Integrative Structure Validation Report

February 18, 2025 - 08:32 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

PDB ID	9A1K
PDB-Dev ID	PDBDEV_00000092
Structure Title	Integrative structure of the COX-AIFM1 complex
Structure Authors	Johannes F. Hevler; Albert J.R. Heck
Deposited on	2021-08-13

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

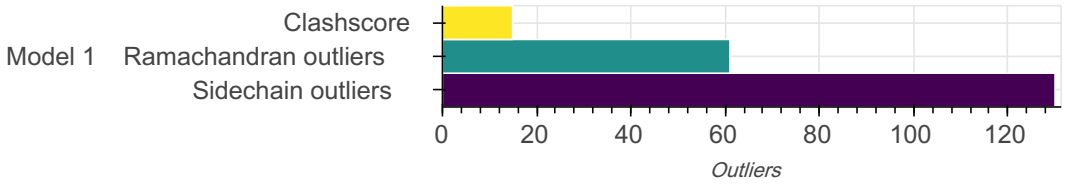
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

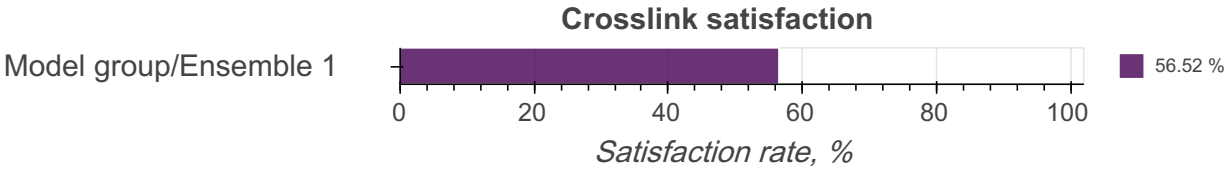
List of references used to build this report is available here.

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 32 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	Cytochrome c oxidase polypeptide I	A	513	-	1-513	100.00 / 0.00	Atomic
		2	Cytochrome c oxidase polypeptide II	B	226	-	1-226	100.00 / 0.00	Atomic
		3	Cytochrome c oxidase polypeptide III	C	259	-	1-259	100.00 / 0.00	Atomic
		4	Cytochrome c oxidase subunit IV isoform 1	D	144	-	1-144	100.00 / 0.00	Atomic
		5	Cytochrome c oxidase polypeptide Va	E	109	-	1-109	100.00 / 0.00	Atomic
		6	Cytochrome c oxidase polypeptide Vb	F	98	-	1-98	100.00 / 0.00	Atomic

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		7	Cytochrome c oxidase polypeptide VIa-heart	G	83	-	1-83	100.00 / 0.00	Atomic
		8	Cytochrome c oxidase polypeptide VIb	H	86	-	1-86	100.00 / 0.00	Atomic
		9	Cytochrome c oxidase polypeptide VIc	I	72	-	1-72	100.00 / 0.00	Atomic
		10	Cytochrome c oxidase polypeptide VIIa-heart	J	58	-	1-58	100.00 / 0.00	Atomic
		11	Cytochrome c oxidase polypeptide VIIb	K	49	-	1-49	100.00 / 0.00	Atomic
		12	Cytochrome c oxidase polypeptide VIIc	L	46	-	1-46	100.00 / 0.00	Atomic
		13	Cytochrome c oxidase polypeptide VIII-heart	M	43	-	1-43	100.00 / 0.00	Atomic
		14	Cytochrome c oxidase subunit NDUFA4	N	80	-	1-80	100.00 / 0.00	Atomic
		15	Apoptosis inducing factor 1	O P	559	-	1-559	100.00 / 0.00	Atomic

Datasets used for modeling

There are 32 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD025102
2	Comparative model	Not available	Not available
3	Comparative model	Not available	Not available
4	Comparative model	Not available	Not available
5	Comparative model	Not available	Not available
6	De Novo model	Not available	Not available
7	Experimental model	PDB	1V54
8	Experimental model	PDB	1OCC
9	Experimental model	PDB	2Y69
10	Experimental model	PDB	3J9M

ID	Dataset type	Database name	Data access code
11	Experimental model	PDB	4G23
12	Experimental model	PDB	4G26
13	Experimental model	PDB	4LEU
14	Experimental model	PDB	5DIZ
15	Experimental model	PDB	5FT9
16	Experimental model	PDB	5IWB
17	Experimental model	PDB	5ORM
18	Experimental model	PDB	5Z62
19	Experimental model	PDB	6F5D
20	Experimental model	PDB	6GAW
21	Experimental model	PDB	6GAZ
22	Experimental model	PDB	6HU9
23	Experimental model	PDB	6LVR
24	Experimental model	PDB	2LQT
25	Experimental model	PDB	5JJ4
26	Experimental model	PDB	5Z62
27	Experimental model	PDB	6NL3
28	Experimental model	PDB	6PCE
29	Experimental model	PDB	6PCF
30	Experimental model	PDB	6TDV
31	Experimental model	PDB	6X89
32	Experimental model	PDB	4BUR

Methodology and software

This entry is a result of 3 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	None	None	None	False	False

There are 5 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
2	trRossetta	Not available	model building	https://yanglab.nankai.edu.cn/trRosetta/

ID	Software name	Software version	Software classification	Software location
1	Robetta	Not available	model building	http://robetta.bakerlab.org
3	DisVis	Not available	prediction of protein-protein interface residues and restraint validation	https://wenmr.science.uu.nl/disvis/
4	Haddock	2.40	Structural docking of protein complexes	https://wenmr.science.uu.nl/haddock2.4/
5	Naccess	Not available	prediction of solvent accessible residues	http://www.bioinf.manchester.ac.uk/naccess/

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.

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 62 bond length outliers in this entry (0.27% of 23079 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	75	PRO	C-N	16.61	1.56	1.33	1	1
P	75	PRO	CA-C	14.67	1.83	1.52	1	1
P	11	ASP	C-N	9.07	1.46	1.33	1	1
P	10	ILE	CA-C	8.92	1.71	1.52	1	1
P	75	PRO	N-CA	7.80	1.58	1.47	1	1
P	76	SER	N-CA	7.75	1.61	1.46	1	1
P	41	TYR	C-N	7.20	1.43	1.33	1	1
P	52	PRO	C-N	6.98	1.43	1.33	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	77	HIS	C-N	6.96	1.43	1.33	1	1
P	30	ALA	N-CA	6.52	1.33	1.46	1	1
P	9	LYS	C-N	6.43	1.24	1.33	1	1
P	30	ALA	CA-CB	5.95	1.72	1.52	1	1
P	7	GLY	CA-C	5.88	1.41	1.52	1	1
P	47	GLY	N-CA	5.81	1.36	1.45	1	1
P	13	SER	C-N	5.67	1.41	1.33	1	1
P	76	SER	C-N	5.63	1.41	1.33	1	1
P	10	ILE	N-CA	5.61	1.35	1.46	1	1
P	4	GLY	CA-C	5.59	1.42	1.52	1	1
P	34	ILE	CA-C	5.49	1.41	1.52	1	1
P	78	VAL	CA-C	5.39	1.64	1.52	1	1
P	5	PRO	N-CD	5.33	1.55	1.47	1	1
P	38	LYS	C-N	5.28	1.40	1.33	1	1
P	54	GLU	C-N	5.13	1.40	1.33	1	1
P	55	LYS	C-N	5.07	1.40	1.33	1	1
P	44	ARG	CA-C	5.05	1.42	1.52	1	1
P	62	SER	C-N	5.05	1.26	1.33	1	1
P	35	LYS	C-N	4.99	1.40	1.33	1	1
P	39	LYS	C-N	4.98	1.40	1.33	1	1
P	76	SER	CA-C	4.97	1.63	1.52	1	1
P	13	SER	CA-C	4.89	1.42	1.52	1	1
P	25	GLY	N-CA	4.87	1.37	1.45	1	1
P	12	ASN	C-N	4.83	1.40	1.33	1	1
P	31	TYR	C-N	4.83	1.40	1.33	1	1
P	50	LEU	C-N	4.82	1.26	1.33	1	1
O	294	LEU	CB-CG	4.73	1.44	1.53	1	1
P	57	LYS	C-N	4.72	1.40	1.33	1	1
P	294	LEU	CB-CG	4.69	1.44	1.53	1	1
P	29	TYR	C-N	4.67	1.39	1.33	1	1
P	45	ILE	C-N	4.67	1.39	1.33	1	1
P	56	GLN	C-N	4.65	1.39	1.33	1	1
P	3	SER	C-N	4.63	1.39	1.33	1	1
P	30	ALA	CA-C	4.62	1.43	1.52	1	1
P	31	TYR	CA-C	4.57	1.43	1.52	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
O	74	ILE	CB-CG1	4.44	1.44	1.53	1	1
P	42	ASN	CA-C	4.43	1.43	1.52	1	1
P	34	ILE	N-CA	4.39	1.37	1.46	1	1
P	59	ALA	CA-C	4.36	1.43	1.52	1	1
P	5	PRO	N-CA	4.34	1.40	1.47	1	1
P	400	HIS	CB-CG	4.34	1.44	1.50	1	1
P	28	ALA	N-CA	4.33	1.38	1.46	1	1
P	43	GLU	C-N	4.29	1.39	1.33	1	1
O	400	HIS	CB-CG	4.27	1.44	1.50	1	1
P	11	ASP	N-CA	4.23	1.54	1.46	1	1
P	20	GLY	N-CA	4.21	1.38	1.45	1	1
P	60	THR	CA-C	4.21	1.44	1.52	1	1
P	46	SER	CA-C	4.17	1.44	1.52	1	1
P	6	SER	CA-C	4.15	1.44	1.52	1	1
P	43	GLU	CA-C	4.12	1.44	1.52	1	1
P	30	ALA	C-N	4.12	1.39	1.33	1	1
P	54	GLU	CA-C	4.12	1.44	1.52	1	1
P	16	VAL	N-CA	4.07	1.38	1.46	1	1
P	16	VAL	C-N	4.01	1.39	1.33	1	1

Standard geometry: angle outliers

There are 137 bond angle outliers in this entry (0.44% of 31327 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)
P	500	PRO	O-C-N	23.94	161.30	123.00	1	1
O	500	PRO	O-C-N	23.88	161.21	123.00	1	1
P	75	PRO	C-N-CA	23.59	164.16	121.70	1	1
P	500	PRO	CA-C-N	17.94	80.31	116.20	1	1
O	500	PRO	CA-C-N	17.93	80.34	116.20	1	1
O	500	PRO	CA-C-O	12.70	80.90	119.00	1	1
P	500	PRO	CA-C-O	12.66	81.01	119.00	1	1
P	1	ALA	N-CA-CB	10.92	94.02	110.40	1	1
P	74	ILE	C-N-CD	9.82	84.74	125.00	1	1
P	37	ASP	CA-C-O	9.00	105.50	120.80	1	1
P	75	PRO	C-CA-CB	8.28	125.83	110.10	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	75	PRO	N-CA-C	8.21	132.62	112.10	1	1
P	34	ILE	CA-C-O	7.74	107.65	120.80	1	1
P	9	LYS	C-N-CA	7.70	107.84	121.70	1	1
P	76	SER	N-CA-C	7.65	132.43	111.00	1	1
P	3	SER	C-N-CA	7.54	108.13	121.70	1	1
P	21	LEU	CA-C-O	7.46	108.12	120.80	1	1
P	62	SER	O-C-N	7.45	111.08	123.00	1	1
P	76	SER	C-N-CA	7.44	135.10	121.70	1	1
P	11	ASP	CA-C-O	7.37	108.28	120.80	1	1
P	16	VAL	CA-C-O	6.99	108.91	120.80	1	1
P	30	ALA	O-C-N	6.93	134.08	123.00	1	1
P	29	TYR	CA-C-O	6.91	109.05	120.80	1	1
P	52	PRO	O-C-N	6.84	133.94	123.00	1	1
P	16	VAL	O-C-N	6.83	133.92	123.00	1	1
P	29	TYR	O-C-N	6.79	133.86	123.00	1	1
P	42	ASN	CA-C-O	6.73	109.35	120.80	1	1
P	41	TYR	O-C-N	6.71	133.74	123.00	1	1
P	77	HIS	C-N-CA	6.66	133.69	121.70	1	1
P	13	SER	O-C-N	6.57	133.51	123.00	1	1
P	58	ARG	O-C-N	6.52	133.42	123.00	1	1
P	14	VAL	CA-C-O	6.48	109.79	120.80	1	1
P	28	ALA	CA-C-O	6.44	109.86	120.80	1	1
P	55	LYS	CA-C-O	6.38	109.95	120.80	1	1
P	34	ILE	O-C-N	6.35	133.16	123.00	1	1
P	43	GLU	O-C-N	6.25	132.99	123.00	1	1
P	17	LEU	O-C-N	6.24	132.99	123.00	1	1
P	26	ALA	CA-C-O	6.24	110.19	120.80	1	1
P	56	GLN	CA-C-O	6.20	110.26	120.80	1	1
P	19	VAL	CA-C-O	6.19	110.27	120.80	1	1
P	1	ALA	C-N-CA	6.17	110.59	121.70	1	1
P	51	THR	CA-C-O	6.17	110.31	120.80	1	1
P	58	ARG	CA-C-O	6.13	110.38	120.80	1	1
P	15	LEU	CA-C-O	6.12	110.39	120.80	1	1
P	57	LYS	O-C-N	6.12	132.79	123.00	1	1
P	55	LYS	O-C-N	6.08	132.73	123.00	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	27	GLY	O-C-N	6.06	132.70	123.00	1	1
P	23	THR	CA-C-O	6.06	110.50	120.80	1	1
P	62	SER	CA-C-O	6.00	131.00	120.80	1	1
P	35	LYS	CA-C-O	5.99	110.61	120.80	1	1
P	38	LYS	O-C-N	5.97	132.56	123.00	1	1
P	22	SER	O-C-N	5.95	132.52	123.00	1	1
P	54	GLU	O-C-N	5.94	132.50	123.00	1	1
P	25	GLY	O-C-N	5.94	132.50	123.00	1	1
P	32	LYS	CA-C-O	5.91	110.75	120.80	1	1
P	45	ILE	O-C-N	5.88	132.41	123.00	1	1
P	53	GLU	O-C-N	5.85	132.37	123.00	1	1
P	61	SER	O-C-N	5.85	132.36	123.00	1	1
P	12	ASN	O-C-N	5.84	132.35	123.00	1	1
P	19	VAL	O-C-N	5.83	132.33	123.00	1	1
P	17	LEU	CA-C-O	5.80	110.94	120.80	1	1
P	10	ILE	C-N-CA	5.80	132.14	121.70	1	1
P	33	THR	O-C-N	5.75	132.20	123.00	1	1
P	57	LYS	CA-C-O	5.71	111.09	120.80	1	1
P	56	GLN	O-C-N	5.70	132.12	123.00	1	1
P	38	LYS	CA-C-O	5.70	111.11	120.80	1	1
P	53	GLU	CA-C-O	5.68	111.14	120.80	1	1
P	43	GLU	CA-C-O	5.68	111.14	120.80	1	1
P	54	GLU	CA-C-O	5.67	111.16	120.80	1	1
P	18	ILE	O-C-N	5.65	132.04	123.00	1	1
P	42	ASN	O-C-N	5.63	132.01	123.00	1	1
P	395	ARG	NE-CZ-NH1	5.60	115.90	121.50	1	1
P	78	VAL	N-CA-C	5.59	126.66	111.00	1	1
P	60	THR	CA-C-O	5.59	111.30	120.80	1	1
P	26	ALA	O-C-N	5.58	131.93	123.00	1	1
P	24	ILE	CA-C-O	5.58	111.32	120.80	1	1
P	60	THR	O-C-N	5.57	131.91	123.00	1	1
P	23	THR	O-C-N	5.57	131.90	123.00	1	1
P	39	LYS	O-C-N	5.56	131.90	123.00	1	1
O	395	ARG	NE-CZ-NH1	5.55	115.95	121.50	1	1
P	39	LYS	CA-C-O	5.55	111.36	120.80	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
P	24	ILE	O-C-N	5.49	131.79	123.00	1	1
P	18	ILE	CA-C-O	5.48	111.49	120.80	1	1
P	40	ARG	CA-C-O	5.46	111.52	120.80	1	1
P	78	VAL	CA-C-N	5.46	125.08	116.90	1	1
P	14	VAL	O-C-N	5.44	131.70	123.00	1	1
P	33	THR	CA-C-O	5.43	111.57	120.80	1	1
P	35	LYS	O-C-N	5.43	131.68	123.00	1	1
P	22	SER	CA-C-O	5.41	111.60	120.80	1	1
P	40	ARG	O-C-N	5.39	131.62	123.00	1	1
P	59	ALA	CA-C-O	5.38	111.66	120.80	1	1
P	12	ASN	CA-C-O	5.35	111.71	120.80	1	1
P	15	LEU	O-C-N	5.24	131.39	123.00	1	1
P	20	GLY	O-C-N	5.23	131.36	123.00	1	1
P	47	GLY	C-N-CA	5.20	112.34	121.70	1	1
P	59	ALA	O-C-N	5.20	131.32	123.00	1	1
P	28	ALA	O-C-N	5.15	131.24	123.00	1	1
P	32	LYS	O-C-N	5.12	131.19	123.00	1	1
P	44	ARG	O-C-N	5.08	131.13	123.00	1	1
P	76	SER	C-CA-CB	5.04	100.52	110.10	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	14.90	668

There are 668 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)
H:67:ILE:CD1	P:194:GLY:HA3	1.61	1	1
N:73:LEU:CD1	P:39:LYS:HD3	1.60	1	1
P:75:PRO:C	P:75:PRO:HA	1.54	1	1
H:10:LYS:C	P:68:PRO:CB	1.50	1	1
P:75:PRO:C	P:75:PRO:CA	1.48	1	1
N:73:LEU:HD13	P:39:LYS:CD	1.47	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
H:10:LYS:C	P:68:PRO:HB3	1.46	1	1
B:115:LEU:CD2	P:192:ASN:O	1.38	1	1
P:76:SER:H	P:160:ALA:CB	1.37	1	1
B:115:LEU:HD23	P:192:ASN:O	1.26	1	1
H:67:ILE:CD1	P:194:GLY:CA	1.24	1	1
N:73:LEU:CD1	P:39:LYS:CD	1.23	1	1
H:9:ILE:HB	P:71:GLN:OE1	1.22	1	1
B:113:GLU:CG	P:178:LYS:HD3	1.21	1	1
P:76:SER:N	P:174:LEU:HD21	1.20	1	1
H:67:ILE:HD11	P:194:GLY:CA	1.18	1	1
H:10:LYS:CA	P:68:PRO:CA	1.17	1	1
H:10:LYS:O	P:68:PRO:CA	1.17	1	1
P:75:PRO:CA	P:160:ALA:HB2	1.14	1	1
H:51:VAL:HG23	P:73:ARG:NH2	1.12	1	1
N:73:LEU:HD11	P:39:LYS:HD3	1.12	1	1
P:75:PRO:HA	P:160:ALA:HB2	1.12	1	1
B:113:GLU:CD	P:178:LYS:HD3	1.11	1	1
B:113:GLU:HG3	P:178:LYS:HD3	1.10	1	1
H:10:LYS:HA	P:68:PRO:CA	1.10	1	1
P:76:SER:HA	P:106:LEU:CD2	1.10	1	1
P:77:HIS:N	P:106:LEU:HD11	1.09	1	1
B:220:LYS:HD3	P:178:LYS:NZ	1.08	1	1
N:73:LEU:HD13	P:39:LYS:CG	1.07	1	1
P:76:SER:N	P:160:ALA:HB1	1.06	1	1
P:76:SER:H	P:160:ALA:HB1	1.05	1	1
B:220:LYS:HD3	P:178:LYS:HZ2	1.05	1	1
H:67:ILE:HD13	P:194:GLY:HA3	1.05	1	1
H:10:LYS:N	P:68:PRO:CB	1.05	1	1
P:76:SER:N	P:160:ALA:CB	1.04	1	1
B:220:LYS:HG3	P:351:GLU:OE2	1.04	1	1
H:10:LYS:HD2	P:63:ALA:HB1	1.03	1	1
P:76:SER:HA	P:106:LEU:HD22	1.03	1	1
N:73:LEU:O	P:43:GLU:OE1	1.00	1	1
P:75:PRO:HA	P:160:ALA:CB	1.00	1	1
H:10:LYS:O	P:68:PRO:N	1.00	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
H:67:ILE:HD12	P:193:ASP:O	1.00	1	1
H:51:VAL:CG2	P:73:ARG:NH2	0.99	1	1
N:73:LEU:HD23	P:40:ARG:CG	0.99	1	1
H:10:LYS:N	P:68:PRO:HG3	0.99	1	1
N:73:LEU:HD23	P:40:ARG:HG3	0.99	1	1
H:51:VAL:CG2	P:73:ARG:HH21	0.97	1	1
H:67:ILE:CD1	P:193:ASP:O	0.97	1	1
H:10:LYS:C	P:68:PRO:CA	0.95	1	1
P:75:PRO:HB2	P:173:VAL:H	0.94	1	1
B:104:TYR:HB2	B:225:MET:SD	0.94	1	1
H:10:LYS:H	P:68:PRO:HG3	0.94	1	1
B:119:SER:HB3	B:225:MET:HB2	0.93	1	1
H:67:ILE:HD11	P:194:GLY:HA3	0.93	1	1
B:141:VAL:HB	I:71:ALA:H	0.93	1	1
D:117:THR:HB	K:45:PRO:HA	0.93	1	1
P:78:VAL:HG13	P:79:PRO:HD3	0.93	1	1
B:220:LYS:CD	P:178:LYS:HZ2	0.93	1	1
A:482:LEU:HD21	M:4:LYS:HB3	0.92	1	1
B:98:THR:HG22	B:153:VAL:HA	0.92	1	1
H:67:ILE:HD12	P:193:ASP:C	0.91	1	1
N:73:LEU:CD2	P:40:ARG:HG3	0.91	1	1
B:124:THR:HA	B:138:ASP:HB3	0.91	1	1
B:152:LEU:HD13	B:178:LEU:HD21	0.90	1	1
H:51:VAL:HG23	P:73:ARG:CZ	0.90	1	1
B:113:GLU:HG3	P:178:LYS:CD	0.90	1	1
P:75:PRO:HB2	P:173:VAL:N	0.89	1	1
B:105:TRP:CD1	B:226:LEU:HB3	0.89	1	1
H:9:ILE:CB	P:71:GLN:OE1	0.88	1	1
A:369:THR:HB	A:431:GLY:HA3	0.87	1	1
P:75:PRO:HB3	P:172:ALA:HB1	0.87	1	1
P:76:SER:N	P:106:LEU:HD22	0.87	1	1
H:51:VAL:HG23	P:73:ARG:HH21	0.86	1	1
H:10:LYS:CD	P:63:ALA:HB1	0.86	1	1
H:10:LYS:O	P:68:PRO:HA	0.85	1	1
B:59:GLU:HB3	E:1:SER:HA	0.85	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:398:LEU:HA	A:497:CYS:HB3	0.85	1	1
A:513:LYS:H	F:61:ILE:HD12	0.84	1	1
B:220:LYS:CD	P:178:LYS:NZ	0.84	1	1
H:67:ILE:HD12	P:194:GLY:HA3	0.83	1	1
A:444:ASP:HB2	K:49:ARG:HG2	0.83	1	1
H:10:LYS:HD3	P:67:GLU:HA	0.82	1	1
D:66:ALA:HB3	E:108:LYS:HA	0.81	1	1
B:117:PHE:CG	B:224:SER:HA	0.81	1	1
B:142:VAL:HG23	B:211:GLU:HB3	0.81	1	1
N:61:TYR:O	P:40:ARG:NH2	0.80	1	1
P:76:SER:CA	P:106:LEU:CD2	0.80	1	1
B:97:LYS:HG3	B:152:LEU:HD12	0.80	1	1
B:101:HIS:HB3	B:156:GLU:HB2	0.80	1	1
B:115:LEU:HD22	P:192:ASN:O	0.80	1	1
B:92:PRO:HG3	B:150:ARG:HB2	0.80	1	1
P:77:HIS:HA	P:106:LEU:HD11	0.79	1	1
B:107:TYR:HB2	B:226:LEU:HA	0.79	1	1
P:75:PRO:C	P:174:LEU:HD21	0.79	1	1
N:73:LEU:HD13	P:39:LYS:HG2	0.78	1	1
P:75:PRO:HG3	P:159:SER:HA	0.78	1	1
P:78:VAL:CG1	P:79:PRO:HD3	0.77	1	1
P:75:PRO:C	P:160:ALA:HB2	0.77	1	1
I:62:MET:HB3	I:67:ILE:HD11	0.77	1	1
B:63:ILE:HD11	P:5:PRO:HB2	0.77	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	2805	2544	200	61

There are 61 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	430	LEU	1
A	434	GLY	1
A	511	ASN	1

Chain	Res	Type	Models (Total)
A	512	LEU	1
B	2	TYR	1
B	59	GLU	1
B	91	ASN	1
B	103	TRP	1
B	110	THR	1
B	111	ASP	1
B	112	TYR	1
B	122	ILE	1
B	128	LYS	1
B	129	PRO	1
B	130	GLY	1
B	137	VAL	1
B	140	ARG	1
B	141	VAL	1
B	142	VAL	1
B	207	PRO	1
B	214	PRO	1
B	216	LYS	1
B	220	LYS	1
B	221	TRP	1
B	223	ALA	1
B	225	MET	1
C	126	GLU	1
C	150	MET	1
D	65	PHE	1
D	113	VAL	1
D	117	THR	1
D	118	LYS	1
F	2	SER	1
F	95	GLN	1
G	3	ALA	1
G	38	SER	1
G	81	TYR	1
H	2	ALA	1

Chain	Res	Type	Models (Total)
H	3	GLU	1
H	83	PRO	1
I	69	GLN	1
I	71	ALA	1
J	2	GLU	1
J	56	PRO	1
K	2	PRO	1
K	42	ARG	1
K	46	LYS	1
K	48	TRP	1
L	3	GLU	1
M	41	LYS	1
N	2	GLN	1
N	3	ILE	1
N	4	ILE	1
N	14	ILE	1
N	49	PRO	1
N	57	PRO	1
N	66	VAL	1
N	68	VAL	1
N	78	PRO	1
P	77	HIS	1
P	78	VAL	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	2393	2142	121	130

There are 130 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.

Chain	Res	Type	Models (Total)
A	5	TRP	1
A	9	THR	1
A	13	ASP	1

Chain	Res	Type	Models (Total)
A	52	ILE	1
A	80	TRP	1
A	90	ASP	1
A	179	GLN	1
A	182	LEU	1
A	211	ASP	1
A	265	GLU	1
A	300	THR	1
A	365	VAL	1
A	406	ASP	1
A	428	HIS	1
A	430	LEU	1
A	432	LEU	1
A	441	ASP	1
A	444	ASP	1
A	480	GLU	1
A	497	CYS	1
A	510	VAL	1
A	512	LEU	1
B	2	TYR	1
B	59	GLU	1
B	63	ILE	1
B	87	ASP	1
B	88	GLU	1
B	97	LYS	1
B	98	THR	1
B	104	TYR	1
B	105	TRP	1
B	108	GLU	1
B	109	TYR	1
B	110	THR	1
B	115	LEU	1
B	117	PHE	1
B	119	SER	1
B	122	ILE	1

Chain	Res	Type	Models (Total)
B	127	LEU	1
B	128	LYS	1
B	134	LEU	1
B	136	GLU	1
B	138	ASP	1
B	139	ASN	1
B	140	ARG	1
B	141	VAL	1
B	142	VAL	1
B	143	LEU	1
B	153	VAL	1
B	157	ASP	1
B	159	LEU	1
B	171	THR	1
B	210	LEU	1
B	211	GLU	1
B	215	LEU	1
B	217	TYR	1
B	218	PHE	1
B	220	LYS	1
B	221	TRP	1
C	2	GLN	1
C	4	HIS	1
C	64	THR	1
C	93	THR	1
C	126	GLU	1
C	188	ASP	1
C	256	TRP	1
C	257	TRP	1
D	2	VAL	1
D	3	VAL	1
D	18	ASP	1
D	55	GLU	1
D	68	MET	1
D	109	GLU	1

Chain	Res	Type	Models (Total)
D	110	GLU	1
D	111	GLU	1
D	112	TRP	1
D	117	THR	1
D	123	MET	1
E	10	GLU	1
E	31	LYS	1
E	66	ARG	1
E	73	ASP	1
E	107	ASP	1
E	108	LYS	1
E	109	VAL	1
F	6	VAL	1
F	61	ILE	1
F	65	ASP	1
F	92	VAL	1
G	16	ARG	1
G	32	LEU	1
G	41	ARG	1
G	56	THR	1
G	67	THR	1
G	81	TYR	1
H	1	MET	1
H	3	GLU	1
H	28	ARG	1
H	30	CYS	1
H	85	LYS	1

Fit of model to data used for modeling

Fit of model(s) to crosslinking-MS data

Restraint types

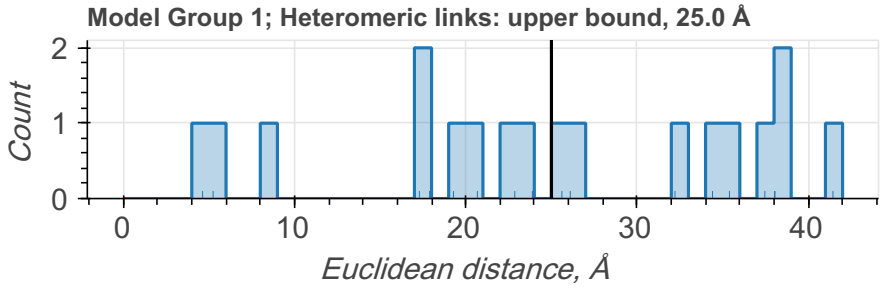
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

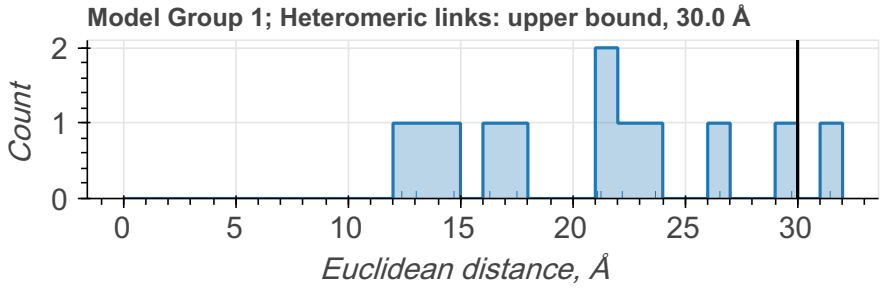
There are 46 crosslinking restraints combined in 46 restraint groups.

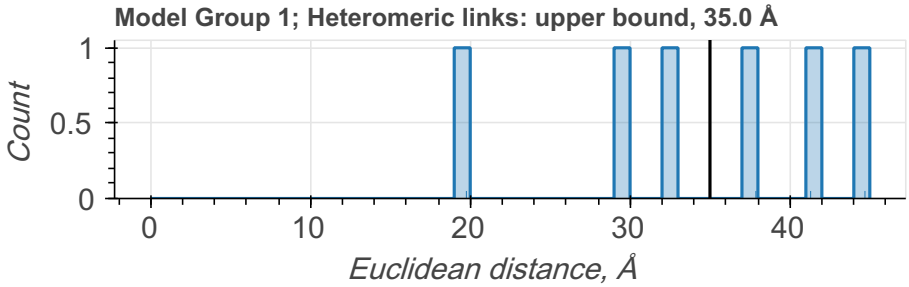
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
Other	ALA	CA	SER	CA	upper bound	30.0	1
Other	ALA	CA	ASP	CA	upper bound	25.0	1
Other	ALA	CA	GLU	CA	upper bound	25.0	1
Other	GLU	CA	LYS	CA	upper bound	25.0	19
Other	ASP	CA	LYS	CA	upper bound	25.0	5
Other	LYS	CA	LYS	CA	upper bound	30.0	13
Other	LYS	CA	LYS	CA	upper bound	35.0	6

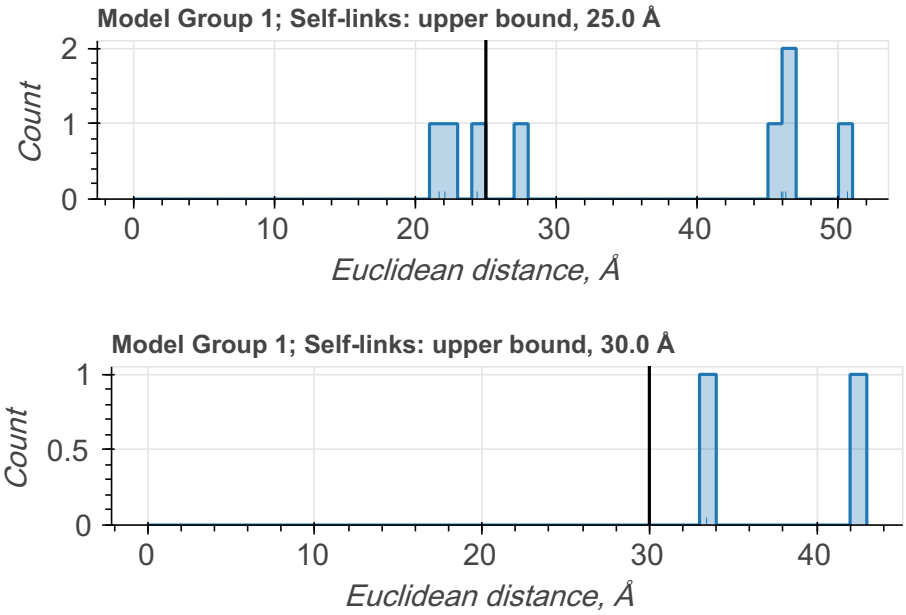
Distograms of individual restraints

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.









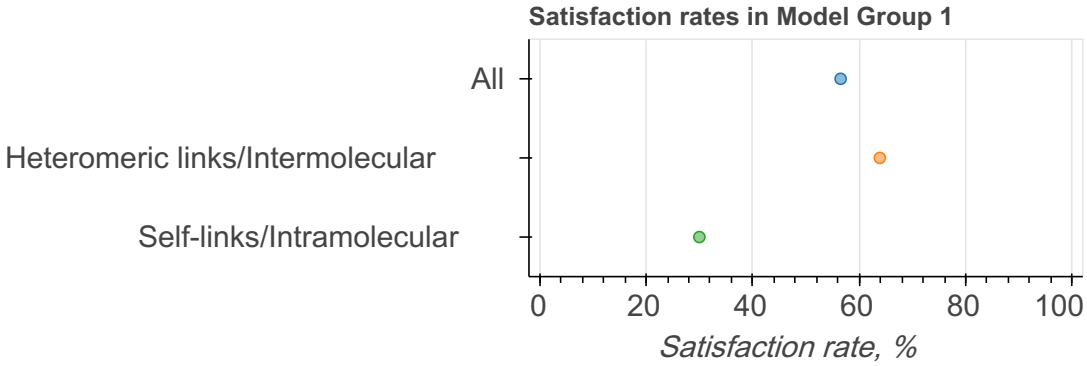
Satisfaction of restraints

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=46)
1	1	1	1/1	All	56.52	43.48	46
				Heteromeric links/ Intermolecular	63.89	36.11	36
				Self-links/ Intramolecular	30.00	70.00	10

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.



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.