

# Integrative Structure Validation Report ?

March 13, 2025 - 11:51 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	9A0H
PDB-Dev ID	PDBDEV_00000053
Structure Title	Integrative model of Nup116 knockout (at 37C) 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](mailto:helpdesk@pdb-ihm.org)*

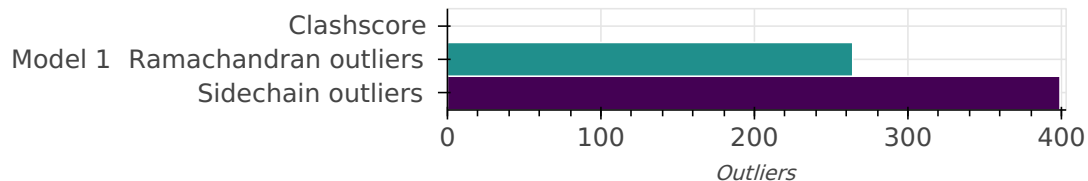
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 7 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	1	Nic96	A1	839	-	1-839	100.00 / 100.00	Atomic
		2	Nup188	B1	1655	-	1-1655	100.00 / 100.00	Atomic
		3	Nup157	D1	1391	-	1-1391	100.00 / 100.00	Atomic
		4	Nup133	K1	1157	-	1-1157	100.00 / 100.00	Atomic
		5	Nup84	L1	726	-	1-726	100.00 / 100.00	Atomic
		6	Nup145c	M1	712	-	1-712	100.00 / 100.00	Atomic
		7	Sec13	N1	297	-	1-297	100.00 / 100.00	Atomic
		8	Seh1	O1	349	-	1-349	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
		9	Nup85	P1	744	-	1-744	100.00 / 100.00	Atomic
		10	Nup120	R1	1037	-	1-1037	100.00 / 100.00	Atomic

### Datasets used for modeling ?

There are 7 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	3DEM volume	EMDB	<a href="#">EMD-10661</a>
2	3DEM volume	Zenodo	<a href="#">10.5281/zenodo.3820319</a>
3	3DEM volume	Zenodo	<a href="#">10.5281/zenodo.3820319</a>
4	Integrative model	PDB	<a href="#">9A0F</a>
5	Integrative model	PDB	<a href="#">9A0F</a>
6	Other	Not available	<a href="https://doi.org/10.1038/nsmb1194">https://doi.org/10.1038/nsmb1194</a>
7	Other	Not available	<a href="https://doi.org/10.1038/nature26003">https://doi.org/10.1038/nature26003</a>

### 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	Monte Carlo simulated annealing optimization of multiple rigid bodies with IMP	Monte Carlo simulated annealing optimization for NR Y-complex and IR asymmetric unit (outer nuclear copy)	None	None	False	False

*There is 1 software package reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="https://integrativemodeling.org">Integrative Modeling Platform (IMP)</a>	2.9.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>

## 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 1192 bond length outliers in this entry (2.04% of 58553 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	597.34	12.81	1.46	1	1
A1	405	ASP	N-CA	426.23	9.56	1.46	1	1
A1	205	ASN	N-CA	395.38	8.97	1.46	1	1
B1	74	THR	CA-C	391.91	9.76	1.52	1	1
B1	75	ILE	N-CA	385.10	8.77	1.46	1	1
B1	508	PRO	N-CD	380.40	6.80	1.47	1	1
D1	309	LEU	CA-C	377.27	9.45	1.52	1	1
B1	407	ALA	N-CA	376.72	8.62	1.46	1	1
D1	481	GLY	N-CA	358.71	7.19	1.45	1	1
D1	339	GLU	N-CA	337.75	7.88	1.46	1	1
B1	1567	GLN	CA-C	324.94	8.35	1.52	1	1
A1	374	TYR	CA-C	308.26	8.00	1.52	1	1
B1	341	PHE	CA-C	303.44	7.90	1.52	1	1
B1	1056	LYS	N-CA	295.71	7.08	1.46	1	1
B1	1593	HIS	N-CA	294.98	7.06	1.46	1	1
B1	649	LYS	N-CA	278.70	6.75	1.46	1	1
B1	74	THR	N-CA	273.98	6.66	1.46	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B1	342	ASP	N-CA	272.69	6.64	1.46	1	1
B1	1383	GLN	N-CA	271.22	6.61	1.46	1	1
B1	131	ASP	N-CA	268.11	6.55	1.46	1	1
A1	455	GLU	N-CA	267.29	6.54	1.46	1	1
B1	726	LYS	N-CA	266.45	6.52	1.46	1	1
B1	256	THR	N-CA	265.29	6.50	1.46	1	1
B1	1157	GLY	N-CA	264.78	5.69	1.45	1	1
A1	515	LEU	CA-C	257.14	6.93	1.52	1	1
B1	406	LYS	CA-C	255.88	6.90	1.52	1	1
B1	1276	LYS	N-CA	245.59	6.12	1.46	1	1
B1	123	ASP	CA-C	240.40	6.57	1.52	1	1
A1	455	GLU	CA-C	238.49	6.53	1.52	1	1
A1	533	ARG	N-CA	234.27	5.91	1.46	1	1
D1	1300	SER	N-CA	230.68	5.84	1.46	1	1
A1	206	ASN	N-CA	229.34	5.82	1.46	1	1
D1	1155	GLN	N-CA	224.26	5.72	1.46	1	1
B1	407	ALA	CA-C	222.84	6.20	1.52	1	1
D1	1039	LEU	N-CA	219.32	5.63	1.46	1	1
D1	89	GLU	N-CA	218.43	5.61	1.46	1	1
D1	309	LEU	N-CA	213.64	5.52	1.46	1	1
B1	1055	GLN	CA-C	212.59	5.99	1.52	1	1
D1	786	THR	N-CA	211.93	5.48	1.46	1	1
B1	1094	SER	N-CA	209.53	5.44	1.46	1	1
B1	1009	PRO	N-CD	207.89	4.38	1.47	1	1
B1	1056	LYS	CA-C	207.42	5.88	1.52	1	1
B1	1133	LYS	CA-C	206.92	5.87	1.52	1	1
D1	482	PRO	N-CD	205.97	4.36	1.47	1	1
D1	481	GLY	CA-C	203.05	5.17	1.52	1	1
B1	1172	SER	CA-C	202.68	5.78	1.52	1	1
B1	508	PRO	N-CA	197.04	4.42	1.47	1	1
B1	1567	GLN	N-CA	193.76	5.14	1.46	1	1
D1	515	ALA	N-CA	191.25	5.09	1.46	1	1
B1	406	LYS	N-CA	190.29	5.07	1.46	1	1
D1	944	LEU	N-CA	188.32	5.04	1.46	1	1
A1	406	PRO	N-CD	185.97	4.08	1.47	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B1	288	LEU	N-CA	185.32	4.98	1.46	1	1
B1	341	PHE	N-CA	184.13	4.96	1.46	1	1
D1	900	ASP	N-CA	180.47	4.89	1.46	1	1
D1	535	GLU	N-CA	180.30	4.88	1.46	1	1
B1	1219	THR	N-CA	178.54	4.85	1.46	1	1
D1	892	PHE	N-CA	176.48	4.81	1.46	1	1
B1	75	ILE	CA-C	176.32	5.23	1.52	1	1
A1	360	ILE	CA-C	176.29	5.23	1.52	1	1
D1	457	SER	CA-C	173.88	5.18	1.52	1	1
B1	1540	LYS	N-CA	173.26	4.75	1.46	1	1
D1	933	ASP	CA-C	171.16	5.12	1.52	1	1
A1	747	PHE	CA-C	169.02	5.07	1.52	1	1
B1	379	ILE	N-CA	168.96	4.67	1.46	1	1
B1	319	PRO	N-CA	168.75	4.00	1.47	1	1
D1	892	PHE	CA-C	168.23	5.06	1.52	1	1
D1	704	VAL	N-CA	167.52	4.64	1.46	1	1
B1	1303	LEU	N-CA	167.07	4.63	1.46	1	1
A1	374	TYR	N-CA	166.78	4.63	1.46	1	1
D1	515	ALA	CA-C	164.38	4.98	1.52	1	1
D1	1299	LYS	CA-C	163.58	4.96	1.52	1	1
D1	921	SER	N-CA	163.56	4.57	1.46	1	1
B1	282	PHE	CA-C	161.86	4.92	1.52	1	1
A1	205	ASN	CA-C	161.19	4.91	1.52	1	1
B1	34	ALA	CA-C	161.18	4.91	1.52	1	1
B1	508	PRO	CA-C	160.63	4.90	1.52	1	1
B1	1241	GLY	N-CA	160.02	4.01	1.45	1	1
B1	203	LYS	N-CA	159.99	4.50	1.46	1	1
B1	551	ASN	N-CA	159.80	4.49	1.46	1	1
B1	408	PRO	N-CD	159.57	3.71	1.47	1	1
D1	339	GLU	CA-C	159.41	4.87	1.52	1	1
B1	1009	PRO	N-CA	156.25	3.81	1.47	1	1
D1	1092	LEU	CA-C	156.10	4.80	1.52	1	1
B1	1093	ASN	CA-C	155.92	4.80	1.52	1	1
B1	1400	PRO	N-CD	155.76	3.65	1.47	1	1
D1	1016	ASP	CA-C	155.45	4.79	1.52	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D1	1391	LYS	N-CA	155.01	4.40	1.46	1	1
D1	830	MET	CA-C	154.79	4.78	1.52	1	1
A1	835	ILE	CA-C	154.33	4.77	1.52	1	1
A1	747	PHE	N-CA	154.27	4.39	1.46	1	1
B1	793	LEU	N-CA	152.16	4.35	1.46	1	1
B1	1332	ILE	N-CA	151.77	4.34	1.46	1	1
B1	1241	GLY	CA-C	151.06	4.24	1.52	1	1
A1	753	ALA	N-CA	148.60	4.28	1.46	1	1
B1	40	ILE	N-CA	148.52	4.28	1.46	1	1
D1	961	PRO	N-CD	147.90	3.54	1.47	1	1
B1	1008	THR	CA-C	147.74	4.63	1.52	1	1
D1	787	ALA	N-CA	147.19	4.25	1.46	1	1
D1	705	LEU	N-CA	146.36	4.24	1.46	1	1

### Standard geometry: angle outliers ?

There are 3645 bond angle outliers in this entry (4.59% of 79339 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	79.67	15.36	103.00	1	1
B1	508	PRO	CA-N-CD	76.13	5.42	112.00	1	1
D1	482	PRO	CA-N-CD	73.96	8.46	112.00	1	1
B1	1566	TYR	C-N-CA	66.63	1.77	121.70	1	1
D1	481	GLY	CA-C-N	65.15	19.18	116.90	1	1
B1	407	ALA	CA-C-N	64.75	19.77	116.90	1	1
A1	405	ASP	CA-C-N	62.84	22.63	116.90	1	1
B1	1400	PRO	CA-N-CD	60.15	27.78	112.00	1	1
B1	90	ALA	C-N-CA	59.56	14.49	121.70	1	1
B1	405	SER	C-N-CA	59.02	15.46	121.70	1	1
D1	932	ILE	C-N-CA	58.59	16.24	121.70	1	1
B1	408	PRO	CA-N-CD	58.52	30.07	112.00	1	1
A1	746	PRO	C-N-CA	58.25	16.84	121.70	1	1
A1	515	LEU	N-CA-CB	58.02	11.86	110.50	1	1
B1	1099	PHE	C-N-CA	58.02	17.26	121.70	1	1
B1	165	ASN	C-N-CA	57.70	17.83	121.70	1	1
D1	961	PRO	CA-N-CD	57.49	31.52	112.00	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A1	359	ASN	C-N-CA	57.09	18.95	121.70	1	1
D1	514	ARG	C-N-CA	56.52	19.96	121.70	1	1
B1	1009	PRO	CA-N-CD	55.73	33.98	112.00	1	1
A1	373	ALA	C-N-CA	55.43	21.93	121.70	1	1
D1	729	PHE	C-N-CA	55.23	22.29	121.70	1	1
D1	829	LEU	C-N-CA	54.88	22.91	121.70	1	1
D1	339	GLU	CA-C-N	54.52	7.17	116.20	1	1
B1	34	ALA	O-C-N	54.12	36.40	123.00	1	1
A1	406	PRO	CA-N-CD	54.10	36.27	112.00	1	1
B1	478	ILE	C-N-CA	53.55	25.31	121.70	1	1
B1	319	PRO	CA-N-CD	53.44	37.18	112.00	1	1
D1	301	LYS	CA-C-N	52.97	10.26	116.20	1	1
B1	1217	ARG	C-N-CA	52.52	27.17	121.70	1	1
D1	536	HIS	C-CA-CB	52.11	11.09	110.10	1	1
D1	1298	ASP	C-N-CA	52.00	28.10	121.70	1	1
B1	1240	PHE	C-N-CA	51.82	28.43	121.70	1	1
D1	288	TYR	C-N-CA	51.48	29.03	121.70	1	1
B1	318	HIS	CA-C-N	51.36	39.86	116.90	1	1
B1	1218	SER	N-CA-CB	50.70	24.31	110.50	1	1
B1	76	ALA	N-CA-CB	50.41	34.78	110.40	1	1
B1	1132	GLU	C-N-CA	50.15	31.43	121.70	1	1
B1	379	ILE	CA-C-O	49.89	35.98	120.80	1	1
B1	1094	SER	CA-C-O	49.33	36.94	120.80	1	1
D1	1015	VAL	C-N-CA	49.00	33.50	121.70	1	1
B1	201	ASN	C-N-CA	48.45	34.50	121.70	1	1
D1	535	GLU	CA-C-N	48.22	19.77	116.20	1	1
B1	340	SER	C-N-CA	48.18	34.97	121.70	1	1
B1	448	ILE	C-N-CA	47.98	35.34	121.70	1	1
B1	358	VAL	CA-C-O	47.90	39.38	120.80	1	1
D1	900	ASP	CA-C-N	47.62	20.95	116.20	1	1
B1	377	THR	C-N-CA	47.50	36.20	121.70	1	1
D1	678	LYS	C-N-CA	47.47	36.26	121.70	1	1
B1	73	SER	N-CA-CB	47.42	29.88	110.50	1	1
B1	647	GLN	C-N-CA	47.41	36.37	121.70	1	1



Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D1	944	LEU	CA-C-N	47.21	21.77	116.20	1	1
B1	87	PRO	CA-N-CD	46.55	46.83	112.00	1	1
B1	618	LEU	C-N-CA	46.38	38.22	121.70	1	1
B1	122	ILE	C-N-CA	46.24	38.47	121.70	1	1
D1	1389	GLY	C-N-CA	45.75	39.36	121.70	1	1
B1	33	ASP	C-N-CA	45.74	39.36	121.70	1	1
B1	40	ILE	CA-C-O	45.71	43.09	120.80	1	1
D1	704	VAL	CA-C-N	45.67	24.86	116.20	1	1
B1	1171	ARG	C-N-CA	44.46	41.68	121.70	1	1
A1	406	PRO	N-CA-CB	43.90	151.29	103.00	1	1
B1	785	ILE	CA-C-O	43.60	46.68	120.80	1	1
A1	443	ILE	C-N-CA	43.18	43.97	121.70	1	1
B1	223	PHE	C-N-CA	42.91	44.47	121.70	1	1
B1	1489	PRO	CA-N-CD	42.55	52.44	112.00	1	1
B1	1056	LYS	CA-C-N	42.29	31.62	116.20	1	1
A1	205	ASN	CA-C-N	42.26	31.68	116.20	1	1
A1	746	PRO	N-CD-CG	41.64	40.74	103.20	1	1
B1	288	LEU	CA-C-N	41.63	32.95	116.20	1	1
B1	1593	HIS	CA-C-N	41.11	33.99	116.20	1	1
D1	836	TYR	CA-C-N	40.99	34.22	116.20	1	1
D1	1156	LEU	N-CA-CB	40.96	40.87	110.50	1	1
A1	834	ASN	CA-C-N	40.83	34.53	116.20	1	1
A1	753	ALA	CA-C-O	40.66	51.67	120.80	1	1
D1	744	GLY	CA-C-O	39.67	37.49	120.80	1	1
B1	1264	SER	C-N-CA	39.51	50.58	121.70	1	1
D1	339	GLU	C-N-CA	39.20	51.13	121.70	1	1
B1	288	LEU	N-CA-C	39.01	1.76	111.00	1	1
B1	1092	SER	C-N-CA	38.88	51.72	121.70	1	1
B1	12	GLN	CA-C-N	38.65	38.90	116.20	1	1
A1	455	GLU	CA-C-N	38.45	39.31	116.20	1	1
B1	174	VAL	CA-C-O	38.12	56.00	120.80	1	1
B1	1007	SER	CA-C-N	38.09	40.02	116.20	1	1
B1	1538	ASP	C-N-CA	37.99	53.32	121.70	1	1
B1	256	THR	CA-C-O	37.94	56.30	120.80	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
K1	626	ASN	CB-CG-OD1	37.86	45.08	120.80	1	1
B1	464	ALA	CA-C-N	37.69	40.82	116.20	1	1
A1	405	ASP	N-CA-C	37.64	5.60	111.00	1	1
B1	508	PRO	N-CA-C	37.39	18.62	112.10	1	1
B1	649	LYS	C-N-CA	37.26	54.63	121.70	1	1
B1	1383	GLN	CA-C-O	37.20	57.56	120.80	1	1
B1	649	LYS	N-CA-C	37.19	6.86	111.00	1	1
B1	34	ALA	N-CA-C	37.18	6.89	111.00	1	1
A1	747	PHE	N-CA-C	36.87	7.75	111.00	1	1
D1	1092	LEU	N-CA-C	36.83	7.87	111.00	1	1
B1	74	THR	N-CA-C	36.75	8.11	111.00	1	1
B1	1540	LYS	CA-C-N	36.69	42.82	116.20	1	1
B1	1119	ASN	CA-C-N	36.67	42.86	116.20	1	1
D1	786	THR	N-CA-C	36.61	8.48	111.00	1	1
B1	726	LYS	C-N-CA	36.35	56.26	121.70	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	7081	6290	527	264

There are 264 unique backbone outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A1	264	LYS	1
A1	268	ILE	1
A1	269	ASN	1

Chain	Res	Type	Models (Total)
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
A1	795	GLN	1
A1	834	ASN	1
B1	14	THR	1
B1	47	ASN	1
B1	73	SER	1
B1	74	THR	1
B1	87	PRO	1
B1	90	ALA	1
B1	122	ILE	1
B1	132	ASN	1
B1	136	ASN	1
B1	175	SER	1
B1	203	LYS	1
B1	281	GLN	1
B1	319	PRO	1

Chain	Res	Type	Models (Total)
B1	321	ILE	1
B1	323	TYR	1
B1	324	SER	1
B1	341	PHE	1
B1	358	VAL	1
B1	372	ASP	1
B1	373	PRO	1
B1	377	THR	1
B1	379	ILE	1
B1	392	ILE	1
B1	405	SER	1
B1	423	LYS	1
B1	425	LEU	1
B1	432	LEU	1
B1	440	ILE	1
B1	441	PRO	1
B1	448	ILE	1
B1	464	ALA	1
B1	466	THR	1
B1	494	PRO	1
B1	496	LEU	1
B1	507	PRO	1
B1	523	SER	1
B1	524	THR	1
B1	573	LEU	1
B1	575	SER	1
B1	585	ASP	1
B1	647	GLN	1
B1	648	ARG	1
B1	649	LYS	1
B1	650	ASP	1
B1	667	ASN	1
B1	680	ASP	1
B1	688	THR	1
B1	702	THR	1

Chain	Res	Type	Models (Total)
B1	727	ASN	1
B1	815	LEU	1
B1	834	ILE	1
B1	836	GLY	1
B1	864	SER	1
B1	868	LEU	1
B1	871	SER	1
B1	893	TYR	1
B1	908	VAL	1
B1	909	GLU	1
B1	915	ASP	1
B1	925	GLU	1
B1	935	VAL	1
B1	942	PRO	1
B1	964	GLN	1
B1	973	THR	1
B1	990	LYS	1
B1	1009	PRO	1
B1	1010	GLU	1
B1	1036	ASP	1
B1	1055	GLN	1
B1	1057	LYS	1
B1	1058	GLU	1
B1	1062	ARG	1
B1	1093	ASN	1
B1	1098	ASN	1
B1	1099	PHE	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	6268	5386	483	399

*There are 399 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.*

Chain	Res	Type	Models (Total)
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
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
B1	41	ARG	1
B1	74	THR	1
B1	87	PRO	1
B1	91	GLN	1
B1	102	PHE	1
B1	120	PRO	1

Chain	Res	Type	Models (Total)
B1	122	ILE	1
B1	135	PHE	1
B1	142	ILE	1
B1	160	LEU	1
B1	175	SER	1
B1	195	LEU	1
B1	204	VAL	1
B1	221	VAL	1
B1	256	THR	1
B1	281	GLN	1
B1	289	TYR	1
B1	319	PRO	1
B1	321	ILE	1
B1	323	TYR	1
B1	340	SER	1
B1	341	PHE	1
B1	355	SER	1
B1	357	ASP	1
B1	358	VAL	1
B1	372	ASP	1
B1	378	VAL	1
B1	380	THR	1
B1	391	PRO	1
B1	408	PRO	1
B1	424	LYS	1
B1	425	LEU	1
B1	432	LEU	1
B1	433	PRO	1
B1	440	ILE	1
B1	449	ASP	1
B1	450	THR	1
B1	451	GLU	1
B1	466	THR	1
B1	469	SER	1
B1	470	LEU	1

Chain	Res	Type	Models (Total)
B1	472	ASP	1
B1	494	PRO	1
B1	501	SER	1
B1	507	PRO	1
B1	508	PRO	1
B1	515	ASN	1
B1	516	CYS	1
B1	529	LEU	1
B1	569	LEU	1
B1	572	LEU	1
B1	573	LEU	1
B1	584	ASP	1
B1	608	ILE	1
B1	648	ARG	1
B1	662	THR	1
B1	666	PRO	1
B1	667	ASN	1
B1	678	LYS	1
B1	684	LYS	1
B1	691	SER	1
B1	725	LEU	1
B1	727	ASN	1
B1	732	LYS	1
B1	741	LYS	1
B1	808	THR	1
B1	811	ASP	1
B1	812	SER	1
B1	814	ASP	1
B1	819	THR	1
B1	833	LYS	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.*