

# Integrative Structure Validation Report ?

February 18, 2025 - 08:45 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	9A8D
PDB-Dev ID	PDBDEV_00000536
Structure Title	Integrative model of SARS-CoV-2 Replicase polypeptide 1ab
Structure Authors	Schneidman, D; Kalisman, N
Deposited on	2023-12-21

*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)*

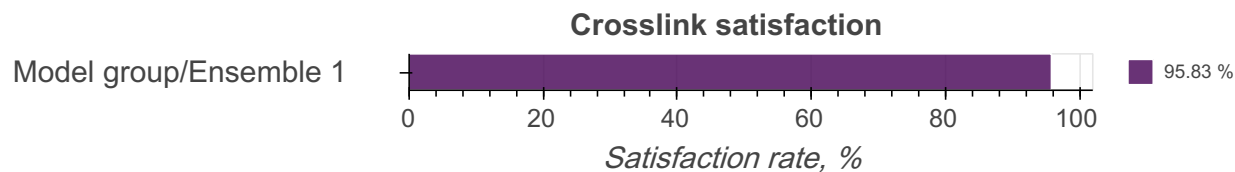
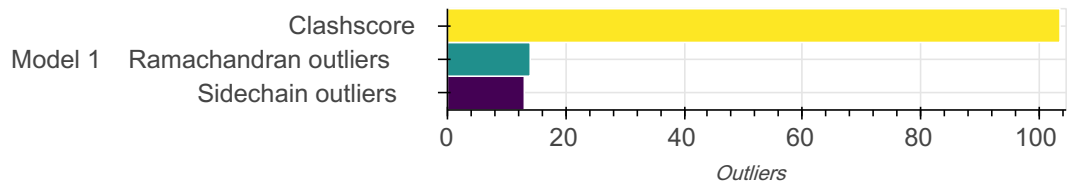
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 4 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	SARS-CoV-2 Replicase polypeptide 1ab	A	638	-	1-104, 105-132, 133-275, 276-345, 346-358, 346-437, 359-511, 512-638	100.00 / 97.96	Atomic

### Datasets used for modeling ?

*There are 4 unique datasets used to build the models in this entry.*

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD023487

ID	Dataset type	Database name	Data access code
2	De Novo model	Not available	Not available
3	Comparative model	Not available	Not available
4	Experimental model	PDB	3LD1

### 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	Modeling with CombDock	None	CombDock with AlphaFold2 domains and crosslinks as an input	None	False	False

*There are 2 software packages reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="#">UCSF ChimeraX</a>	1.2/v9	model building	<a href="https://www.rbvi.ucsf.edu/chimerax/">https://www.rbvi.ucsf.edu/chimerax/</a>
2	<a href="#">CombDock</a>	Not available	assembly	<a href="http://bioinfo3d.cs.tau.ac.il/CombDock/download/">http://bioinfo3d.cs.tau.ac.il/CombDock/download/</a>

### 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 17 bond length outliers in this entry (0.34% of 5036 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	347	LYS	C-N	15.75	1.55	1.33	1	1
A	348	SER	N-CA	11.57	1.68	1.46	1	1
A	511	ASP	C-N	8.66	1.45	1.33	1	1
A	275	GLN	C-N	7.66	1.44	1.33	1	1
A	346	GLN	C-N	6.89	1.43	1.33	1	1
A	274	LEU	C-N	5.88	1.41	1.33	1	1
A	348	SER	C-N	5.66	1.41	1.33	1	1
A	534	LYS	CA-CB	5.22	1.63	1.53	1	1
A	347	LYS	CA-C	4.91	1.63	1.52	1	1
A	511	ASP	CA-C	4.74	1.62	1.52	1	1
A	512	SER	C-N	4.73	1.40	1.33	1	1
A	105	GLN	CA-C	4.71	1.43	1.52	1	1
A	463	ARG	CA-C	4.52	1.43	1.52	1	1
A	105	GLN	N-CA	4.41	1.37	1.46	1	1
A	106	PRO	N-CA	4.37	1.40	1.47	1	1
A	533	SER	C-N	4.31	1.39	1.33	1	1
A	275	GLN	CA-C	4.26	1.61	1.52	1	1

### Standard geometry: angle outliers ?

There are 161 bond angle outliers in this entry (2.36% of 6810 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)
A	275	GLN	C-N-CA	20.52	158.64	121.70	1	1
A	347	LYS	C-N-CA	13.49	145.98	121.70	1	1
A	368	PHE	CA-CB-CG	12.65	101.15	113.80	1	1
A	348	SER	C-N-CA	12.28	143.80	121.70	1	1
A	104	ILE	C-N-CA	11.06	141.61	121.70	1	1
A	492	LYS	N-CA-CB	10.75	128.78	110.50	1	1
A	92	ASN	CA-CB-CG	10.49	102.11	112.60	1	1
A	511	ASP	C-N-CA	10.12	139.92	121.70	1	1
A	351	SER	CA-C-N	9.98	131.88	116.90	1	1
A	103	THR	C-N-CA	9.43	138.68	121.70	1	1
A	338	LYS	C-CA-CB	9.32	92.38	110.10	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	463	ARG	C-CA-CB	8.86	93.26	110.10	1	1
A	606	ASN	CA-CB-CG	8.69	103.91	112.60	1	1
A	420	TYR	CA-CB-CG	8.35	98.87	113.90	1	1
A	498	PHE	CA-CB-CG	8.07	105.73	113.80	1	1
A	102	LYS	C-N-CA	7.98	107.33	121.70	1	1
A	347	LYS	N-CA-C	7.96	133.28	111.00	1	1
A	116	PHE	CA-CB-CG	7.95	105.85	113.80	1	1
A	437	PHE	CA-CB-CG	7.87	105.93	113.80	1	1
A	347	LYS	CA-C-N	7.78	131.76	116.20	1	1
A	84	ASP	CA-CB-CG	7.55	105.05	112.60	1	1
A	347	LYS	CA-C-O	7.54	107.99	120.80	1	1
A	276	LYS	N-CA-C	7.41	90.26	111.00	1	1
A	300	PHE	CA-CB-CG	7.27	106.53	113.80	1	1
A	275	GLN	N-CA-C	7.26	131.32	111.00	1	1
A	104	ILE	CA-C-N	7.13	101.95	116.20	1	1
A	348	SER	N-CA-CB	6.98	122.36	110.50	1	1
A	163	PHE	CA-CB-CG	6.90	106.90	113.80	1	1
A	496	GLN	C-N-CA	6.90	109.28	121.70	1	1
A	435	ASN	CA-CB-CG	6.90	105.70	112.60	1	1
A	534	LYS	N-CA-CB	6.53	121.60	110.50	1	1
A	96	PRO	C-CA-CB	6.45	97.84	110.10	1	1
A	456	LYS	N-CA-CB	6.43	121.43	110.50	1	1
A	347	LYS	CA-CB-CG	6.30	126.70	114.10	1	1
A	347	LYS	C-CA-CB	6.27	98.18	110.10	1	1
A	275	GLN	C-CA-CB	6.22	98.27	110.10	1	1
A	503	ASN	CA-CB-CG	6.14	106.46	112.60	1	1
A	505	PHE	CA-CB-CG	6.05	107.75	113.80	1	1
A	267	ASN	CA-CB-CG	6.03	106.57	112.60	1	1
A	346	GLN	CA-C-N	5.96	128.12	116.20	1	1
A	9	ASN	CA-CB-CG	5.96	106.64	112.60	1	1
A	83	PHE	CA-CB-CG	5.77	108.03	113.80	1	1
A	346	GLN	C-CA-CB	5.75	121.03	110.10	1	1
A	23	ASP	CA-CB-CG	5.75	106.85	112.60	1	1
A	114	ASP	CA-CB-CG	5.72	106.88	112.60	1	1
A	537	TYR	CA-CB-CG	5.71	103.62	113.90	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	277	GLU	C-CA-CB	5.66	99.34	110.10	1	1
A	364	VAL	N-CA-CB	5.64	121.09	111.50	1	1
A	414	ASN	C-CA-CB	5.64	99.39	110.10	1	1
A	350	LEU	C-N-CA	5.63	131.84	121.70	1	1
A	493	GLU	C-N-CA	5.62	111.59	121.70	1	1
A	286	ASP	CA-CB-CG	5.57	107.03	112.60	1	1
A	194	HIS	CA-CB-CG	5.54	108.26	113.80	1	1
A	156	PHE	CA-CB-CG	5.49	108.31	113.80	1	1
A	631	ASN	CA-CB-CG	5.43	107.17	112.60	1	1
A	98	ASN	CA-CB-CG	5.42	107.18	112.60	1	1
A	277	GLU	C-N-CA	5.39	112.00	121.70	1	1
A	292	GLU	CB-CG-CD	5.33	103.53	112.60	1	1
A	464	ASP	CA-CB-CG	5.32	107.28	112.60	1	1
A	499	PHE	C-CA-CB	5.29	100.05	110.10	1	1
A	10	PHE	CA-CB-CG	5.29	108.51	113.80	1	1
A	233	TYR	C-N-CA	5.28	131.21	121.70	1	1
A	351	SER	N-CA-C	5.28	125.77	111.00	1	1
A	471	PHE	N-CA-CB	5.28	119.47	110.50	1	1
A	349	ILE	C-N-CA	5.24	131.14	121.70	1	1
A	351	SER	O-C-N	5.22	114.65	123.00	1	1
A	615	ASP	CA-CB-CG	5.21	107.39	112.60	1	1
A	455	PHE	C-CA-CB	5.18	100.26	110.10	1	1
A	557	LYS	C-N-CA	5.17	131.00	121.70	1	1
A	275	GLN	CB-CG-CD	5.16	103.82	112.60	1	1
A	463	ARG	N-CA-CB	5.13	119.22	110.50	1	1
A	348	SER	CA-CB-OG	5.12	121.34	111.10	1	1
A	406	PHE	CA-CB-CG	5.10	108.70	113.80	1	1
A	268	ASP	CA-CB-CG	5.09	107.51	112.60	1	1
A	247	ALA	C-CA-CB	5.05	102.93	110.50	1	1
A	413	ASN	CA-CB-CG	4.98	107.62	112.60	1	1
A	292	GLU	C-CA-CB	4.95	100.70	110.10	1	1
A	349	ILE	N-CA-C	4.90	124.72	111.00	1	1
A	276	LYS	N-CA-CB	4.83	118.72	110.50	1	1
A	237	HIS	CD2-NE2-CE1	4.81	104.19	109.00	1	1
A	328	ASN	CA-CB-CG	4.80	107.80	112.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	254	ASN	CA-CB-CG	4.79	107.81	112.60	1	1
A	471	PHE	CA-CB-CG	4.77	109.03	113.80	1	1
A	346	GLN	CA-C-O	4.74	112.74	120.80	1	1
A	321	GLN	CB-CG-CD	4.72	104.57	112.60	1	1
A	404	MET	C-CA-CB	4.72	101.13	110.10	1	1
A	346	GLN	CB-CG-CD	4.71	120.61	112.60	1	1
A	75	PHE	C-CA-CB	4.71	101.16	110.10	1	1
A	41	PHE	CA-CB-CG	4.68	109.12	113.80	1	1
A	329	PHE	CA-CB-CG	4.66	109.14	113.80	1	1
A	537	TYR	C-CA-CB	4.65	101.26	110.10	1	1
A	43	ASP	CA-CB-CG	4.64	107.96	112.60	1	1
A	398	LEU	C-N-CA	4.63	130.03	121.70	1	1
A	145	HIS	CD2-NE2-CE1	4.60	104.40	109.00	1	1
A	344	GLY	C-N-CA	4.59	113.43	121.70	1	1
A	238	ASN	CA-CB-CG	4.59	108.01	112.60	1	1
A	483	GLN	C-CA-CB	4.58	101.39	110.10	1	1
A	399	ARG	CD-NE-CZ	4.58	117.98	124.40	1	1
A	555	ALA	CA-C-N	4.58	123.77	116.90	1	1
A	363	VAL	C-N-CA	4.58	113.46	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	103.58	1028

There are 1028 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:348:SER:CA	A:348:SER:N	1.56	1	1
A:410:LEU:HD12	A:412:THR:HG22	1.16	1	1
A:96:PRO:HD3	A:259:VAL:HG12	1.12	1	1
A:453:GLU:HB3	A:557:LYS:HB3	1.12	1	1
A:347:LYS:CB	A:444:LEU:HD11	1.11	1	1
A:338:LYS:HE2	A:539:LYS:HB2	1.11	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:377:ASN:HB2	A:380:ARG:HG3	1.11	1	1
A:381:VAL:HA	A:384:LYS:HB2	1.11	1	1
A:489:LYS:HD3	A:502:VAL:HG21	1.11	1	1
A:556:PRO:HG3	A:607:GLY:HA2	1.11	1	1
A:347:LYS:HB2	A:444:LEU:HD11	1.11	1	1
A:453:GLU:HG3	A:558:GLU:HB2	1.10	1	1
A:347:LYS:CA	A:426:VAL:HG11	1.09	1	1
A:389:ILE:HG21	A:398:LEU:HD21	1.08	1	1
A:103:THR:HG21	A:106:PRO:HD3	1.08	1	1
A:275:GLN:HB2	A:277:GLU:H	1.08	1	1
A:505:PHE:HA	A:514:ILE:HD12	1.07	1	1
A:251:ILE:HB	A:271:LEU:HD21	1.07	1	1
A:577:VAL:HG12	A:603:VAL:HG12	1.07	1	1
A:485:VAL:HG22	A:491:ILE:HD11	1.07	1	1
A:132:CYS:HA	A:183:ASN:HB2	1.06	1	1
A:338:LYS:HE3	A:445:LYS:HB2	1.06	1	1
A:341:TRP:HB2	A:348:SER:HB3	1.06	1	1
A:443:LYS:HE3	A:513:ILE:HG22	1.05	1	1
A:375:ALA:HA	A:382:LEU:HD21	1.05	1	1
A:520:LEU:HD13	A:534:LYS:HE2	1.05	1	1
A:335:LYS:HG2	A:546:GLU:HB2	1.04	1	1
A:96:PRO:HB3	A:259:VAL:HA	1.04	1	1
A:341:TRP:HB2	A:348:SER:CB	1.03	1	1
A:381:VAL:HG12	A:385:ALA:HB2	1.02	1	1
A:116:PHE:HB2	A:234:VAL:HA	1.02	1	1
A:94:VAL:HA	A:225:ALA:HB1	1.01	1	1
A:258:VAL:HG21	A:266:LEU:HD23	1.00	1	1
A:465:GLY:HA2	A:468:ILE:HG12	1.00	1	1
A:34:THR:HG21	A:548:GLY:HA3	0.99	1	1
A:338:LYS:HD2	A:541:VAL:HG23	0.98	1	1
A:415:LEU:HA	A:418:MET:HE2	0.98	1	1
A:505:PHE:CD2	A:514:ILE:HB	0.98	1	1
A:446:PRO:HD3	A:539:LYS:HD3	0.98	1	1
A:447:VAL:HG22	A:448:LEU:HD22	0.98	1	1
A:338:LYS:HG3	A:445:LYS:CG	0.98	1	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:490:GLU:HA	A:495:VAL:HB	0.98	1	1
A:347:LYS:HA	A:426:VAL:HG11	0.97	1	1
A:348:SER:HA	A:348:SER:N	0.97	1	1
A:348:SER:HA	A:441:TYR:OH	0.97	1	1
A:398:LEU:HD23	A:405:MET:HG3	0.96	1	1
A:14:ASP:HB3	A:216:ILE:HD12	0.96	1	1
A:94:VAL:HG21	A:230:VAL:CG2	0.95	1	1
A:338:LYS:CD	A:541:VAL:HG23	0.95	1	1
A:338:LYS:HG3	A:445:LYS:HG2	0.94	1	1
A:374:THR:HG22	A:381:VAL:HG11	0.94	1	1
A:75:PHE:HB3	A:106:PRO:HD2	0.94	1	1
A:488:ALA:HA	A:496:GLN:HB3	0.94	1	1
A:95:PHE:HB3	A:96:PRO:HD2	0.94	1	1
A:116:PHE:CG	A:234:VAL:HG13	0.94	1	1
A:486:THR:H	A:503:ASN:HD21	0.93	1	1
A:445:LYS:HD3	A:539:LYS:CD	0.93	1	1
A:570:GLU:HB3	A:599:VAL:HG12	0.93	1	1
A:341:TRP:CZ2	A:427:GLN:HG2	0.93	1	1
A:410:LEU:CD1	A:412:THR:HG22	0.93	1	1
A:347:LYS:HB3	A:444:LEU:HD21	0.92	1	1
A:515:ILE:HD12	A:520:LEU:HD12	0.92	1	1
A:338:LYS:HG2	A:539:LYS:HG3	0.92	1	1
A:377:ASN:HB2	A:380:ARG:CG	0.91	1	1
A:338:LYS:HD2	A:541:VAL:CG2	0.91	1	1
A:22:LYS:HD3	A:219:LYS:CE	0.91	1	1
A:415:LEU:CA	A:418:MET:HE2	0.91	1	1
A:483:GLN:HG2	A:507:ALA:HA	0.91	1	1
A:489:LYS:HD3	A:502:VAL:CG2	0.91	1	1
A:455:PHE:CZ	A:472:ILE:HB	0.91	1	1
A:116:PHE:CD1	A:234:VAL:HG22	0.91	1	1
A:341:TRP:CB	A:348:SER:HB3	0.91	1	1
A:258:VAL:HG21	A:266:LEU:CD2	0.90	1	1
A:451:LEU:HD12	A:502:VAL:HG12	0.90	1	1
A:491:ILE:HD13	A:503:ASN:HB3	0.90	1	1
A:341:TRP:HA	A:347:LYS:C	0.90	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:508:LEU:HD11	A:519:LYS:CD	0.90	1	1
A:116:PHE:HE2	A:129:PRO:HG3	0.90	1	1
A:336:ALA:HB2	A:346:GLN:HG3	0.90	1	1
A:490:GLU:CA	A:495:VAL:HB	0.90	1	1
A:132:CYS:HA	A:183:ASN:CB	0.89	1	1
A:290:ASN:HB2	A:420:TYR:CZ	0.89	1	1
A:96:PRO:CB	A:259:VAL:HA	0.89	1	1
A:381:VAL:CG1	A:385:ALA:HB2	0.89	1	1
A:531:THR:HB	A:534:LYS:HD3	0.89	1	1
A:275:GLN:HB2	A:277:GLU:N	0.89	1	1
A:520:LEU:CD1	A:534:LYS:HE2	0.89	1	1
A:347:LYS:HD3	A:449:ASP:CA	0.88	1	1
A:338:LYS:CE	A:445:LYS:HB2	0.88	1	1
A:341:TRP:HA	A:347:LYS:O	0.88	1	1
A:116:PHE:CD2	A:234:VAL:HG13	0.88	1	1
A:389:ILE:HG23	A:393:ILE:HG13	0.88	1	1
A:348:SER:HA	A:441:TYR:CZ	0.87	1	1
A:418:MET:SD	A:472:ILE:HG21	0.87	1	1
A:486:THR:HB	A:489:LYS:HD2	0.87	1	1
A:476:ALA:HB3	A:487:CYS:SG	0.86	1	1
A:251:ILE:HB	A:271:LEU:CD2	0.86	1	1
A:75:PHE:CD1	A:106:PRO:HG2	0.86	1	1
A:103:THR:CG2	A:106:PRO:HD3	0.86	1	1
A:335:LYS:HG2	A:546:GLU:CB	0.86	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	636	593	29	14

There are 14 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	105	GLN	1
A	276	LYS	1
A	345	GLU	1

Chain	Res	Type	Models (Total)
A	349	ILE	1
A	350	LEU	1
A	362	ARG	1
A	380	ARG	1
A	399	ARG	1
A	408	SER	1
A	434	THR	1
A	447	VAL	1
A	489	LYS	1
A	492	LYS	1
A	556	PRO	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	545	496	36	13

There are 13 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	75	PHE	1
A	111	LYS	1
A	223	THR	1
A	251	ILE	1
A	346	GLN	1
A	347	LYS	1
A	364	VAL	1
A	408	SER	1
A	422	THR	1
A	445	LYS	1
A	519	LYS	1
A	539	LYS	1
A	558	GLU	1

## Fit of model to data used for modeling ?

### Fit of model(s) to crosslinking-MS data

#### Restraint types

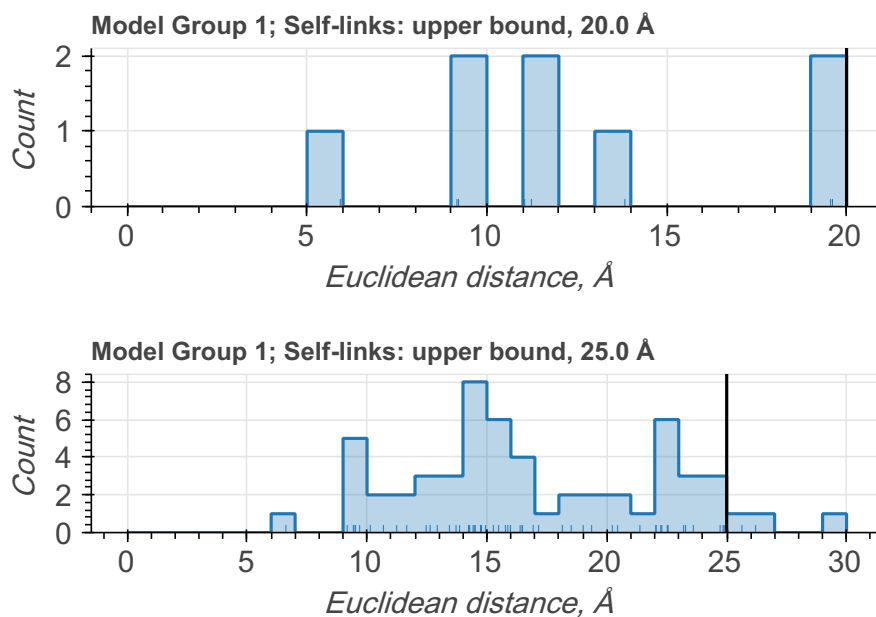
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

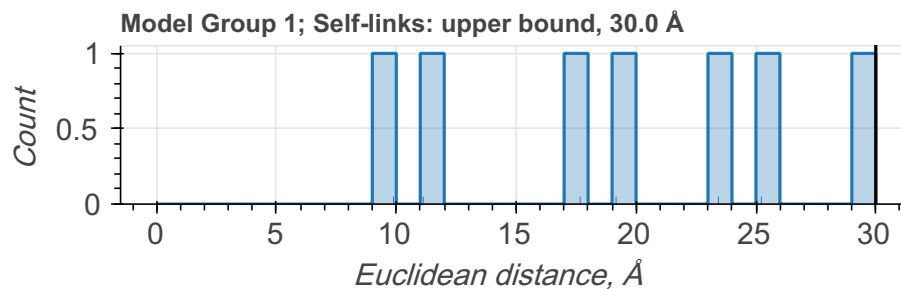
There are 72 crosslinking restraints combined in 72 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	LYS	CA	upper bound	25.0	57
BS3	GLU	CA	LYS	CA	upper bound	30.0	7
BS3	ARG	CA	LYS	CA	upper bound	20.0	5
BS3	GLY	CA	LYS	CA	upper bound	20.0	1
BS3	LYS	CA	LYS	CA	upper bound	20.0	2

#### 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.





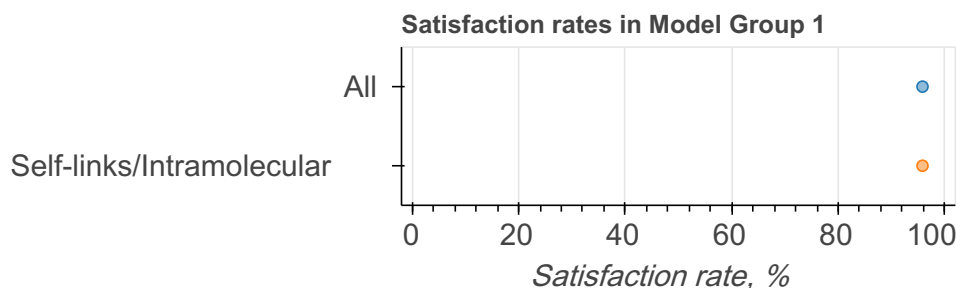
### Satisfaction of restraints

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=72)
1	1	1	1/1	All	95.83	4.17	72
				Self-links/Intramolecular	95.83	4.17	72

### 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 Trehwella, 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.