

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	9A47
PDB-Dev ID	PDBDEV_00000228
Structure Title	Man9 fully-glycosylated model of mouse N-cadherin EC4-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	2023-12-16

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

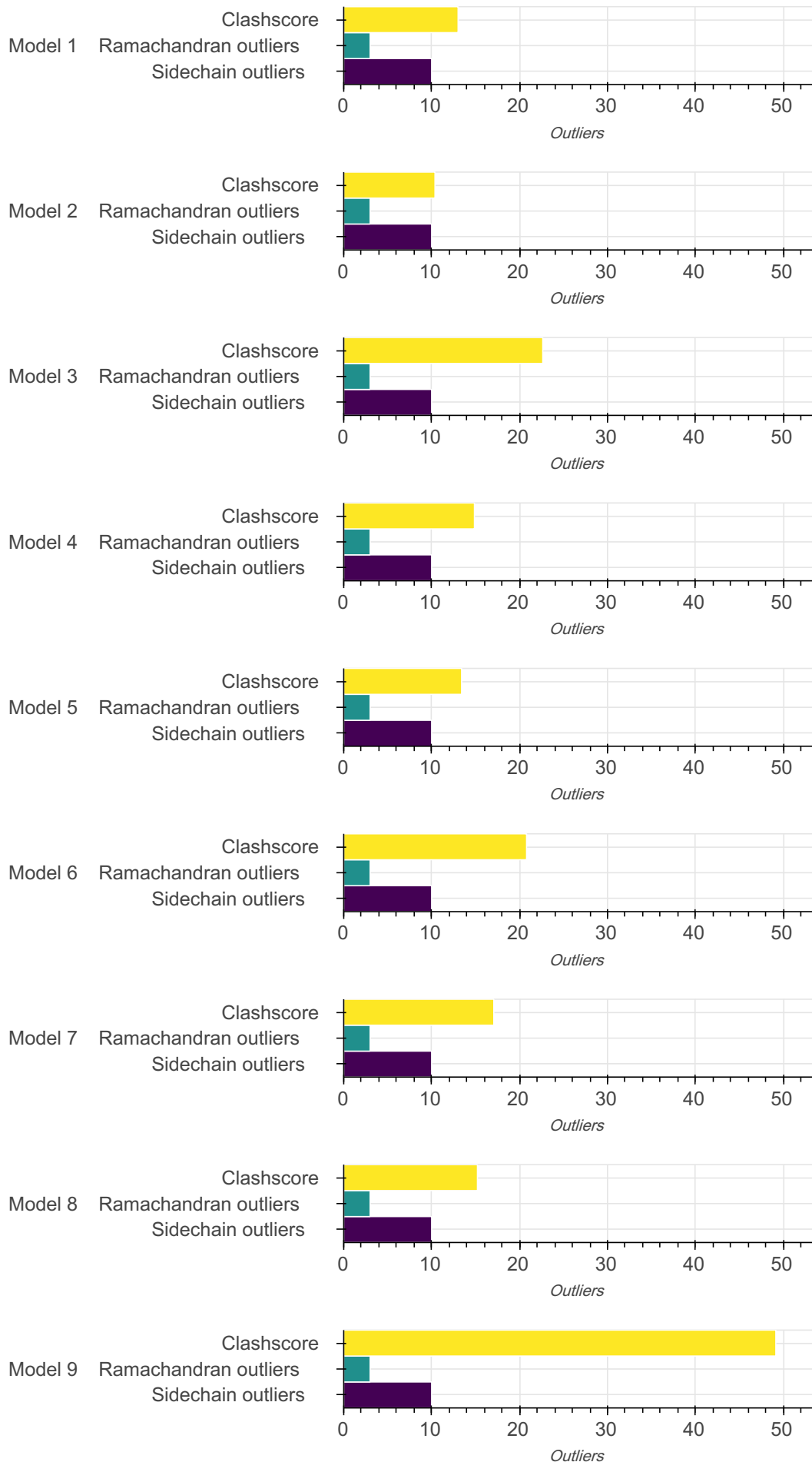
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

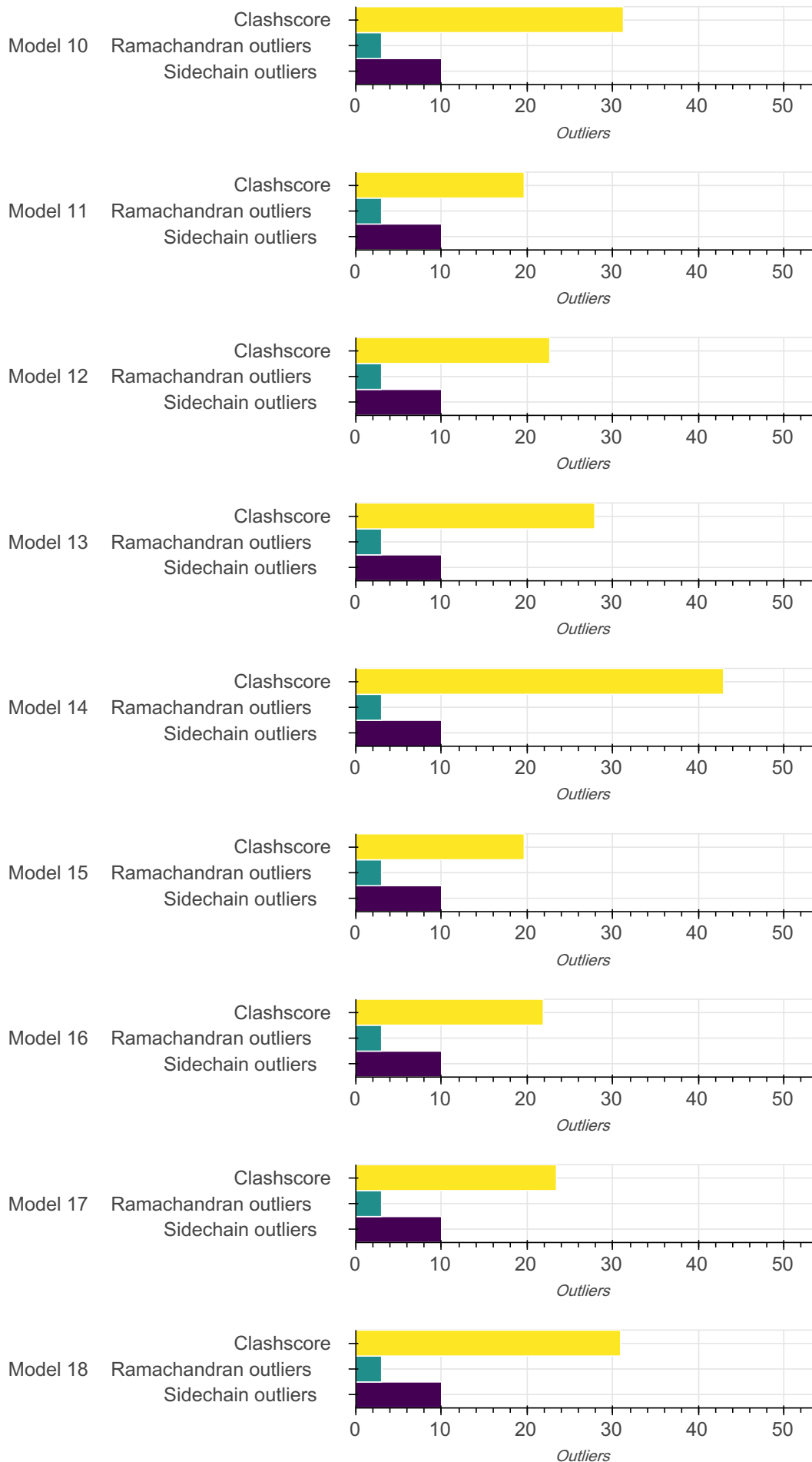
List of references used to build this report is available [here](#).

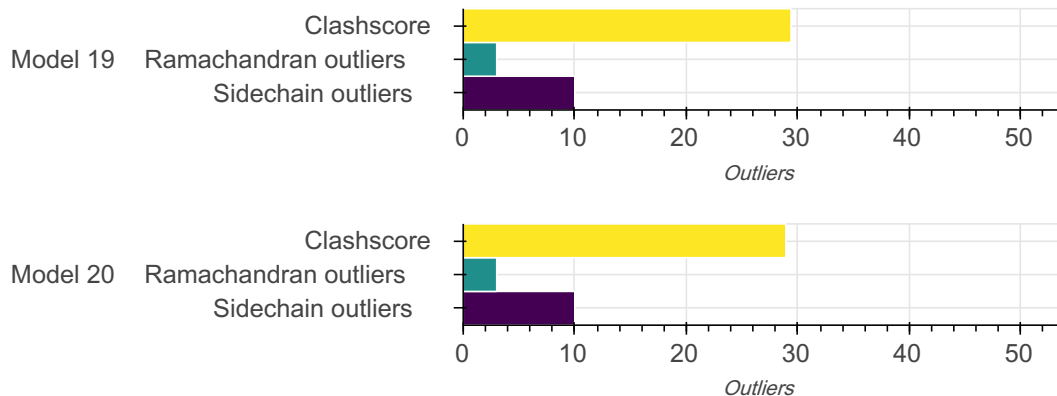
Overall quality ?

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	211	-	1-211	100.00 / 100.00	Atomic

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		2	alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	B C D E	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	SASDT45
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 ectodomains 4 to 5 of 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 288 bond length outliers in this entry (0.66% of 43873 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)
D	3	BMA	C2-C3	8.45	1.37	1.54	16	1
E	3	BMA	C2-C3	8.28	1.38	1.54	16	1
B	3	BMA	C2-C3	8.13	1.38	1.54	2	1
C	3	BMA	C2-C3	8.01	1.38	1.54	7	1
B	5	MAN	C1-C2	6.63	1.39	1.53	15	3
B	6	MAN	C1-O5	6.56	1.53	1.40	10	2
B	5	MAN	C1-O5	6.48	1.53	1.40	12	2
B	10	MAN	C2-C3	6.22	1.40	1.52	13	1
C	2	NAG	C1-C2	5.98	1.41	1.53	4	1
D	2	NAG	C1-C2	5.86	1.41	1.53	7	3
C	4	MAN	C1-O5	5.81	1.52	1.40	17	2
D	3	BMA	C3-O3	5.80	1.52	1.41	3	2
E	10	MAN	C2-O2	5.71	1.52	1.41	4	3
C	1	NAG	C1-C2	5.70	1.42	1.53	14	1
B	4	MAN	C1-O5	5.59	1.51	1.40	8	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	10	MAN	C2-O2	5.59	1.52	1.41	13	3
E	2	NAG	C1-C2	5.59	1.42	1.53	7	2
C	3	BMA	C3-O3	5.57	1.52	1.41	1	4
E	3	BMA	C3-O3	5.54	1.52	1.41	3	3
E	7	MAN	C3-O3	5.44	1.52	1.41	19	2
B	11	MAN	C1-O5	5.39	1.51	1.40	12	1
E	9	MAN	C1-C2	5.39	1.42	1.53	10	3
C	9	MAN	C2-O2	5.37	1.51	1.41	12	1
D	7	MAN	C3-O3	5.34	1.51	1.41	19	2
B	1	NAG	C1-C2	5.32	1.43	1.53	6	2
B	7	MAN	C3-O3	5.31	1.51	1.41	4	2
C	7	MAN	C6-O6	5.30	1.51	1.41	10	2
B	9	MAN	C2-O2	5.23	1.51	1.41	5	1
C	5	MAN	C1-C2	5.20	1.42	1.53	18	1
B	8	MAN	C2-O2	5.20	1.51	1.41	12	1
D	10	MAN	C3-C4	5.19	1.63	1.52	7	1
C	2	NAG	C5-C6	5.19	1.62	1.51	14	1
D	10	MAN	C2-O2	5.19	1.51	1.41	4	3
B	3	BMA	C3-O3	5.18	1.51	1.41	20	2
C	5	MAN	C2-O2	5.18	1.51	1.41	1	1
D	6	MAN	C5-C6	5.18	1.62	1.51	12	1
C	3	BMA	C1-O5	5.17	1.51	1.41	20	1
E	5	MAN	C2-O2	5.13	1.51	1.41	3	1
C	7	MAN	C3-O3	5.12	1.51	1.41	10	3
B	11	MAN	C5-O5	5.11	1.52	1.42	11	1
D	3	BMA	C4-C5	5.09	1.63	1.53	17	1
D	5	MAN	C2-O2	5.08	1.51	1.41	3	2
E	10	MAN	C3-C4	5.01	1.62	1.52	7	1
E	6	MAN	C5-C6	4.99	1.61	1.51	13	2
C	3	BMA	C4-C5	4.95	1.63	1.53	8	1
C	10	MAN	C3-C4	4.94	1.62	1.52	4	1
D	11	MAN	C6-O6	4.94	1.51	1.41	20	2
E	10	MAN	C1-C2	4.93	1.43	1.53	5	1
C	3	BMA	C3-C4	4.91	1.64	1.54	11	2
C	9	MAN	C1-C2	4.91	1.43	1.53	4	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	10	MAN	C2-C3	4.90	1.43	1.52	13	2
B	6	MAN	C3-O3	4.90	1.51	1.41	1	1
D	8	MAN	C1-C2	4.90	1.43	1.53	16	1
C	6	MAN	C1-O5	4.88	1.50	1.40	19	2
E	11	MAN	C1-O5	4.84	1.50	1.40	4	1
D	7	MAN	C6-O6	4.83	1.50	1.41	19	2
C	3	BMA	C5-C6	4.82	1.43	1.53	19	2
B	9	MAN	C1-C2	4.81	1.43	1.53	20	2
E	9	MAN	C1-O5	4.81	1.50	1.40	3	4
B	8	MAN	C1-C2	4.79	1.43	1.53	2	2
E	7	MAN	C6-O6	4.79	1.50	1.41	19	2
E	1	NAG	C5-C6	4.77	1.61	1.51	19	2
D	8	MAN	C2-O2	4.76	1.50	1.41	13	2
D	8	MAN	C1-O5	4.76	1.49	1.40	19	1
B	2	NAG	C6-O6	4.73	1.50	1.41	14	1
E	10	MAN	C2-C3	4.70	1.62	1.52	2	2
D	3	BMA	C3-C4	4.70	1.45	1.54	6	2
B	6	MAN	C2-O2	4.70	1.50	1.41	11	1
D	9	MAN	C1-O5	4.69	1.49	1.40	3	3
D	11	MAN	C5-O5	4.69	1.51	1.42	10	2
C	2	NAG	C4-O4	4.68	1.50	1.41	20	1
B	4	MAN	C1-C2	4.68	1.43	1.53	13	2
C	6	MAN	C5-O5	4.68	1.51	1.42	5	2
B	3	BMA	C4-C5	4.68	1.62	1.53	3	2
D	3	BMA	C1-O5	4.68	1.50	1.41	14	1
C	7	MAN	C1-O5	4.68	1.49	1.40	11	1
E	11	MAN	C6-O6	4.67	1.50	1.41	20	2
E	9	MAN	C3-O3	4.67	1.50	1.41	18	1
B	7	MAN	C1-O5	4.67	1.49	1.40	14	3
E	3	BMA	C1-O5	4.67	1.50	1.41	14	2
C	9	MAN	C1-O5	4.67	1.49	1.40	16	4
B	9	MAN	C1-O5	4.66	1.49	1.40	4	2
D	2	NAG	C6-O6	4.65	1.50	1.41	5	2
C	8	MAN	C1-C2	4.63	1.43	1.53	7	2
E	6	MAN	C3-O3	4.62	1.50	1.41	6	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	4	MAN	C2-O2	4.62	1.50	1.41	20	1
E	8	MAN	C1-O5	4.62	1.49	1.40	19	1
B	2	NAG	C4-O4	4.60	1.50	1.41	19	1
E	10	MAN	C6-O6	4.60	1.50	1.41	19	1
D	2	NAG	C4-C5	4.59	1.44	1.53	9	1
E	4	MAN	C2-O2	4.58	1.50	1.41	13	1
C	6	MAN	C2-O2	4.58	1.50	1.41	13	1
C	6	MAN	C3-O3	4.58	1.50	1.41	3	1
B	7	MAN	C2-O2	4.57	1.50	1.41	17	1
E	7	MAN	C5-O5	4.56	1.51	1.42	7	1
D	7	MAN	C1-C2	4.56	1.43	1.53	8	2
D	1	NAG	C5-C6	4.55	1.60	1.51	9	2
E	10	MAN	C4-C5	4.55	1.44	1.53	7	1
C	3	BMA	C1-C2	4.55	1.61	1.52	16	1
C	7	MAN	C1-C2	4.54	1.44	1.53	5	1

Standard geometry: angle outliers ?

There are 87 bond angle outliers in this entry (0.15% of 58824 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	171	ASP	N-CA-CB	11.69	90.63	110.50	17	20
A	171	ASP	N-CA-C	8.19	133.93	111.00	17	20
E	2	NAG	C3-C4-O4	5.43	123.59	107.29	10	6
D	2	NAG	C3-C4-O4	5.22	122.95	107.29	7	5
C	2	NAG	C3-C4-O4	5.11	122.63	107.29	4	6
B	1	NAG	C3-C4-O4	5.06	122.47	107.29	8	2
C	1	NAG	C3-C4-O4	4.99	122.27	107.29	17	2
E	3	BMA	C1-O5-C5	4.87	104.20	118.82	11	1
B	2	NAG	C3-C4-O4	4.87	121.89	107.29	6	2
C	3	BMA	C1-O5-C5	4.73	104.62	118.82	13	1
E	7	MAN	C1-C2-O2	4.60	120.59	106.80	18	1
D	7	MAN	C1-C2-O2	4.55	120.45	106.80	18	1
C	7	MAN	C1-C2-O2	4.53	120.39	106.80	9	1
E	1	NAG	C3-C4-O4	4.38	120.44	107.29	9	1
D	1	NAG	C3-C4-O4	4.38	120.43	107.29	9	1
C	5	MAN	C1-C2-O2	4.32	119.75	106.80	20	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	1	NAG	C5-C4-O4	4.27	98.89	111.70	1	2
B	1	NAG	C5-C4-O4	4.22	99.05	111.70	8	1
E	3	BMA	C1-C2-O2	4.17	120.92	108.40	10	1
C	6	MAN	C2-C3-O3	4.16	120.05	107.58	19	1
B	3	BMA	C1-C2-O2	4.15	120.85	108.40	15	1
D	10	MAN	C1-C2-O2	4.14	119.21	106.80	16	1
C	4	MAN	C4-C5-C6	4.14	124.09	111.68	16	2
C	9	MAN	C1-C2-O2	4.04	118.92	106.80	6	1
D	1	NAG	C5-C4-O4	4.02	99.63	111.70	3	1
E	11	MAN	C1-C2-O2	4.02	118.86	106.80	10	1
E	9	MAN	C1-C2-O2	4.02	118.86	106.80	15	1
D	2	NAG	C4-C5-O5	4.02	97.01	109.06	8	1
E	1	NAG	C5-C4-O4	4.00	99.70	111.70	3	1
B	4	MAN	C3-C4-O4	4.00	119.06	107.06	5	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	13.01	35
2	10.38	28
3	22.63	61
4	14.86	40
5	13.41	36
6	20.79	56
7	17.07	46
8	15.21	41
9	49.14	132
10	31.23	84
11	19.65	53
12	22.63	61
13	27.89	75
14	42.91	115
15	19.65	53
16	21.88	59

Model ID	Clash score	Number of clashes
17	23.41	63
18	30.90	83
19	29.39	79
20	28.92	78

There are 1278 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:158:THR:CG2	B:2:NAG:C1	1.64	19	1
A:158:THR:HG21	B:2:NAG:C1	1.63	19	2
A:185:ILE:CG2	B:3:BMA:H61	1.57	14	1
A:207:ARG:CG	B:11:MAN:H5	1.56	14	1
A:22:HIS:NE2	D:6:MAN:C2	1.56	9	2
A:22:HIS:CD2	D:6:MAN:C2	1.55	9	1
A:158:THR:HB	B:1:NAG:C4	1.53	19	2
A:133:ASN:ND2	E:1:NAG:C1	1.50	6	5
A:78:LYS:HZ1	C:7:MAN:C1	1.49	13	1
A:156:PRO:HG2	B:2:NAG:CT	1.47	19	1
A:207:ARG:HG2	B:11:MAN:C5	1.44	14	1
A:78:LYS:NZ	C:7:MAN:C1	1.43	13	1
A:130:ASN:OD1	E:1:NAG:CT	1.43	7	3
A:211:CYS:SG	E:11:MAN:H4	1.42	12	1
A:158:THR:CB	B:2:NAG:C1	1.42	19	1
A:78:LYS:NZ	C:3:BMA:C1	1.42	17	3
A:78:LYS:HZ2	C:3:BMA:C1	1.41	17	2
A:83:ASN:ND2	C:1:NAG:C1	1.41	9	8
A:78:LYS:HB2	C:2:NAG:C1	1.41	19	6
A:78:LYS:HD3	C:2:NAG:C3	1.41	17	3
A:158:THR:HG21	B:2:NAG:N	1.39	6	2
A:51:PRO:HG2	C:1:NAG:C6	1.39	13	1
A:198:PRO:CD	D:11:MAN:H62	1.37	9	1
A:158:THR:HG23	B:2:NAG:CT	1.37	6	1
A:211:CYS:SG	E:11:MAN:C4	1.36	12	1
A:158:THR:HB	B:1:NAG:C6	1.36	8	1
A:79:ASN:OD1	C:11:MAN:C6	1.35	10	1
A:125:GLU:OE2	B:2:NAG:CT	1.35	4	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:78:LYS:CB	C:2:NAG:N	1.35	9	4
A:185:ILE:CG2	B:3:BMA:C6	1.35	14	1
A:129:PRO:CG	E:11:MAN:O6	1.33	18	1
A:205:ILE:CG2	B:11:MAN:H61	1.32	9	1
A:207:ARG:HG3	B:10:MAN:C1	1.32	14	1
A:185:ILE:HG22	B:3:BMA:C6	1.32	14	1
A:141:ILE:HD13	C:10:MAN:C4	1.32	9	1
A:158:THR:CB	B:1:NAG:H62	1.31	8	1
A:141:ILE:CD1	C:10:MAN:O4	1.31	9	1
A:78:LYS:HZ3	C:3:BMA:C1	1.30	20	2
A:187:GLU:OE1	B:7:MAN:H62	1.29	9	1
A:154:LEU:HB3	D:5:MAN:O6	1.29	3	1
A:78:LYS:CD	C:2:NAG:H3	1.28	17	3
A:185:ILE:HD11	B:5:MAN:O6	1.28	10	1
A:78:LYS:HB2	C:2:NAG:C2	1.27	16	5
A:207:ARG:HG3	B:10:MAN:C2	1.27	14	1
A:78:LYS:HG2	C:3:BMA:O5	1.27	19	3
A:158:THR:CG2	B:2:NAG:N	1.27	6	2
A:78:LYS:N	C:2:NAG:N	1.27	4	6
A:79:ASN:OD1	C:11:MAN:O6	1.27	10	1
A:187:GLU:OE1	B:7:MAN:H2	1.27	15	1
A:126:THR:OG1	E:11:MAN:O6	1.26	9	1
A:205:ILE:CG2	B:11:MAN:O5	1.26	9	1
A:131:SER:O	E:1:NAG:H61	1.26	5	6
A:126:THR:CG2	E:10:MAN:O6	1.26	18	1
A:124:CYS:SG	E:11:MAN:H62	1.25	20	1
A:205:ILE:O	B:11:MAN:C6	1.25	14	1
A:168:LEU:HD23	E:1:NAG:O	1.24	3	1
A:158:THR:OG1	B:1:NAG:O6	1.24	13	2
A:141:ILE:HD13	C:10:MAN:O4	1.24	9	1
A:124:CYS:HB2	E:11:MAN:C6	1.24	20	1
A:198:PRO:CG	D:11:MAN:H62	1.24	9	1
A:182:GLU:OE1	B:8:MAN:O3	1.23	3	1
A:205:ILE:CG2	B:11:MAN:C6	1.23	9	1
A:130:ASN:CG	E:1:NAG:CT	1.23	7	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:78:LYS:CG	C:3:BMA:O5	1.23	19	2
A:182:GLU:N	B:2:NAG:O6	1.22	18	2
A:78:LYS:HG3	C:3:BMA:C5	1.22	19	2
A:156:PRO:CG	B:2:NAG:CT	1.22	19	2
A:22:HIS:CG	D:6:MAN:O3	1.21	9	1
A:141:ILE:HG21	C:10:MAN:O4	1.21	9	1
A:78:LYS:HG3	C:3:BMA:C6	1.20	20	3
A:22:HIS:NE2	D:6:MAN:H2	1.20	20	1
A:118:PRO:HB3	E:2:NAG:C	1.20	12	1
A:187:GLU:OE2	B:8:MAN:C6	1.20	15	1
A:207:ARG:NH1	B:7:MAN:O2	1.19	15	1
A:158:THR:HB	B:1:NAG:H4	1.19	19	1
A:78:LYS:CG	C:3:BMA:H62	1.19	20	4
A:158:THR:CB	B:1:NAG:C6	1.19	8	1
A:207:ARG:CG	B:10:MAN:C1	1.18	14	1
A:187:GLU:CB	B:7:MAN:H2	1.18	14	1
A:78:LYS:HD3	C:2:NAG:H3	1.18	18	3
A:126:THR:HG21	E:10:MAN:O6	1.17	18	1
A:207:ARG:NH2	B:10:MAN:O6	1.16	13	1
A:187:GLU:OE1	B:3:BMA:H62	1.16	13	1
A:128:GLU:HG3	E:11:MAN:C5	1.15	18	1
A:129:PRO:HG2	E:11:MAN:O6	1.15	18	1
A:51:PRO:HG2	C:1:NAG:O6	1.14	13	1
A:211:CYS:HG	E:11:MAN:C4	1.14	12	1
A:154:LEU:HD11	D:8:MAN:C4	1.14	17	1
A:155:SER:HB2	B:8:MAN:H61	1.14	19	1
A:185:ILE:CD1	B:11:MAN:H62	1.14	11	1
A:205:ILE:HG22	B:11:MAN:H61	1.13	9	1
A:78:LYS:NZ	C:3:BMA:H5	1.13	17	2
A:185:ILE:HD12	B:11:MAN:H62	1.13	11	1
A:187:GLU:HB3	B:7:MAN:H2	1.13	14	1
A:124:CYS:HB2	E:11:MAN:H61	1.13	20	1
A:187:GLU:OE2	B:8:MAN:O6	1.13	15	1
A:79:ASN:OD1	C:11:MAN:H62	1.13	10	1
A:129:PRO:CD	E:11:MAN:O6	1.13	18	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:154:LEU:CD1	D:8:MAN:H4	1.12	17	1
A:198:PRO:HD3	D:11:MAN:C6	1.12	9	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	207	178	26	3
2	207	178	26	3
3	207	178	26	3
4	207	178	26	3
5	207	178	26	3
6	207	178	26	3
7	207	178	26	3
8	207	178	26	3
9	207	178	26	3
10	207	178	26	3
11	207	178	26	3
12	207	178	26	3
13	207	178	26	3
14	207	178	26	3
15	207	178	26	3
16	207	178	26	3
17	207	178	26	3
18	207	178	26	3
19	207	178	26	3
20	207	178	26	3

There are 3 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	12	PRO	20
A	170	GLY	20
A	171	ASP	20

Torsion angles : Protein sidechains ?

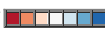
In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	185	144	31	10
2	185	144	31	10
3	185	144	31	10
4	185	144	31	10
5	185	144	31	10
6	185	144	31	10
7	185	144	31	10
8	185	144	31	10
9	185	144	31	10
10	185	144	31	10
11	185	144	31	10
12	185	144	31	10
13	185	144	31	10
14	185	144	31	10
15	185	144	31	10
16	185	144	31	10
17	185	144	31	10
18	185	144	31	10
19	185	144	31	10
20	185	144	31	10

There are 10 unique sidechain outliers. Detailed list of outliers are tabulated below.

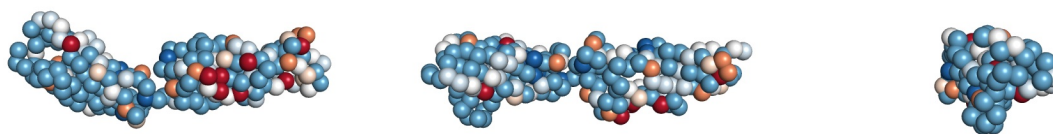
Chain	Res	Type	Models (Total)
A	8	PHE	20
A	18	GLU	20
A	43	ILE	20
A	73	GLU	20
A	79	ASN	20
A	135	THR	20
A	152	LEU	20
A	169	ASN	20
A	177	LEU	20
A	185	ILE	20

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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