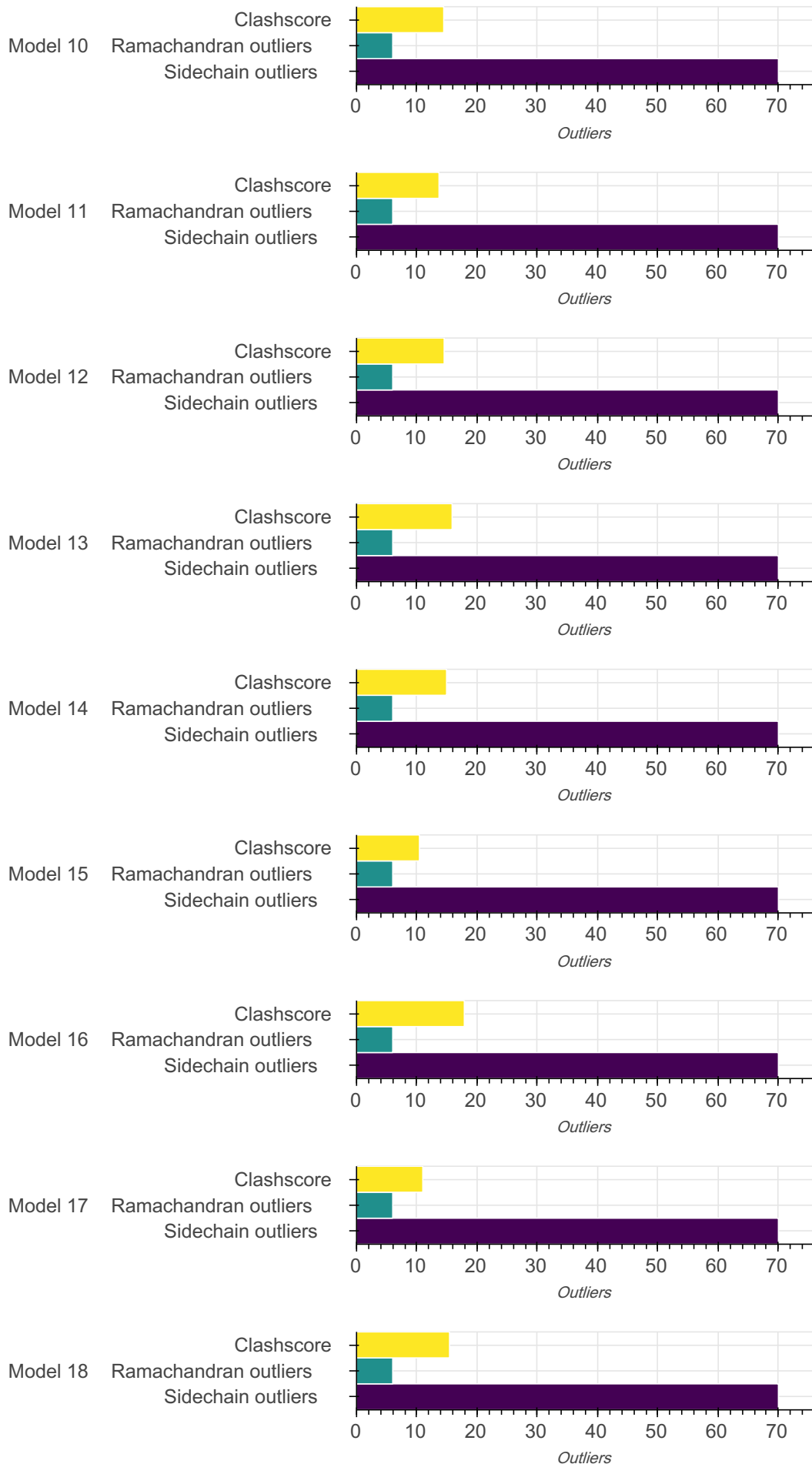
List of references used to build this report is available [here](#).

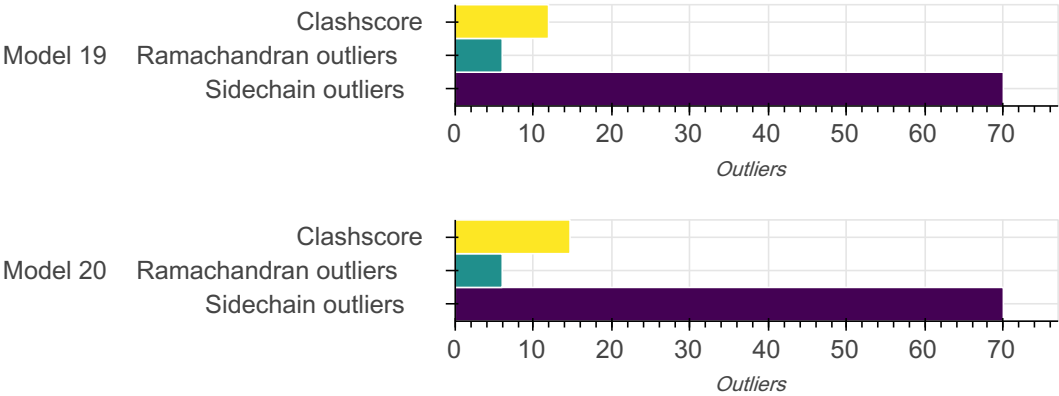
Overall quality ?

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					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		2	N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose	C D E F G H I J K L M N O P Q R	Non-polymeric	-	-	Not available / Not available	Atomic

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
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 1696 bond length outliers in this entry (0.70% of 241420 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)
C	3	BMA	C2-C3	6.90	1.41	1.54	1	3
K	3	BMA	C2-C3	6.90	1.41	1.54	1	3
D	3	BMA	C2-C3	6.88	1.41	1.54	1	3
L	3	BMA	C2-C3	6.88	1.41	1.54	1	3
E	3	BMA	C2-C3	6.75	1.41	1.54	1	3
M	3	BMA	C2-C3	6.75	1.41	1.54	1	3
H	3	BMA	C2-C3	6.70	1.41	1.54	1	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	3	BMA	C2-C3	6.70	1.41	1.54	1	3
Q	3	BMA	C2-C3	6.69	1.41	1.54	1	3
I	3	BMA	C2-C3	6.69	1.41	1.54	1	3
D	15	NAG	C6-O6	6.63	1.54	1.41	18	2
L	15	NAG	C6-O6	6.63	1.54	1.41	18	2
E	8	NAG	C1-C2	6.63	1.40	1.53	19	1
M	8	NAG	C1-C2	6.63	1.40	1.53	19	1
F	15	NAG	C6-O6	6.51	1.54	1.41	14	2
N	15	NAG	C6-O6	6.51	1.54	1.41	14	2
C	15	NAG	C6-O6	6.43	1.54	1.41	19	2
K	15	NAG	C6-O6	6.43	1.54	1.41	19	2
N	18	FUC	C5-C6	6.36	1.64	1.51	20	2
F	18	FUC	C5-C6	6.36	1.64	1.51	20	2
P	15	NAG	C6-O6	6.32	1.53	1.41	15	1
H	15	NAG	C6-O6	6.32	1.53	1.41	15	1
G	15	NAG	C6-O6	6.26	1.53	1.41	14	1
O	15	NAG	C6-O6	6.26	1.53	1.41	14	1
H	5	NAG	C5-C6	6.26	1.64	1.51	19	1
P	5	NAG	C5-C6	6.26	1.64	1.51	19	1
C	10	SIA	C4-C5	6.24	1.41	1.53	7	2
K	10	SIA	C4-C5	6.24	1.41	1.53	7	2
F	3	BMA	C2-C3	6.18	1.42	1.54	6	2
N	3	BMA	C2-C3	6.18	1.42	1.54	6	2
Q	5	NAG	C5-C6	6.11	1.64	1.51	13	1
I	5	NAG	C5-C6	6.11	1.64	1.51	13	1
R	3	BMA	C5-O5	6.09	1.54	1.42	10	2
J	3	BMA	C5-O5	6.09	1.54	1.42	10	2
O	5	NAG	C5-C6	6.09	1.63	1.51	17	1
G	5	NAG	C5-C6	6.09	1.63	1.51	17	1
I	8	NAG	C5-O5	6.01	1.53	1.41	1	1
Q	8	NAG	C5-O5	6.01	1.53	1.41	1	1
F	5	NAG	C5-C6	6.00	1.63	1.51	18	1
N	5	NAG	C5-C6	6.00	1.63	1.51	18	1
G	18	FUC	C5-C6	6.00	1.63	1.51	3	2
O	18	FUC	C5-C6	6.00	1.63	1.51	3	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	14	SIA	C1-C2	5.98	1.47	1.58	5	1
K	14	SIA	C1-C2	5.98	1.47	1.58	5	1
L	14	SIA	C3-C4	5.97	1.41	1.53	6	4
D	14	SIA	C3-C4	5.97	1.41	1.53	6	4
O	3	BMA	C2-C3	5.94	1.43	1.54	6	1
G	3	BMA	C2-C3	5.94	1.43	1.54	6	1
H	16	GAL	C6-O6	5.91	1.53	1.41	18	1
P	16	GAL	C6-O6	5.91	1.53	1.41	18	1
P	14	SIA	C3-C4	5.89	1.41	1.53	5	2
H	14	SIA	C3-C4	5.89	1.41	1.53	5	2
O	9	GAL	C1-O5	5.88	1.52	1.41	1	1
G	9	GAL	C1-O5	5.88	1.52	1.41	1	1
H	8	NAG	C5-O5	5.88	1.53	1.41	1	1
P	8	NAG	C5-O5	5.88	1.53	1.41	1	1
N	16	GAL	C1-C2	5.84	1.41	1.52	11	1
F	16	GAL	C1-C2	5.84	1.41	1.52	11	1
Q	14	SIA	C1-C2	5.83	1.47	1.58	6	2
I	14	SIA	C1-C2	5.83	1.47	1.58	6	2
I	18	FUC	C5-C6	5.83	1.63	1.51	6	2
Q	18	FUC	C5-C6	5.83	1.63	1.51	6	2
G	16	GAL	C6-O6	5.80	1.52	1.41	16	1
O	16	GAL	C6-O6	5.80	1.52	1.41	16	1
F	16	GAL	C6-O6	5.79	1.52	1.41	17	1
N	16	GAL	C6-O6	5.79	1.52	1.41	17	1
J	1	NAG	C5-O5	5.79	1.53	1.41	13	3
R	1	NAG	C5-O5	5.79	1.53	1.41	13	3
F	9	GAL	C1-O5	5.77	1.52	1.41	1	1
N	9	GAL	C1-O5	5.77	1.52	1.41	1	1
G	2	NAG	C3-C4	5.76	1.41	1.52	20	1
O	2	NAG	C3-C4	5.76	1.41	1.52	20	1
E	8	NAG	C5-O5	5.73	1.53	1.41	1	1
M	8	NAG	C5-O5	5.73	1.53	1.41	1	1
D	8	NAG	C5-O5	5.73	1.53	1.41	1	2
L	8	NAG	C5-O5	5.73	1.53	1.41	1	2
E	2	NAG	C2-C3	5.72	1.64	1.53	18	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
M	2	NAG	C2-C3	5.72	1.64	1.53	18	1
N	2	NAG	C3-C4	5.71	1.41	1.52	20	1
F	2	NAG	C3-C4	5.71	1.41	1.52	20	1
C	9	GAL	C1-O5	5.69	1.52	1.41	3	1
K	9	GAL	C1-O5	5.69	1.52	1.41	3	1
E	18	FUC	C5-C6	5.69	1.63	1.51	13	2
M	18	FUC	C5-C6	5.69	1.63	1.51	13	2
D	14	SIA	C1-C2	5.67	1.47	1.58	7	1
L	14	SIA	C1-C2	5.67	1.47	1.58	7	1
E	7	SIA	C6-C7	5.66	1.43	1.55	15	1
M	7	SIA	C6-C7	5.66	1.43	1.55	15	1
O	5	NAG	C4-C5	5.64	1.42	1.53	2	2
G	5	NAG	C4-C5	5.64	1.42	1.53	2	2
H	7	SIA	C6-O6	5.64	1.54	1.42	15	1
P	7	SIA	C6-O6	5.64	1.54	1.42	15	1
C	7	SIA	C6-O6	5.63	1.54	1.42	19	1
K	7	SIA	C6-O6	5.63	1.54	1.42	19	1
L	5	NAG	C4-C5	5.63	1.42	1.53	5	2
D	5	NAG	C4-C5	5.63	1.42	1.53	5	2
C	3	BMA	C6-O6	5.62	1.52	1.41	2	1
K	3	BMA	C6-O6	5.62	1.52	1.41	2	1
Q	7	SIA	C6-C7	5.61	1.44	1.55	17	1
I	7	SIA	C6-C7	5.61	1.44	1.55	17	1

Standard geometry: angle outliers ?

There are 390 bond angle outliers in this entry (0.12% of 321610 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	501	ASP	N-CA-CB	11.69	90.63	110.50	4	20
B	501	ASP	N-CA-CB	11.69	90.63	110.50	4	20
B	501	ASP	N-CA-C	8.19	133.93	111.00	20	20
A	501	ASP	N-CA-C	8.19	133.93	111.00	20	20
D	11	MAN	C1-C2-O2	5.80	124.19	106.80	1	1
L	11	MAN	C1-C2-O2	5.80	124.19	106.80	1	1
I	11	MAN	C1-C2-O2	5.61	123.64	106.80	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
Q	11	MAN	C1-C2-O2	5.61	123.64	106.80	1	2
C	11	MAN	C1-C2-O2	5.61	123.64	106.80	1	1
K	11	MAN	C1-C2-O2	5.61	123.64	106.80	1	1
E	11	MAN	C1-C2-O2	5.55	123.46	106.80	1	2
M	11	MAN	C1-C2-O2	5.55	123.46	106.80	1	2
J	17	SIA	C7-C8-C9	5.55	127.69	111.05	17	1
R	17	SIA	C7-C8-C9	5.55	127.69	111.05	17	1
H	11	MAN	C1-C2-O2	5.47	123.21	106.80	1	1
P	11	MAN	C1-C2-O2	5.47	123.21	106.80	1	1
J	3	BMA	C2-C3-O3	5.22	122.33	106.67	13	1
R	3	BMA	C2-C3-O3	5.22	122.33	106.67	13	1
N	4	MAN	C3-C4-O4	5.19	122.64	107.06	18	2
F	4	MAN	C3-C4-O4	5.19	122.64	107.06	18	2
G	4	MAN	C3-C4-O4	5.18	122.59	107.06	17	2
O	4	MAN	C3-C4-O4	5.18	122.59	107.06	17	2
P	4	MAN	C3-C4-O4	5.14	122.49	107.06	19	2
H	4	MAN	C3-C4-O4	5.14	122.49	107.06	19	2
I	4	MAN	C3-C4-O4	5.11	122.38	107.06	13	1
Q	4	MAN	C3-C4-O4	5.11	122.38	107.06	13	1
R	3	BMA	C2-C1-O5	5.02	96.38	111.45	12	2
J	3	BMA	C2-C1-O5	5.02	96.38	111.45	12	2
D	3	BMA	C1-C2-O2	5.02	123.45	108.40	9	1
L	3	BMA	C1-C2-O2	5.02	123.45	108.40	9	1
E	3	BMA	C1-C2-O2	5.01	123.42	108.40	4	1
M	3	BMA	C1-C2-O2	5.01	123.42	108.40	4	1
G	3	BMA	C2-C3-O3	4.99	121.63	106.67	10	2
O	3	BMA	C2-C3-O3	4.99	121.63	106.67	10	2
I	3	BMA	C2-C3-O3	4.91	121.40	106.67	10	1
Q	3	BMA	C2-C3-O3	4.91	121.40	106.67	10	1
O	12	NAG	C3-C4-O4	4.90	121.98	107.29	19	1
G	12	NAG	C3-C4-O4	4.90	121.98	107.29	19	1
C	3	BMA	C1-C2-O2	4.87	123.00	108.40	8	1
K	3	BMA	C1-C2-O2	4.87	123.00	108.40	8	1
M	4	MAN	C3-C4-O4	4.85	121.60	107.06	6	1
E	4	MAN	C3-C4-O4	4.85	121.60	107.06	6	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
N	3	BMA	C2-C3-O3	4.84	121.20	106.67	12	2
F	3	BMA	C2-C3-O3	4.84	121.20	106.67	12	2
R	16	GAL	C5-C6-O6	4.84	123.61	109.08	11	1
J	16	GAL	C5-C6-O6	4.84	123.61	109.08	11	1
J	4	MAN	C3-C4-O4	4.84	121.57	107.06	6	3
R	4	MAN	C3-C4-O4	4.84	121.57	107.06	6	3
D	3	BMA	C2-C3-O3	4.83	121.15	106.67	16	1
L	3	BMA	C2-C3-O3	4.83	121.15	106.67	16	1
C	4	MAN	C3-C4-O4	4.79	121.43	107.06	2	2
K	4	MAN	C3-C4-O4	4.79	121.43	107.06	2	2
C	3	BMA	C2-C3-O3	4.78	121.02	106.67	15	2
K	3	BMA	C2-C3-O3	4.78	121.02	106.67	15	2
L	4	MAN	C3-C4-O4	4.77	121.37	107.06	12	2
D	4	MAN	C3-C4-O4	4.77	121.37	107.06	12	2
H	3	BMA	C2-C3-O3	4.75	120.91	106.67	12	1
P	3	BMA	C2-C3-O3	4.75	120.91	106.67	12	1
C	11	MAN	C3-C2-O2	4.74	97.55	111.77	14	1
K	11	MAN	C3-C2-O2	4.74	97.55	111.77	14	1
R	11	MAN	C3-C2-O2	4.71	97.64	111.77	2	1
J	11	MAN	C3-C2-O2	4.71	97.64	111.77	2	1
C	7	SIA	C7-C6-O6	4.68	117.75	103.71	7	1
K	7	SIA	C7-C6-O6	4.68	117.75	103.71	7	1
R	11	MAN	C1-C2-O2	4.67	120.81	106.80	18	2
J	11	MAN	C1-C2-O2	4.67	120.81	106.80	18	2
C	17	SIA	C7-C6-O6	4.67	117.71	103.71	7	1
K	17	SIA	C7-C6-O6	4.67	117.71	103.71	7	1
D	14	SIA	C7-C6-O6	4.64	117.63	103.71	2	1
L	14	SIA	C7-C6-O6	4.64	117.63	103.71	2	1
C	14	SIA	C7-C6-O6	4.63	117.60	103.71	2	1
K	14	SIA	C7-C6-O6	4.63	117.60	103.71	2	1
J	3	BMA	C3-C4-O4	4.59	119.55	105.79	5	2
R	3	BMA	C3-C4-O4	4.59	119.55	105.79	5	2
E	7	SIA	C7-C6-O6	4.58	117.44	103.71	19	1
M	7	SIA	C7-C6-O6	4.58	117.44	103.71	19	1
D	10	SIA	C3-C4-O4	4.54	98.13	111.75	11	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	10	SIA	C3-C4-O4	4.54	98.13	111.75	11	1
N	15	NAG	C3-C4-O4	4.51	120.83	107.29	10	1
F	15	NAG	C3-C4-O4	4.51	120.83	107.29	10	1
O	10	SIA	C3-C4-O4	4.51	98.22	111.75	6	1
G	10	SIA	C3-C4-O4	4.51	98.22	111.75	6	1
Q	10	SIA	C3-C4-O4	4.49	98.27	111.75	5	1
I	10	SIA	C3-C4-O4	4.49	98.27	111.75	5	1
H	15	NAG	C3-C4-O4	4.48	120.72	107.29	12	1
P	15	NAG	C3-C4-O4	4.48	120.72	107.29	12	1
O	9	GAL	C4-C3-O3	4.47	99.84	113.26	19	1
G	9	GAL	C4-C3-O3	4.47	99.84	113.26	19	1
C	10	SIA	C3-C4-O4	4.47	98.33	111.75	10	1
K	10	SIA	C3-C4-O4	4.47	98.33	111.75	10	1
J	15	NAG	C3-C4-O4	4.47	120.71	107.29	20	1
R	15	NAG	C3-C4-O4	4.47	120.71	107.29	20	1
H	14	SIA	C5-C4-O4	4.47	120.29	106.87	5	1
P	14	SIA	C5-C4-O4	4.47	120.29	106.87	5	1
G	15	NAG	C3-C4-O4	4.46	120.68	107.29	10	1
O	15	NAG	C3-C4-O4	4.46	120.68	107.29	10	1
E	10	SIA	C3-C4-O4	4.45	98.39	111.75	5	1
M	10	SIA	C3-C4-O4	4.45	98.39	111.75	5	1
C	10	SIA	C5-C6-C7	4.44	123.88	110.56	7	1
K	10	SIA	C5-C6-C7	4.44	123.88	110.56	7	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	24.70	356
2	14.60	211
3	11.75	170
4	22.66	327
5	14.31	207
6	21.60	312
7	18.52	268

Model ID	Clash score	Number of clashes
8	21.89	316
9	10.03	145
10	14.47	209
11	13.68	198
12	14.54	210
13	15.86	229
14	14.94	216
15	10.44	151
16	17.88	258
17	10.99	159
18	15.43	223
19	11.92	172
20	14.66	212

There are 4549 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)
B:445:GLN:HB2	R:18:FUC:C6	1.63	4	1
A:445:GLN:HB2	J:18:FUC:C6	1.63	4	1
A:488:THR:CB	I:1:NAG:H4	1.59	1	1
A:511:PHE:CB	I:18:FUC:H61	1.59	5	1
B:511:PHE:CB	Q:18:FUC:H61	1.58	5	1
B:488:THR:CB	Q:1:NAG:H4	1.58	1	1
A:488:THR:HA	J:1:NAG:CT	1.58	6	1
B:488:THR:HA	R:1:NAG:CT	1.58	6	1
A:384:TRP:CZ2	J:13:GAL:H62	1.58	12	1
B:384:TRP:CZ2	R:13:GAL:H62	1.58	12	1
B:488:THR:HA	Q:1:NAG:CT	1.58	7	5
A:488:THR:HA	I:1:NAG:CT	1.57	7	5
A:488:THR:CA	J:1:NAG:CT	1.57	6	1
B:488:THR:CA	R:1:NAG:CT	1.57	6	1
O:7:SIA:CT	P:17:SIA:CT	1.57	8	1
B:399:VAL:HG23	R:12:NAG:C	1.56	12	1
B:488:THR:CG2	Q:2:NAG:C1	1.56	1	1
G:7:SIA:CT	H:17:SIA:CT	1.56	8	1
A:399:VAL:HG23	J:12:NAG:C	1.56	12	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:488:THR:CG2	I:2:NAG:C1	1.56	1	1
A:510:LYS:CB	I:2:NAG:H61	1.55	10	1
B:510:LYS:CB	Q:2:NAG:H61	1.55	10	1
A:498:LEU:CD2	H:1:NAG:H62	1.54	7	3
B:148:ARG:CA	M:18:FUC:H4	1.54	19	1
B:498:LEU:CD2	P:1:NAG:H62	1.54	7	3
A:148:ARG:CA	E:18:FUC:H4	1.54	19	1
B:502:PHE:C	P:18:FUC:H62	1.53	7	1
A:502:PHE:C	H:18:FUC:H62	1.52	7	1
B:463:ASN:ND2	P:1:NAG:C1	1.52	2	10
B:352:HIS:HB3	R:17:SIA:CT	1.52	8	1
A:445:GLN:HG2	J:1:NAG:C2	1.51	1	1
A:352:HIS:HB3	J:17:SIA:CT	1.51	8	1
B:510:LYS:CA	Q:2:NAG:H62	1.51	10	1
B:445:GLN:HG2	R:1:NAG:C2	1.51	1	1
A:463:ASN:ND2	H:1:NAG:C1	1.51	2	10
A:469:TYR:HE2	J:2:NAG:C2	1.51	3	1
B:445:GLN:HG3	R:18:FUC:C5	1.51	4	1
A:510:LYS:CA	I:2:NAG:H62	1.51	10	1
B:469:TYR:HE2	R:2:NAG:C2	1.51	3	1
A:445:GLN:HG3	J:18:FUC:C5	1.50	4	1
B:408:LYS:CG	O:2:NAG:H62	1.50	8	1
A:445:GLN:CG	J:18:FUC:H5	1.50	4	1
B:445:GLN:CG	R:18:FUC:H5	1.50	4	1
A:408:LYS:CG	G:2:NAG:H62	1.50	8	1
A:498:LEU:HB2	H:18:FUC:C6	1.49	7	1
A:110:HIS:CE1	D:18:FUC:H4	1.49	6	1
B:110:HIS:CE1	L:18:FUC:H4	1.48	6	1
B:498:LEU:HB2	P:18:FUC:C6	1.48	7	1
A:433:GLN:HE22	G:18:FUC:C5	1.48	17	1
B:243:ASN:ND2	N:1:NAG:C1	1.48	13	11
B:433:GLN:HE22	O:18:FUC:C5	1.48	17	1
A:510:LYS:CB	I:2:NAG:C6	1.48	10	1
A:243:ASN:ND2	F:1:NAG:C1	1.47	13	11
B:445:GLN:NE2	R:1:NAG:N	1.47	12	3

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:510:LYS:CB	Q:2:NAG:C6	1.47	10	1
B:148:ARG:HB3	M:1:NAG:C5	1.47	13	2
B:510:LYS:C	Q:2:NAG:H62	1.47	10	1
A:488:THR:CB	J:1:NAG:CT	1.47	6	1
A:445:GLN:NE2	J:1:NAG:N	1.47	12	3
B:488:THR:CB	R:1:NAG:CT	1.47	6	1
A:469:TYR:CD2	J:14:SIA:C9	1.47	8	1
A:148:ARG:HB3	E:1:NAG:C5	1.47	13	2
B:469:TYR:CD2	R:14:SIA:C9	1.47	8	1
A:510:LYS:C	I:2:NAG:H62	1.47	10	1
A:138:PRO:HD2	D:10:SIA:C4	1.46	4	1
A:199:PRO:HG2	E:2:NAG:C3	1.46	18	1
B:199:PRO:HG2	M:2:NAG:C3	1.46	18	1
A:138:PRO:HD2	D:10:SIA:C5	1.46	4	1
B:138:PRO:HD2	L:10:SIA:C4	1.46	4	1
B:138:PRO:HD2	L:10:SIA:C5	1.45	4	1
B:408:LYS:HG2	O:2:NAG:C6	1.45	8	2
A:408:LYS:HG2	G:2:NAG:C6	1.44	8	2
A:199:PRO:CG	E:2:NAG:O4	1.44	16	1
A:488:THR:CG2	I:18:FUC:H4	1.44	4	1
B:488:THR:CG2	Q:18:FUC:H4	1.44	4	1
B:199:PRO:CG	M:2:NAG:O4	1.44	16	1
B:488:THR:CB	Q:1:NAG:N	1.44	7	1
A:488:THR:CB	I:1:NAG:N	1.44	7	1
A:114:ASN:ND2	D:1:NAG:C1	1.43	17	7
B:114:ASN:ND2	L:1:NAG:C1	1.43	17	7
A:445:GLN:CB	J:18:FUC:C6	1.43	4	1
B:445:GLN:CB	R:18:FUC:C6	1.43	4	1
B:148:ARG:HH21	M:2:NAG:CT	1.43	5	2
A:498:LEU:CB	H:18:FUC:H61	1.43	7	2
B:498:LEU:CB	P:18:FUC:H61	1.43	7	2
G:8:NAG:O	H:9:GAL:C6	1.43	6	1
A:148:ARG:HH21	E:2:NAG:CT	1.42	5	2
O:8:NAG:O	P:9:GAL:C6	1.42	6	1
A:463:ASN:HD22	H:1:NAG:C1	1.42	20	8

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:491:ARG:HH21	J:1:NAG:C	1.42	6	1
A:488:THR:HB	I:1:NAG:N	1.42	7	2
B:90:ASN:ND2	C:9:GAL:H61	1.42	20	1
A:90:ASN:ND2	K:9:GAL:H61	1.42	20	1
B:463:ASN:HD22	P:1:NAG:C1	1.41	20	9
A:174:VAL:HA	E:8:NAG:CT	1.41	1	1
B:32:LEU:HG	K:18:FUC:C6	1.41	8	1
B:491:ARG:HH21	R:1:NAG:C	1.41	6	1
B:488:THR:HB	Q:1:NAG:N	1.41	7	2
A:32:LEU:HG	C:18:FUC:C6	1.41	8	1
B:174:VAL:HA	M:8:NAG:CT	1.41	1	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

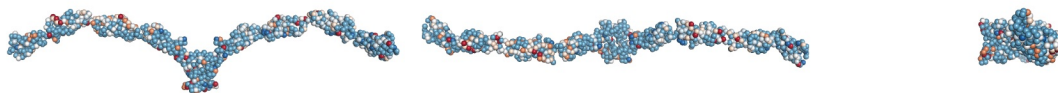
Chain	Res	Type	Models (Total)
A	22	VAL	20
A	24	ILE	20
A	28	ARG	20
A	31	ASN	20
A	38	VAL	20
A	60	LEU	20
A	62	VAL	20
A	81	VAL	20
A	83	ILE	20
A	94	ILE	20
A	98	VAL	20
A	131	THR	20
A	145	LEU	20
A	180	ARG	20
A	208	THR	20
A	227	THR	20
A	234	GLU	20
A	237	VAL	20
A	269	THR	20
A	271	ARG	20
A	286	THR	20
A	291	ILE	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

Chain	Res	Type	Models (Total)
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
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.

Acknowledgments

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

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

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