

Integrative Structure Validation Report

March 27, 2025 - 10:01 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	9A0J
PDB-Dev ID	PDBDEV_00000055
Structure Title	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM
Structure Authors	Farrell DP; Anishchenko I; Shakeel S; Lauko A; Passmore LA; Baker D; DiMaio F
Deposited on	2020-08-11

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

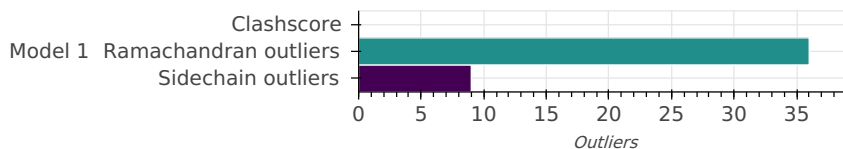
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the  symbol.

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

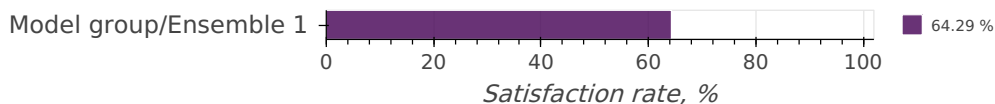
Overall quality

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



Crosslink satisfaction



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 model(s). A total of 93 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	fancB	B	867	1-235, 1-370, 231-365, 378-434, 441-660, 441-780, 466-626, 651-770	435-440	89.16 / 99.22	Atomic
				b					
		2	fancC	C	595	1-175, 1-335, 176-335, 331-570	-	95.80 / 100.00	Atomic
		3	fancE	E	520	1-150, 261-520, 266-520	151-170	82.69 / 95.35	Atomic
		4	fancF	F	350	140-341	342-350	60.29 / 95.73	Atomic
		5	fancG	G	648	1-175, 1-320, 44-645, 181-320, 201-435, 204-315, 321-648	-	100.00 / 100.00	Atomic
				g					
		6	fancL	L	373	1-100, 2-91, 101-205, 101-300, 104-373, 191-300, 301-373	-	100.00 / 100.00	Atomic
				I					
		7	faap100	P	888	1-200, 1-300, 28-442, 186-480, 301-480, 453-507, 491-615, 491-820, 510-609, 711-820, 714-803, 804-888	-	100.00 / 100.00	Atomic
				p					

Datasets used for modeling

There are 93 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	De Novo model	Zenodo	10.5281/zenodo.3979898
2	De Novo model	Zenodo	10.5281/zenodo.3979898
3	De Novo model	Zenodo	10.5281/zenodo.3979898
4	De Novo model	Zenodo	10.5281/zenodo.3979898
5	De Novo model	Zenodo	10.5281/zenodo.3979898
6	De Novo model	Zenodo	10.5281/zenodo.3979898
7	De Novo model	Zenodo	10.5281/zenodo.3979898
8	De Novo model	Zenodo	10.5281/zenodo.3979898
9	De Novo model	Zenodo	10.5281/zenodo.3979898
10	De Novo model	Zenodo	10.5281/zenodo.3979898
11	De Novo model	Zenodo	10.5281/zenodo.3979898
12	De Novo model	Zenodo	10.5281/zenodo.3979898

ID	Dataset type	Database name	Data access code
13	De Novo model	Zenodo	10.5281/zenodo.3979898
14	De Novo model	Zenodo	10.5281/zenodo.3979898
15	De Novo model	Zenodo	10.5281/zenodo.3979898
16	De Novo model	Zenodo	10.5281/zenodo.3979898
17	De Novo model	Zenodo	10.5281/zenodo.3979898
18	De Novo model	Zenodo	10.5281/zenodo.3979898
19	De Novo model	Zenodo	10.5281/zenodo.3979898
20	De Novo model	Zenodo	10.5281/zenodo.3979898
21	De Novo model	Zenodo	10.5281/zenodo.3979898
22	De Novo model	Zenodo	10.5281/zenodo.3979898
23	De Novo model	Zenodo	10.5281/zenodo.3979898
24	De Novo model	Zenodo	10.5281/zenodo.3979898
25	De Novo model	Zenodo	10.5281/zenodo.3979898
26	De Novo model	Zenodo	10.5281/zenodo.3979898
27	De Novo model	Zenodo	10.5281/zenodo.3979898
28	De Novo model	Zenodo	10.5281/zenodo.3979898
29	De Novo model	Zenodo	10.5281/zenodo.3979898
30	De Novo model	Zenodo	10.5281/zenodo.3979898
31	De Novo model	Zenodo	10.5281/zenodo.3979898
32	De Novo model	Zenodo	10.5281/zenodo.3979898
33	De Novo model	Zenodo	10.5281/zenodo.3979898
34	De Novo model	Zenodo	10.5281/zenodo.3979898
35	De Novo model	Zenodo	10.5281/zenodo.3979898
36	3DEM volume	EMDB	EMD-10291
37	3DEM volume	EMDB	EMD-10292
38	3DEM volume	EMDB	EMD-10293
39	Crosslinking-MS data	PRIDE	PXD014282
40	Comparative model	Zenodo	10.5281/zenodo.3979898
41	Comparative model	Zenodo	10.5281/zenodo.3979898
42	Comparative model	Zenodo	10.5281/zenodo.3979898
43	Comparative model	Zenodo	10.5281/zenodo.3979898
44	Comparative model	Zenodo	10.5281/zenodo.3979898
45	Comparative model	Zenodo	10.5281/zenodo.3979898
46	Comparative model	Zenodo	10.5281/zenodo.3979898
47	Comparative model	Zenodo	10.5281/zenodo.3979898
48	Comparative model	Zenodo	10.5281/zenodo.3979898
49	Comparative model	Zenodo	10.5281/zenodo.3979898
50	Comparative model	Zenodo	10.5281/zenodo.3979898
51	Experimental model	PDB	4ccg
52	Experimental model	PDB	4zdt
53	Experimental model	PDB	5o6c
54	Experimental model	PDB	2d8s
55	Experimental model	PDB	1vyx
56	Experimental model	PDB	3k1l

ID	Dataset type	Database name	Data access code
57	Experimental model	PDB	2iqc
58	Experimental model	PDB	1r5m
59	Experimental model	PDB	5m23
60	Experimental model	PDB	6chg
61	Experimental model	PDB	6f9n
62	Experimental model	PDB	2pbi
63	Experimental model	PDB	5m89
64	Experimental model	PDB	4ggc
65	Experimental model	PDB	6eoj
66	Experimental model	PDB	5kdo
67	Experimental model	PDB	5oql
68	Experimental model	PDB	5opt
69	Experimental model	PDB	3odt
70	Experimental model	PDB	5a31
71	Experimental model	PDB	5xyi
72	Experimental model	PDB	2ilr
73	Experimental model	PDB	5orq
74	Experimental model	PDB	1fch
75	Experimental model	PDB	3hym
76	Experimental model	PDB	3fp2
77	Experimental model	PDB	2gw1
78	Experimental model	PDB	6c9m
79	Experimental model	PDB	6eou
80	Experimental model	PDB	3ieg
81	Experimental model	PDB	4rg9
82	Experimental model	PDB	2xpi
83	Experimental model	PDB	3cvp
84	Experimental model	PDB	5i9f
85	Experimental model	PDB	5aio
86	Experimental model	PDB	5dse
87	Experimental model	PDB	4g1t
88	Experimental model	PDB	4zlh
89	Experimental model	PDB	2y4t
90	Experimental model	PDB	3u4t
91	Experimental model	PDB	4pjr
92	Experimental model	PDB	4buj
93	3DEM volume	Zenodo	10.5281/zenodo.3979898

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
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Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Production sampling	Monte Carlo	None	None	False	False
2	1	Rosetta Hybridize	Rosetta Hybridize	None	None	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Rosetta	Rosetta version unknown:ff8ee24ee5f65423d5064cba818ede41d012fa87 2020-08-10 10:39:53 -0700 from git@github.com:RosettaCommons/main.git	RosettaCM/hybridize and unpublished 'complex assembly'	https://www.rosettacommons.org/
2	trRosetta	1.0.0	trRosetta	https://github.com/gjoni/trRosetta
3	HHpred	website	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred

Data quality ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

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 150 bond length outliers in this entry (0.37% of 40718 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	333	PHE	CB-CG	9.41	1.29	1.50	1	1
B	286	LEU	CG-CD2	8.44	1.24	1.52	1	1
G	480	LEU	CB-CG	8.38	1.70	1.53	1	1
p	278	HIS	CE1-NE2	7.44	1.25	1.32	1	1
b	333	PHE	CB-CG	7.42	1.33	1.50	1	1
B	287	ILE	CB-CG1	7.23	1.39	1.53	1	1
B	435	HIS	CB-CG	7.17	1.40	1.50	1	1
p	346	ARG	NE-CZ	7.10	1.40	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	346	ARG	NE-CZ	6.93	1.40	1.33	1	1
g	648	ARG	NE-CZ	6.74	1.40	1.33	1	1
P	849	HIS	CB-CG	6.69	1.40	1.50	1	1
G	648	ARG	NE-CZ	6.64	1.40	1.33	1	1
P	636	LEU	CB-CG	6.61	1.66	1.53	1	1
g	472	LEU	CG-CD2	6.55	1.30	1.52	1	1
E	92	HIS	CB-CG	6.47	1.41	1.50	1	1
g	540	ARG	CB-CG	6.39	1.33	1.52	1	1
b	435	HIS	CB-CG	6.30	1.41	1.50	1	1
B	528	LEU	CB-CG	6.23	1.65	1.53	1	1
b	606	HIS	CB-CG	6.15	1.41	1.50	1	1
b	47	ARG	CD-NE	6.05	1.37	1.46	1	1
G	77	ASN	CB-CG	5.90	1.37	1.52	1	1
b	528	LEU	CB-CG	5.90	1.65	1.53	1	1
p	658	LEU	CB-CG	5.89	1.65	1.53	1	1
P	312	PHE	CB-CG	5.87	1.64	1.50	1	1
P	79	LEU	CB-CG	5.84	1.65	1.53	1	1
B	666	PHE	CB-CG	5.78	1.37	1.50	1	1
P	658	LEU	CB-CG	5.73	1.64	1.53	1	1
C	347	HIS	CB-CG	5.70	1.42	1.50	1	1
B	779	PHE	CG-CD1	5.68	1.50	1.38	1	1
b	261	GLN	CA-C	5.66	1.64	1.52	1	1
b	340	GLN	CG-CD	5.66	1.37	1.52	1	1
B	738	HIS	CB-CG	5.66	1.42	1.50	1	1
P	888	LEU	CB-CG	5.62	1.64	1.53	1	1
E	129	ARG	CG-CD	5.58	1.35	1.52	1	1
P	82	HIS	CB-CG	5.51	1.57	1.50	1	1
p	350	LEU	CB-CG	5.48	1.64	1.53	1	1
g	573	TYR	CB-CG	5.45	1.39	1.51	1	1
G	509	PHE	CB-CG	5.43	1.38	1.50	1	1
P	887	LEU	CB-CG	5.39	1.42	1.53	1	1
p	312	PHE	CG-CD1	5.39	1.50	1.38	1	1
P	312	PHE	CG-CD1	5.39	1.50	1.38	1	1
C	343	TYR	CB-CG	5.38	1.39	1.51	1	1
P	312	PHE	CG-CD2	5.35	1.50	1.38	1	1
B	388	LEU	CB-CG	5.34	1.64	1.53	1	1
P	611	LEU	CB-CG	5.34	1.42	1.53	1	1
p	430	LEU	CB-CG	5.30	1.64	1.53	1	1
p	312	PHE	CG-CD2	5.28	1.49	1.38	1	1
L	15	LEU	CG-CD1	5.27	1.35	1.52	1	1
b	343	LEU	CB-CG	5.24	1.43	1.53	1	1
P	609	TYR	CB-CG	5.23	1.40	1.51	1	1
b	591	HIS	CB-CG	5.17	1.42	1.50	1	1
I	38	ARG	CG-CD	5.16	1.37	1.52	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
G	190	ARG	CD-NE	5.16	1.39	1.46	1	1
P	95	ARG	CD-NE	5.16	1.53	1.46	1	1
g	648	ARG	CD-NE	5.08	1.53	1.46	1	1
p	173	PHE	CG-CD1	5.04	1.49	1.38	1	1
B	261	GLN	CA-C	5.04	1.63	1.52	1	1
p	278	HIS	ND1-CE1	5.02	1.27	1.32	1	1
b	14	HIS	CB-CG	5.02	1.43	1.50	1	1
p	378	LEU	CB-CG	4.98	1.63	1.53	1	1
B	260	THR	CB-OG1	4.98	1.35	1.43	1	1
C	432	TYR	CG-CD2	4.96	1.49	1.39	1	1
p	173	PHE	CG-CD2	4.95	1.49	1.38	1	1
p	115	PRO	N-CD	4.93	1.40	1.47	1	1
C	432	TYR	CG-CD1	4.93	1.49	1.39	1	1
G	345	LEU	CB-CG	4.90	1.43	1.53	1	1
P	430	LEU	CB-CG	4.90	1.63	1.53	1	1
P	173	PHE	CG-CD2	4.87	1.49	1.38	1	1
L	33	ARG	CG-CD	4.86	1.37	1.52	1	1
L	74	HIS	CB-CG	4.86	1.43	1.50	1	1
g	472	LEU	CB-CG	4.85	1.43	1.53	1	1
b	590	PHE	CB-CG	4.82	1.39	1.50	1	1
B	779	PHE	CG-CD2	4.79	1.48	1.38	1	1
G	591	TRP	NE1-CE2	4.79	1.32	1.37	1	1
B	152	TYR	CB-CG	4.77	1.41	1.51	1	1
P	346	ARG	CD-NE	4.76	1.52	1.46	1	1
G	648	ARG	CD-NE	4.74	1.52	1.46	1	1
P	572	PHE	CB-CG	4.73	1.39	1.50	1	1
L	67	HIS	CB-CG	4.73	1.43	1.50	1	1
b	459	SER	C-N	4.72	1.40	1.33	1	1
b	330	VAL	CB-CG1	4.71	1.37	1.52	1	1
G	479	TYR	CE2-CZ	4.70	1.27	1.38	1	1
B	606	HIS	CB-CG	4.68	1.43	1.50	1	1
P	173	PHE	CG-CD1	4.67	1.48	1.38	1	1
P	510	PRO	N-CA	4.65	1.40	1.47	1	1
g	462	LEU	CB-CG	4.63	1.62	1.53	1	1
P	77	TYR	CB-CG	4.63	1.41	1.51	1	1
L	82	PHE	CB-CG	4.62	1.40	1.50	1	1
g	540	ARG	CG-CD	4.59	1.38	1.52	1	1
p	491	LEU	CB-CG	4.58	1.44	1.53	1	1
B	231	HIS	CB-CG	4.58	1.43	1.50	1	1
b	173	MET	CG-SD	4.57	1.69	1.80	1	1
L	33	ARG	CD-NE	4.56	1.39	1.46	1	1
b	779	PHE	CG-CD2	4.56	1.48	1.38	1	1
B	32	ARG	NE-CZ	4.52	1.38	1.33	1	1
p	346	ARG	CD-NE	4.52	1.52	1.46	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	524	LEU	CB-CG	4.50	1.44	1.53	1	1
I	36	HIS	CB-CG	4.49	1.43	1.50	1	1
E	34	LEU	CG-CD2	4.49	1.37	1.52	1	1
P	378	LEU	CB-CG	4.47	1.62	1.53	1	1

Standard geometry: angle outliers ?

There are 236 bond angle outliers in this entry (0.43% of 55184 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	303	PHE	CA-CB-CG	12.80	101.00	113.80	1	1
b	459	SER	C-N-CA	10.25	140.14	121.70	1	1
b	280	PRO	N-CA-CB	9.34	92.73	103.00	1	1
B	463	SER	C-N-CA	9.22	138.30	121.70	1	1
L	179	ASP	CA-CB-CG	9.20	121.80	112.60	1	1
b	626	LEU	C-N-CA	9.04	137.98	121.70	1	1
B	280	PRO	N-CA-CB	8.45	93.71	103.00	1	1
p	27	ARG	C-N-CA	8.06	136.20	121.70	1	1
B	626	LEU	C-N-CA	7.96	136.02	121.70	1	1
G	499	PHE	CA-CB-CG	7.88	121.68	113.80	1	1
p	312	PHE	CA-CB-CG	7.88	121.68	113.80	1	1
b	433	ARG	C-N-CA	7.75	135.66	121.70	1	1
P	27	ARG	C-N-CA	7.55	135.28	121.70	1	1
P	122	ILE	C-N-CA	7.51	135.22	121.70	1	1
B	261	GLN	N-CA-C	7.40	131.72	111.00	1	1
p	122	ILE	C-N-CA	7.25	134.75	121.70	1	1
b	261	GLN	N-CA-C	7.12	130.93	111.00	1	1
b	341	LEU	C-N-CA	7.09	134.46	121.70	1	1
P	570	PHE	CA-CB-CG	7.03	120.83	113.80	1	1
p	476	PHE	CA-CB-CG	6.98	106.82	113.80	1	1
B	71	HIS	CA-CB-CG	6.92	106.88	113.80	1	1
G	64	ALA	C-N-CA	6.60	133.58	121.70	1	1
p	123	PHE	N-CA-C	6.55	129.35	111.00	1	1
P	312	PHE	CA-CB-CG	6.54	120.34	113.80	1	1
B	299	PHE	CA-CB-CG	6.50	120.30	113.80	1	1
b	672	ASP	CA-CB-CG	6.49	119.09	112.60	1	1
b	501	ASP	CA-CB-CG	6.49	119.09	112.60	1	1
p	610	SER	O-C-N	6.43	112.71	123.00	1	1
B	341	LEU	C-N-CA	6.34	133.11	121.70	1	1
L	309	TYR	N-CA-C	6.29	93.37	111.00	1	1
B	299	PHE	C-CA-CB	6.23	98.26	110.10	1	1
P	123	PHE	N-CA-C	6.19	128.34	111.00	1	1
B	277	CYS	C-N-CA	6.18	132.83	121.70	1	1
C	344	PHE	CA-CB-CG	6.16	119.96	113.80	1	1
E	137	PRO	N-CA-C	6.10	127.34	112.10	1	1
G	36	ALA	C-N-CA	6.08	132.64	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
b	458	VAL	C-N-CA	6.04	132.58	121.70	1	1
p	465	SER	C-N-CA	5.97	132.44	121.70	1	1
b	262	LYS	C-N-CA	5.93	132.37	121.70	1	1
P	115	PRO	C-N-CA	5.89	132.30	121.70	1	1
P	161	ASP	CA-CB-CG	5.86	118.46	112.60	1	1
b	281	TYR	N-CA-CB	5.85	120.45	110.50	1	1
b	230	PRO	C-N-CA	5.85	132.22	121.70	1	1
P	285	PHE	CA-CB-CG	5.84	119.64	113.80	1	1
P	114	PHE	CA-CB-CG	5.82	119.62	113.80	1	1
p	43	PHE	CA-CB-CG	5.81	119.61	113.80	1	1
b	600	HIS	CA-CB-CG	5.78	108.02	113.80	1	1
G	544	PHE	CA-CB-CG	5.76	119.56	113.80	1	1
C	213	ALA	C-N-CA	5.72	131.99	121.70	1	1
C	303	ASN	CA-CB-CG	5.72	106.88	112.60	1	1
p	285	PHE	CA-CB-CG	5.62	119.42	113.80	1	1
B	281	TYR	N-CA-CB	5.59	120.01	110.50	1	1
B	345	PHE	CA-CB-CG	5.57	119.37	113.80	1	1
E	138	PRO	C-CA-CB	5.57	120.68	110.10	1	1
p	887	LEU	C-N-CA	5.53	131.66	121.70	1	1
B	231	HIS	CA-CB-CG	5.53	108.27	113.80	1	1
L	200	ASP	CA-CB-CG	5.50	118.10	112.60	1	1
G	311	TYR	CA-CB-CG	5.50	104.00	113.90	1	1
g	499	PHE	CA-CB-CG	5.46	119.26	113.80	1	1
b	435	HIS	CA-CB-CG	5.46	108.34	113.80	1	1
p	127	SER	C-N-CA	5.44	131.49	121.70	1	1
B	287	ILE	C-CA-CB	5.43	100.73	111.60	1	1
E	137	PRO	CA-C-N	5.40	124.99	116.90	1	1
b	626	LEU	C-CA-CB	5.39	120.35	110.10	1	1
P	887	LEU	C-CA-CB	5.32	99.99	110.10	1	1
P	163	PRO	CA-C-N	5.27	124.81	116.90	1	1
b	362	PHE	CA-CB-CG	5.27	119.07	113.80	1	1
b	263	ASN	N-CA-C	5.26	125.73	111.00	1	1
B	340	GLN	C-N-CA	5.25	131.14	121.70	1	1
p	653	ASP	C-N-CA	5.18	131.03	121.70	1	1
L	140	ASP	CA-CB-CG	5.18	117.78	112.60	1	1
b	338	THR	C-N-CA	5.18	131.02	121.70	1	1
G	138	HIS	CA-CB-CG	5.18	118.98	113.80	1	1
p	610	SER	CA-C-O	5.12	112.09	120.80	1	1
B	626	LEU	C-CA-CB	5.11	119.81	110.10	1	1
p	606	ALA	C-N-CA	5.10	112.51	121.70	1	1
b	626	LEU	CA-C-N	5.09	126.38	116.20	1	1
l	45	SER	C-N-CA	5.09	130.85	121.70	1	1
p	120	ALA	C-N-CA	5.08	130.84	121.70	1	1
B	509	ASP	CA-CB-CG	5.08	117.68	112.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
B	263	ASN	N-CA-C	5.05	125.15	111.00	1	1
G	647	SER	C-N-CA	5.04	130.77	121.70	1	1
L	301	PHE	CA-CB-CG	5.03	118.83	113.80	1	1
b	433	ARG	CA-C-N	5.02	126.24	116.20	1	1
B	262	LYS	C-N-CA	5.01	130.72	121.70	1	1
B	463	SER	CA-C-N	5.01	126.22	116.20	1	1
B	277	CYS	N-CA-C	5.00	97.00	111.00	1	1
p	610	SER	C-CA-CB	4.98	119.57	110.10	1	1
B	649	GLY	N-CA-C	4.98	98.86	113.30	1	1
G	481	HIS	CA-CB-CG	4.96	108.84	113.80	1	1
b	38	ASP	CA-CB-CG	4.96	117.56	112.60	1	1
b	266	ILE	C-CA-CB	4.94	101.72	111.60	1	1
G	33	ARG	C-N-CA	4.91	112.86	121.70	1	1
B	695	HIS	CA-CB-CG	4.91	108.89	113.80	1	1
P	43	PHE	CA-CB-CG	4.91	118.71	113.80	1	1
B	279	LEU	N-CA-C	4.90	124.71	111.00	1	1
B	365	ILE	C-N-CA	4.90	130.51	121.70	1	1
B	626	LEU	CA-C-N	4.89	125.98	116.20	1	1
P	166	ARG	N-CA-C	4.86	97.39	111.00	1	1
b	80	ASP	N-CA-C	4.86	97.40	111.00	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	5079	4875	168	36

There are 36 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	39	ARG	1
B	68	ARG	1
B	202	THR	1
B	285	CYS	1
B	326	LYS	1
B	337	GLY	1
B	464	LEU	1
B	624	ILE	1
B	692	LYS	1
E	10	ALA	1

Chain	Res	Type	Models (Total)
G	65	LEU	1
G	299	GLU	1
G	338	THR	1
P	28	VAL	1
P	114	PHE	1
P	162	SER	1
P	621	SER	1
P	785	MET	1
b	68	ARG	1
b	202	THR	1
b	340	GLN	1
b	459	SER	1
b	591	HIS	1
b	624	ILE	1
b	651	MET	1
b	666	PHE	1
b	755	SER	1
g	328	PHE	1
g	338	THR	1
l	6	SER	1
p	114	PHE	1
p	116	VAL	1
p	425	SER	1
p	555	SER	1
p	610	SER	1
p	618	GLY	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	4426	4367	50	9

There are 9 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	427	ILE	1
G	33	ARG	1
P	100	THR	1
P	240	CYS	1
b	427	ILE	1
b	441	LYS	1
b	669	MET	1
g	213	THR	1
p	150	MET	1

Fit of model to data used for modeling

Fit of model(s) to crosslinking-MS data

Restraint types

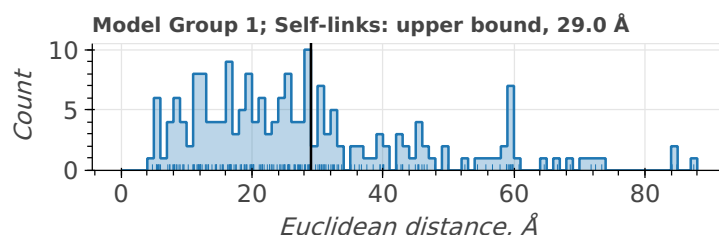
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". **Restraint group** represents a set of crosslinking restraints applied collectively in the modeling.

There are 445 crosslinking restraints combined in 445 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	SER	CA	upper bound	29.0	103
BS3	LYS	CA	LYS	CA	upper bound	29.0	293
BS3	LYS	CA	THR	CA	upper bound	29.0	22
BS3	SER	CA	SER	CA	upper bound	29.0	12
BS3	LYS	CA	TYR	CA	upper bound	29.0	8
BS3	SER	CA	TYR	CA	upper bound	29.0	1
BS3	SER	CA	THR	CA	upper bound	29.0	3
BS3	LYS	CA	MET	CA	upper bound	29.0	1
BS3	TYR	CA	TYR	CA	upper bound	29.0	1
BS3	THR	CA	TYR	CA	upper bound	29.0	1

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



Satisfaction of restraints

Satisfaction of restraints is calculated on a **restraint group** (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=445)
1	1	1	1/1	All	64.29	35.71	196
				Self-links/ Intramolecular	64.29	35.71	196

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



3DEM volume

Validation for this section is under development.

Fit of model to data used for validation ①

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 Trewella, 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.