

Integrative Structure Validation Report ?

March 13, 2025 - 11:38 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

PDB ID	9A0F
PDB-Dev ID	PDBDEV_00000051
Structure Title	Integrative model of the wild type yeast nuclear pore complex
Structure Authors	Vasileios Rantos; Matteo Allegretti; Christian E. Zimmerli; Florian Wilfling; Paolo Ronchi; Herman K.H. Fung; Chia-Wei Lee; Wim Hagen; Beata Turonova; Kai Karius; Mandy Boermel; Xiaojie Zhang; Christoph Mueller; Yannick Schwab; Julia Mahamid; Boris Pfander; Martin Beck; Jan Kosinski
Deposited on	2020-06-04

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

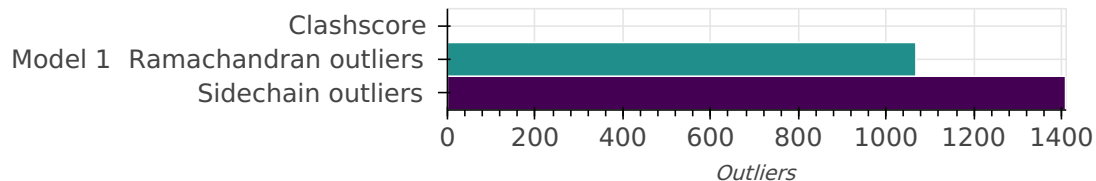
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 0 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 10 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	8	Dyn2	91	92	-	1-92	100.00 / 100.00	Atomic
				92					
		12	Nic96	A1	839	-	1-839	100.00 / 100.00	Atomic
				A2					
				A3					
				A4					
		13	Nup188	B1	1655	-	1-1655	100.00 / 100.00	Atomic
				B2					
		17	Nup192	C1	1683	-	1-1683	100.00 / 100.00	Atomic
				C2					
		14	Nup157	D1	1391	-	1-1391	100.00 / 100.00	Atomic
				D2					
		15	Nup57	H1	541	-	1-541	100.00 / 100.00	Atomic
				H2					
				H3					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				H4					
		16	Nup49	I1	472	-	1-472	100.00 / 100.00	Atomic
				I2					
				I3					
				I4					
		11	Nsp1	J1	823	-	1-823	100.00 / 100.00	Atomic
				J2					
				J3					
				J4					
				J5					
				J6					
		1	Nup133	K1	1157	-	1-1157	100.00 / 100.00	Atomic
				K2					
		2	Nup84	L1	726	-	1-726	100.00 / 100.00	Atomic
				L2					
		3	Nup145c	M1	712	-	1-712	100.00 / 100.00	Atomic
				M2					
		4	Sec13	N1	297	-	1-297	100.00 / 100.00	Atomic
				N2					
		5	Seh1	O1	349	-	1-349	100.00 / 100.00	Atomic
				O2					
		6	Nup85	P1	744	-	1-744	100.00 / 100.00	Atomic
				P2					
		7	Nup120	R1	1037	-	1-1037	100.00 / 100.00	Atomic
				R2					
		10	Nup159	V1	1460	-	1-1460	100.00 / 100.00	Atomic
				V2					
		9	Nup82	W1	713	-	1-713	100.00 / 100.00	Atomic
				W2					
		18	Nup170	d1	1502	-	1-1502	100.00 / 100.00	Atomic
				d2					

Datasets used for modeling ?

There are 10 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	3DEM volume	EMDB	EMD-10198
2	3DEM volume	Zenodo	10.5281/zenodo.3820319
3	3DEM volume	Zenodo	10.5281/zenodo.3820319
4	Experimental model	PDB	4XMM
5	Comparative model	Zenodo	10.5281/zenodo.1194547
6	Comparative model	Zenodo	10.5281/zenodo.1194547
7	Integrative model	PDB	8ZZA
8	Integrative model	PDB	8ZZA
9	Integrative model	PDB	8ZZA
10	Other	Not available	https://doi.org/10.1038/nsmb1194

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	Systematic fitting to EM maps with Global search from UCSF Chimera	Systematic fitting of CR Y-complex, NR Y-complex, IR asymmetric unit and P-complex rigid bodies	None	None	False	False
2	1	Monte Carlo simulated annealing optimization of multiple rigid bodies with IMP	Monte Carlo simulated annealing optimization for CR Y-complex, NR Y-complex and IR asymmetric unit	None	None	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	2.9.0	integrative model building	https://integrativemodeling.org
2	UCSF Chimera	1.14	rigid body fitting to EM maps	https://www.cgl.ucsf.edu/chimera/

Data quality ?

3DEM volume

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 5994 bond length outliers in this entry (2.90% of 206673 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)
D1	88	SER	N-CA	597.49	12.81	1.46	1	1
D2	88	SER	N-CA	597.41	12.81	1.46	1	1
A3	56	LEU	CA-C	534.50	12.75	1.52	1	1
A2	56	LEU	CA-C	534.46	12.75	1.52	1	1
A4	56	LEU	CA-C	475.10	11.50	1.52	1	1
A1	56	LEU	CA-C	475.05	11.50	1.52	1	1
W1	522	GLU	N-CA	460.47	10.21	1.46	1	1
d1	98	SER	N-CA	446.89	9.95	1.46	1	1
d2	98	SER	N-CA	446.88	9.95	1.46	1	1
A1	405	ASP	N-CA	426.20	9.56	1.46	1	1
A4	405	ASP	N-CA	426.16	9.56	1.46	1	1
A1	205	ASN	N-CA	395.33	8.97	1.46	1	1
A4	205	ASN	N-CA	395.30	8.97	1.46	1	1
B2	74	THR	CA-C	391.90	9.75	1.52	1	1
B1	74	THR	CA-C	391.85	9.75	1.52	1	1
B2	75	ILE	N-CA	385.14	8.78	1.46	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B1	75	ILE	N-CA	385.10	8.77	1.46	1	1
C1	1651	ASP	N-CA	382.37	8.72	1.46	1	1
C2	1651	ASP	N-CA	382.35	8.72	1.46	1	1
J5	727	SER	CA-C	380.85	9.52	1.52	1	1
J3	727	SER	CA-C	380.81	9.52	1.52	1	1
J6	727	SER	CA-C	380.75	9.52	1.52	1	1
J4	727	SER	CA-C	380.75	9.52	1.52	1	1
B1	508	PRO	N-CD	380.46	6.80	1.47	1	1
B2	508	PRO	N-CD	380.43	6.80	1.47	1	1
D2	309	LEU	CA-C	377.26	9.45	1.52	1	1
D1	309	LEU	CA-C	377.23	9.45	1.52	1	1
B2	407	ALA	N-CA	376.77	8.62	1.46	1	1
B1	407	ALA	N-CA	376.66	8.61	1.46	1	1
V1	1126	LEU	CA-C	362.47	9.14	1.52	1	1
D1	481	GLY	N-CA	358.86	7.19	1.45	1	1
D2	481	GLY	N-CA	358.73	7.19	1.45	1	1
W2	452	SER	CA-C	350.15	8.88	1.52	1	1
I1	270	PRO	N-CD	347.67	6.34	1.47	1	1
I4	270	PRO	N-CD	347.58	6.34	1.47	1	1
I1	270	PRO	N-CA	342.88	6.61	1.47	1	1
I4	270	PRO	N-CA	342.77	6.61	1.47	1	1
D2	339	GLU	N-CA	337.74	7.88	1.46	1	1
D1	339	GLU	N-CA	337.69	7.87	1.46	1	1
V2	1126	LEU	CA-C	334.06	8.54	1.52	1	1
A2	405	ASP	N-CA	329.74	7.72	1.46	1	1
A3	405	ASP	N-CA	329.72	7.72	1.46	1	1
V1	1429	LYS	N-CA	328.63	7.70	1.46	1	1
B2	1567	GLN	CA-C	324.92	8.35	1.52	1	1
B1	1567	GLN	CA-C	324.85	8.35	1.52	1	1
W1	452	SER	CA-C	323.04	8.31	1.52	1	1
C1	814	ASN	N-CA	321.81	7.57	1.46	1	1
C2	814	ASN	N-CA	321.81	7.57	1.46	1	1
J1	637	LEU	N-CA	314.69	7.44	1.46	1	1
C1	1644	ASP	CA-C	313.81	8.12	1.52	1	1
C2	1644	ASP	CA-C	313.78	8.11	1.52	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
d1	992	CYS	CA-C	312.75	8.09	1.52	1	1
d2	992	CYS	CA-C	312.72	8.09	1.52	1	1
A4	374	TYR	CA-C	308.26	8.00	1.52	1	1
A1	374	TYR	CA-C	308.24	8.00	1.52	1	1
I1	359	THR	CA-C	306.54	7.96	1.52	1	1
I3	359	THR	CA-C	306.53	7.96	1.52	1	1
I2	359	THR	CA-C	306.52	7.96	1.52	1	1
I4	359	THR	CA-C	306.45	7.96	1.52	1	1
B1	341	PHE	CA-C	303.51	7.90	1.52	1	1
B2	341	PHE	CA-C	303.42	7.90	1.52	1	1
A2	205	ASN	N-CA	301.80	7.19	1.46	1	1
A3	205	ASN	N-CA	301.74	7.19	1.46	1	1
J2	637	LEU	N-CA	300.30	7.16	1.46	1	1
H2	476	GLN	CA-C	298.52	7.79	1.52	1	1
H4	476	GLN	CA-C	298.52	7.79	1.52	1	1
H3	476	GLN	CA-C	298.52	7.79	1.52	1	1
H1	476	GLN	CA-C	298.44	7.79	1.52	1	1
I2	433	LYS	N-CA	297.94	7.12	1.46	1	1
I1	433	LYS	N-CA	297.92	7.12	1.46	1	1
I4	433	LYS	N-CA	297.89	7.12	1.46	1	1
I3	433	LYS	N-CA	297.89	7.12	1.46	1	1
B1	1056	LYS	N-CA	295.77	7.08	1.46	1	1
B2	1056	LYS	N-CA	295.71	7.08	1.46	1	1
B1	1593	HIS	N-CA	295.05	7.06	1.46	1	1
B2	1593	HIS	N-CA	294.99	7.06	1.46	1	1
C1	798	ASN	CA-C	292.80	7.67	1.52	1	1
C2	798	ASN	CA-C	292.79	7.67	1.52	1	1
V1	1117	TYR	N-CA	289.75	6.96	1.46	1	1
I4	271	PRO	N-CD	287.72	5.50	1.47	1	1
I1	271	PRO	N-CD	287.63	5.50	1.47	1	1
V2	1382	VAL	N-CA	287.48	6.92	1.46	1	1
W2	522	GLU	N-CA	284.38	6.86	1.46	1	1
d1	992	CYS	N-CA	284.36	6.86	1.46	1	1
d2	992	CYS	N-CA	284.35	6.86	1.46	1	1
H4	287	GLN	N-CA	283.05	6.84	1.46	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
H1	287	GLN	N-CA	282.97	6.83	1.46	1	1
I4	369	LEU	N-CA	280.41	6.79	1.46	1	1
I2	369	LEU	N-CA	280.38	6.79	1.46	1	1
I1	369	LEU	N-CA	280.32	6.78	1.46	1	1
I3	369	LEU	N-CA	280.22	6.78	1.46	1	1
B2	649	LYS	N-CA	278.65	6.75	1.46	1	1
B1	649	LYS	N-CA	278.64	6.75	1.46	1	1
V2	1332	LYS	N-CA	276.68	6.71	1.46	1	1
B2	74	THR	N-CA	274.01	6.66	1.46	1	1
B1	74	THR	N-CA	273.90	6.66	1.46	1	1
B1	342	ASP	N-CA	272.73	6.64	1.46	1	1
B2	342	ASP	N-CA	272.64	6.64	1.46	1	1
B2	1383	GLN	N-CA	271.21	6.61	1.46	1	1
B1	1383	GLN	N-CA	271.20	6.61	1.46	1	1

Standard geometry: angle outliers ?

There are 17381 bond angle outliers in this entry (6.23% of 279206 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)
A1	746	PRO	N-CA-CB	79.70	15.33	103.00	1	1
A4	746	PRO	N-CA-CB	79.66	15.38	103.00	1	1
B1	508	PRO	CA-N-CD	76.15	5.39	112.00	1	1
B2	508	PRO	CA-N-CD	76.14	5.40	112.00	1	1
D2	482	PRO	CA-N-CD	73.95	8.46	112.00	1	1
D1	482	PRO	CA-N-CD	73.94	8.48	112.00	1	1
C1	293	PRO	CA-N-CD	72.37	10.68	112.00	1	1
C2	293	PRO	CA-N-CD	72.33	10.74	112.00	1	1
W2	123	PRO	CA-N-CD	67.20	17.93	112.00	1	1
B1	1566	TYR	C-N-CA	66.63	1.77	121.70	1	1
B2	1566	TYR	C-N-CA	66.61	1.81	121.70	1	1
C2	1584	ASN	CA-C-N	65.87	18.10	116.90	1	1
C1	1584	ASN	CA-C-N	65.86	18.12	116.90	1	1
D1	481	GLY	CA-C-N	65.14	19.20	116.90	1	1
D2	481	GLY	CA-C-N	65.13	19.20	116.90	1	1
B1	407	ALA	CA-C-N	64.77	19.75	116.90	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B2	407	ALA	CA-C-N	64.74	19.79	116.90	1	1
I1	270	PRO	CA-N-CD	64.61	21.54	112.00	1	1
I4	270	PRO	CA-N-CD	64.60	21.55	112.00	1	1
C2	1126	PRO	CA-N-CD	64.25	22.05	112.00	1	1
C1	1126	PRO	CA-N-CD	64.20	22.11	112.00	1	1
A2	746	PRO	N-CA-CB	63.50	172.85	103.00	1	1
A3	746	PRO	N-CA-CB	63.41	172.76	103.00	1	1
A1	405	ASP	CA-C-N	62.83	22.65	116.90	1	1
A4	405	ASP	CA-C-N	62.81	22.69	116.90	1	1
A4	55	GLN	C-N-CA	62.46	9.26	121.70	1	1
A1	55	GLN	C-N-CA	62.45	9.29	121.70	1	1
I4	271	PRO	CA-N-CD	62.22	24.89	112.00	1	1
I1	271	PRO	CA-N-CD	62.21	24.90	112.00	1	1
J6	726	VAL	C-N-CA	62.19	9.75	121.70	1	1
J5	726	VAL	C-N-CA	62.18	9.78	121.70	1	1
J4	726	VAL	C-N-CA	62.18	9.78	121.70	1	1
J3	726	VAL	C-N-CA	62.16	9.81	121.70	1	1
A2	405	ASP	CA-C-N	61.13	25.21	116.90	1	1
A3	405	ASP	CA-C-N	61.12	25.22	116.90	1	1
d1	1015	GLU	C-N-CA	60.88	12.11	121.70	1	1
C2	797	LEU	C-N-CA	60.87	12.14	121.70	1	1
d2	1015	GLU	C-N-CA	60.86	12.16	121.70	1	1
C1	797	LEU	C-N-CA	60.82	12.22	121.70	1	1
I2	271	PRO	CA-N-CD	60.61	27.14	112.00	1	1
I3	271	PRO	CA-N-CD	60.60	27.16	112.00	1	1
d2	831	LYS	CA-C-O	60.36	18.19	120.80	1	1
d1	831	LYS	CA-C-O	60.35	18.20	120.80	1	1
B1	1400	PRO	CA-N-CD	60.15	27.79	112.00	1	1
A3	359	ASN	C-N-CA	60.14	13.45	121.70	1	1
B2	1400	PRO	CA-N-CD	60.13	27.82	112.00	1	1
A2	359	ASN	C-N-CA	60.09	13.54	121.70	1	1
B2	90	ALA	C-N-CA	59.56	14.49	121.70	1	1
B1	90	ALA	C-N-CA	59.52	14.56	121.70	1	1
I3	270	PRO	CA-N-CD	59.41	28.82	112.00	1	1
I2	270	PRO	CA-N-CD	59.41	28.83	112.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J2	777	ASN	C-N-CA	59.09	15.33	121.70	1	1
B2	405	SER	C-N-CA	59.03	15.44	121.70	1	1
B1	405	SER	C-N-CA	59.00	15.50	121.70	1	1
D1	932	ILE	C-N-CA	58.66	16.12	121.70	1	1
D2	932	ILE	C-N-CA	58.62	16.19	121.70	1	1
B2	408	PRO	CA-N-CD	58.53	30.06	112.00	1	1
B1	408	PRO	CA-N-CD	58.51	30.09	112.00	1	1
A1	746	PRO	C-N-CA	58.25	16.85	121.70	1	1
A4	746	PRO	C-N-CA	58.24	16.87	121.70	1	1
A2	20	LYS	CA-C-O	58.14	21.96	120.80	1	1
A3	20	LYS	CA-C-O	58.13	21.98	120.80	1	1
A1	515	LEU	N-CA-CB	58.04	11.83	110.50	1	1
A4	515	LEU	N-CA-CB	58.04	11.83	110.50	1	1
B1	1099	PHE	C-N-CA	58.00	17.29	121.70	1	1
B2	1099	PHE	C-N-CA	58.00	17.30	121.70	1	1
B2	165	ASN	C-N-CA	57.70	17.83	121.70	1	1
B1	165	ASN	C-N-CA	57.70	17.83	121.70	1	1
D2	961	PRO	CA-N-CD	57.51	31.48	112.00	1	1
D1	961	PRO	CA-N-CD	57.49	31.51	112.00	1	1
d1	1061	PRO	CA-N-CD	57.49	31.52	112.00	1	1
d2	1061	PRO	CA-N-CD	57.46	31.56	112.00	1	1
C2	1072	PRO	N-CA-CB	57.22	165.95	103.00	1	1
C1	1072	PRO	N-CA-CB	57.10	165.81	103.00	1	1
A1	359	ASN	C-N-CA	57.10	18.92	121.70	1	1
A4	359	ASN	C-N-CA	57.09	18.94	121.70	1	1
D2	514	ARG	C-N-CA	56.53	19.95	121.70	1	1
D1	514	ARG	C-N-CA	56.51	19.98	121.70	1	1
V2	1238	PHE	C-N-CA	56.06	20.78	121.70	1	1
B1	1009	PRO	CA-N-CD	55.74	33.97	112.00	1	1
B2	1009	PRO	CA-N-CD	55.73	33.97	112.00	1	1
I3	358	LEU	C-N-CA	55.69	21.45	121.70	1	1
I2	358	LEU	C-N-CA	55.68	21.47	121.70	1	1
I1	358	LEU	C-N-CA	55.62	21.58	121.70	1	1
I4	358	LEU	C-N-CA	55.62	21.58	121.70	1	1
A4	373	ALA	C-N-CA	55.43	21.92	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A1	373	ALA	C-N-CA	55.39	21.99	121.70	1	1
I1	406	PHE	C-N-CA	55.34	22.09	121.70	1	1
W1	625	HIS	CA-C-O	55.32	26.75	120.80	1	1
I3	406	PHE	C-N-CA	55.32	22.13	121.70	1	1
I4	406	PHE	C-N-CA	55.30	22.15	121.70	1	1
I2	406	PHE	C-N-CA	55.28	22.20	121.70	1	1
D1	729	PHE	C-N-CA	55.25	22.25	121.70	1	1
C2	1272	LEU	CA-C-O	55.23	26.92	120.80	1	1
D2	729	PHE	C-N-CA	55.22	22.31	121.70	1	1
C1	1272	LEU	CA-C-O	55.20	26.96	120.80	1	1
V2	1125	ASP	C-N-CA	55.06	22.58	121.70	1	1
D2	829	LEU	C-N-CA	54.90	22.89	121.70	1	1
D1	829	LEU	C-N-CA	54.88	22.92	121.70	1	1
D1	339	GLU	CA-C-N	54.53	7.14	116.20	1	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	0.00	0

There are no too-close contacts.

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	24713	21896	1749	1068

There are 1068 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
91	65	PHE	1
91	77	VAL	1
91	82	GLY	1
91	83	PRO	1
92	37	LEU	1
92	54	GLY	1

Chain	Res	Type	Models (Total)
92	55	ASN	1
92	65	PHE	1
92	77	VAL	1
92	82	GLY	1
92	83	PRO	1
A1	21	LYS	1
A1	35	ALA	1
A1	37	SER	1
A1	46	ILE	1
A1	47	ASN	1
A1	55	GLN	1
A1	264	LYS	1
A1	268	ILE	1
A1	269	ASN	1
A1	297	GLY	1
A1	316	ALA	1
A1	317	ASP	1
A1	328	ILE	1
A1	346	ILE	1
A1	359	ASN	1
A1	406	PRO	1
A1	423	LYS	1
A1	470	GLY	1
A1	474	PHE	1
A1	475	SER	1
A1	476	ASN	1
A1	613	VAL	1
A1	675	VAL	1
A1	697	PHE	1
A1	732	TRP	1
A1	744	LEU	1
A1	746	PRO	1
A1	764	ASP	1
A1	765	ASP	1

Chain	Res	Type	Models (Total)
A1	795	GLN	1
A1	834	ASN	1
A2	35	ALA	1
A2	37	SER	1
A2	46	ILE	1
A2	47	ASN	1
A2	55	GLN	1
A2	264	LYS	1
A2	268	ILE	1
A2	269	ASN	1
A2	297	GLY	1
A2	316	ALA	1
A2	317	ASP	1
A2	328	ILE	1
A2	346	ILE	1
A2	359	ASN	1
A2	373	ALA	1
A2	406	PRO	1
A2	423	LYS	1
A2	470	GLY	1
A2	474	PHE	1
A2	475	SER	1
A2	476	ASN	1
A2	613	VAL	1
A2	675	VAL	1
A2	697	PHE	1
A2	732	TRP	1
A2	744	LEU	1
A2	746	PRO	1
A2	764	ASP	1
A2	765	ASP	1
A2	795	GLN	1
A3	35	ALA	1
A3	37	SER	1
A3	46	ILE	1

Chain	Res	Type	Models (Total)
A3	47	ASN	1
A3	55	GLN	1
A3	264	LYS	1
A3	268	ILE	1
A3	269	ASN	1
A3	297	GLY	1
A3	316	ALA	1
A3	317	ASP	1
A3	328	ILE	1
A3	346	ILE	1
A3	359	ASN	1
A3	373	ALA	1
A3	406	PRO	1
A3	423	LYS	1
A3	470	GLY	1
A3	474	PHE	1
A3	475	SER	1
A3	476	ASN	1
A3	613	VAL	1
A3	675	VAL	1
A3	697	PHE	1
A3	732	TRP	1
A3	744	LEU	1
A3	746	PRO	1
A3	764	ASP	1

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	22485	19359	1717	1409

There are 1409 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
91	7	SER	1

Chain	Res	Type	Models (Total)
91	8	THR	1
91	17	THR	1
91	44	THR	1
91	52	LYS	1
91	76	PHE	1
92	17	THR	1
92	52	LYS	1
92	55	ASN	1
92	76	PHE	1
A1	22	LEU	1
A1	37	SER	1
A1	47	ASN	1
A1	56	LEU	1
A1	205	ASN	1
A1	206	ASN	1
A1	232	PHE	1
A1	272	GLU	1
A1	312	LYS	1
A1	313	LEU	1
A1	318	LYS	1
A1	360	ILE	1
A1	374	TYR	1
A1	405	ASP	1
A1	406	PRO	1
A1	429	THR	1
A1	439	HIS	1
A1	444	LYS	1
A1	500	GLU	1
A1	515	LEU	1
A1	542	THR	1
A1	625	GLU	1
A1	668	SER	1
A1	672	GLN	1
A1	683	THR	1
A1	697	PHE	1

Chain	Res	Type	Models (Total)
A1	746	PRO	1
A1	747	PHE	1
A1	754	ARG	1
A1	765	ASP	1
A1	795	GLN	1
A1	834	ASN	1
A1	835	ILE	1
A2	20	LYS	1
A2	22	LEU	1
A2	37	SER	1
A2	47	ASN	1
A2	56	LEU	1
A2	232	PHE	1
A2	272	GLU	1
A2	312	LYS	1
A2	313	LEU	1
A2	318	LYS	1
A2	360	ILE	1
A2	367	PHE	1
A2	374	TYR	1
A2	405	ASP	1
A2	429	THR	1
A2	439	HIS	1
A2	500	GLU	1
A2	515	LEU	1
A2	542	THR	1
A2	625	GLU	1
A2	668	SER	1
A2	672	GLN	1
A2	683	THR	1
A2	697	PHE	1
A2	746	PRO	1
A2	747	PHE	1
A2	754	ARG	1
A2	765	ASP	1

Chain	Res	Type	Models (Total)
A2	795	GLN	1
A3	20	LYS	1
A3	22	LEU	1
A3	37	SER	1
A3	47	ASN	1
A3	56	LEU	1
A3	232	PHE	1
A3	272	GLU	1
A3	312	LYS	1
A3	313	LEU	1
A3	318	LYS	1
A3	360	ILE	1
A3	367	PHE	1
A3	374	TYR	1
A3	405	ASP	1
A3	429	THR	1
A3	439	HIS	1
A3	500	GLU	1
A3	515	LEU	1
A3	542	THR	1
A3	625	GLU	1
A3	668	SER	1
A3	672	GLN	1
A3	683	THR	1
A3	697	PHE	1
A3	746	PRO	1
A3	747	PHE	1
A3	754	ARG	1
A3	765	ASP	1

Fit of model to data used for modeling ?

3DEM volume

Validation for this section is under development.

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 Trewhella, 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.