

# Integrative Structure Validation Report ?

April 09, 2025 - 08:13 PM 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	9A40
PDB-Dev ID	PDBDEV_00000221
Structure Title	model of Cullin4
Structure Authors	Kolja Stahl; Oliver Brock; Juri Rappsilber
Deposited on	2023-12-18

*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)*

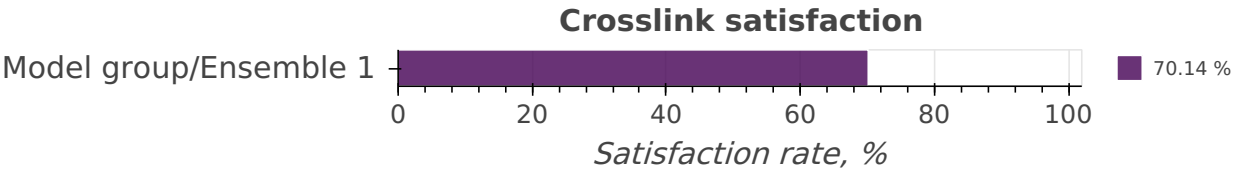
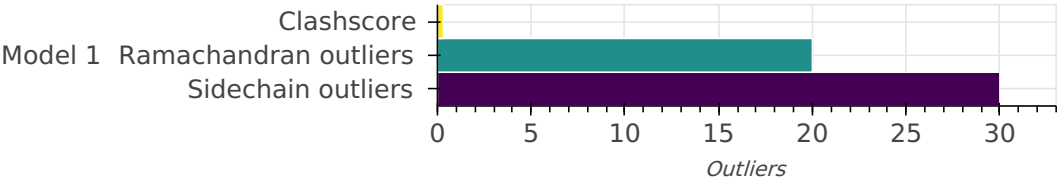
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 1 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	CUL4A_HUMAN	A	739	-	1-739	100.00 / 0.00	Atomic
		2	DCAF1_HUMAN	B	373	-	1-373	100.00 / 0.00	Atomic
		3	DDB1_HUMAN	C	1142	-	1-1142	100.00 / 0.00	Atomic
		4	RBX1_HUMAN	D	98	-	1-98	100.00 / 0.00	Atomic
		5	G7N4W9_MACMU	E	628	-	1-628	100.00 / 0.00	Atomic
		6	A4UDG5_SIV	F	138	-	1-138	100.00 / 0.00	Atomic

## Datasets used for modeling ?

*There is 1 unique dataset used to build the models in this entry.*

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	<a href="#">PXD020453</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	AlphaLink2	AlphaLink2	No starting models were used in the modeling	1	False	False

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

ID	Software name	Software version	Software classification	Software location
1	<a href="#">AlphaLink2</a>	1.00	model building	<a href="https://github.com/Rappsilber-Laboratory/AlphaLink2">https://github.com/Rappsilber-Laboratory/AlphaLink2</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 no bond length outliers.

### Standard geometry: angle outliers ?

There are 175 bond angle outliers in this entry (0.51% of 34489 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)
E	7	ASP	C-N-CA	6.19	132.84	121.70	1	1
C	1095	ASP	CA-CB-CG	5.91	118.51	112.60	1	1
F	53	ASP	CA-CB-CG	5.83	118.43	112.60	1	1
E	355	ASP	CA-CB-CG	5.76	118.36	112.60	1	1
E	7	ASP	O-C-N	5.67	113.92	123.00	1	1
E	503	ASP	CA-CB-CG	5.55	118.15	112.60	1	1
B	272	ASP	CA-CB-CG	5.49	118.09	112.60	1	1
C	189	GLN	OE1-CD-NE2	5.47	117.13	122.60	1	1
E	449	GLN	OE1-CD-NE2	5.44	117.16	122.60	1	1
A	702	GLN	OE1-CD-NE2	5.39	117.21	122.60	1	1
C	799	GLN	OE1-CD-NE2	5.31	117.29	122.60	1	1
F	126	THR	CA-C-N	5.27	124.81	116.90	1	1
E	7	ASP	CA-C-N	5.27	126.73	116.20	1	1
A	14	PRO	CA-N-CD	5.26	104.63	112.00	1	1
A	575	GLN	OE1-CD-NE2	5.24	117.36	122.60	1	1
B	275	ASP	CA-CB-CG	5.22	117.82	112.60	1	1
C	1109	GLN	OE1-CD-NE2	5.20	117.40	122.60	1	1
A	398	ARG	CD-NE-CZ	5.17	131.64	124.40	1	1
E	8	SER	C-N-CA	5.13	130.94	121.70	1	1
A	85	GLN	OE1-CD-NE2	5.13	117.47	122.60	1	1
C	566	ASP	C-N-CA	5.09	130.87	121.70	1	1
D	1	MET	C-N-CA	5.09	130.86	121.70	1	1
C	435	GLN	OE1-CD-NE2	4.94	117.66	122.60	1	1
C	708	ASP	CA-CB-CG	4.93	117.53	112.60	1	1
A	37	ASN	OD1-CG-ND2	4.93	117.67	122.60	1	1
C	973	ASN	CA-CB-CG	4.92	117.52	112.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
E	318	PHE	CA-CB-CG	4.91	118.71	113.80	1	1
C	973	ASN	OD1-CG-ND2	4.88	117.72	122.60	1	1
A	734	GLN	OE1-CD-NE2	4.87	117.73	122.60	1	1
A	493	GLN	OE1-CD-NE2	4.82	117.78	122.60	1	1
C	278	ASP	CA-CB-CG	4.81	117.41	112.60	1	1
E	164	HIS	CB-CG-CD2	4.80	124.96	131.20	1	1
C	746	GLN	OE1-CD-NE2	4.80	117.80	122.60	1	1
C	497	GLN	OE1-CD-NE2	4.80	117.80	122.60	1	1
F	134	TYR	C-N-CA	4.79	130.32	121.70	1	1
A	273	GLN	OE1-CD-NE2	4.79	117.81	122.60	1	1
A	670	GLN	OE1-CD-NE2	4.78	117.82	122.60	1	1
F	44	ARG	CD-NE-CZ	4.75	131.05	124.40	1	1
E	8	SER	CA-C-N	4.75	125.70	116.20	1	1
C	570	ARG	NH1-CZ-NH2	4.75	113.13	119.30	1	1
F	129	LEU	N-CA-C	4.75	124.29	111.00	1	1
E	237	GLN	OE1-CD-NE2	4.74	117.86	122.60	1	1
C	734	GLN	OE1-CD-NE2	4.74	117.86	122.60	1	1
B	273	ASP	CA-CB-CG	4.73	117.33	112.60	1	1
B	276	ASP	CA-CB-CG	4.73	117.33	112.60	1	1
C	1073	HIS	CB-CG-CD2	4.72	125.06	131.20	1	1
A	120	GLN	OE1-CD-NE2	4.72	117.88	122.60	1	1
A	284	GLN	OE1-CD-NE2	4.71	117.89	122.60	1	1
C	599	PHE	CA-CB-CG	4.70	118.50	113.80	1	1
A	653	GLN	OE1-CD-NE2	4.69	117.91	122.60	1	1
E	51	GLN	OE1-CD-NE2	4.69	117.91	122.60	1	1
A	361	GLN	OE1-CD-NE2	4.68	117.92	122.60	1	1
A	92	ASP	CA-CB-CG	4.67	117.27	112.60	1	1
E	467	GLN	OE1-CD-NE2	4.66	117.94	122.60	1	1
A	531	GLN	OE1-CD-NE2	4.65	117.95	122.60	1	1
A	137	ASP	CA-CB-CG	4.64	117.24	112.60	1	1
C	527	GLN	OE1-CD-NE2	4.64	117.96	122.60	1	1
E	621	GLN	OE1-CD-NE2	4.61	117.99	122.60	1	1
A	12	GLN	OE1-CD-NE2	4.60	118.00	122.60	1	1
A	232	GLN	OE1-CD-NE2	4.60	118.00	122.60	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
E	580	PHE	CA-CB-CG	4.60	118.40	113.80	1	1
C	470	GLN	OE1-CD-NE2	4.59	118.01	122.60	1	1
C	346	GLN	OE1-CD-NE2	4.57	118.03	122.60	1	1
C	848	GLN	OE1-CD-NE2	4.57	118.03	122.60	1	1
C	688	ASP	CA-CB-CG	4.53	117.13	112.60	1	1
C	637	GLN	OE1-CD-NE2	4.53	118.07	122.60	1	1
A	304	GLN	OE1-CD-NE2	4.53	118.07	122.60	1	1
E	169	HIS	CB-CG-CD2	4.52	125.33	131.20	1	1
C	525	HIS	CB-CG-CD2	4.52	125.33	131.20	1	1
D	47	GLN	OE1-CD-NE2	4.51	118.09	122.60	1	1
C	534	HIS	CB-CG-CD2	4.49	125.36	131.20	1	1
A	736	HIS	CB-CG-CD2	4.49	125.37	131.20	1	1
C	177	GLN	OE1-CD-NE2	4.48	118.12	122.60	1	1
B	178	ASN	OD1-CG-ND2	4.48	118.12	122.60	1	1
A	495	GLN	OE1-CD-NE2	4.48	118.12	122.60	1	1
C	711	GLN	OE1-CD-NE2	4.47	118.13	122.60	1	1
E	607	GLN	OE1-CD-NE2	4.47	118.13	122.60	1	1
D	38	HIS	CB-CG-CD2	4.46	125.40	131.20	1	1
F	67	GLN	OE1-CD-NE2	4.46	118.14	122.60	1	1
A	661	GLN	OE1-CD-NE2	4.45	118.15	122.60	1	1
F	126	THR	N-CA-C	4.45	123.45	111.00	1	1
D	70	HIS	CB-CG-CD2	4.44	125.42	131.20	1	1
B	271	ALA	C-N-CA	4.44	129.70	121.70	1	1
F	25	GLN	OE1-CD-NE2	4.44	118.16	122.60	1	1
C	1028	GLN	OE1-CD-NE2	4.43	118.17	122.60	1	1
E	196	ARG	CD-NE-CZ	4.42	130.59	124.40	1	1
A	382	PRO	C-N-CA	4.42	129.66	121.70	1	1
C	800	HIS	CB-CG-CD2	4.42	125.45	131.20	1	1
F	94	HIS	CB-CG-CD2	4.42	125.46	131.20	1	1
E	111	GLN	OE1-CD-NE2	4.41	118.19	122.60	1	1
C	1018	GLN	OE1-CD-NE2	4.41	118.19	122.60	1	1
C	762	GLN	OE1-CD-NE2	4.41	118.19	122.60	1	1
C	908	HIS	CB-CG-CD2	4.41	125.47	131.20	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
D	50	GLN	OE1-CD-NE2	4.40	118.20	122.60	1	1
E	10	GLN	OE1-CD-NE2	4.40	118.20	122.60	1	1
D	82	GLN	OE1-CD-NE2	4.40	118.20	122.60	1	1
C	270	ASN	OD1-CG-ND2	4.39	118.21	122.60	1	1
A	477	ASP	CA-CB-CG	4.39	116.99	112.60	1	1
A	116	ASN	CA-CB-CG	4.39	108.21	112.60	1	1
E	208	HIS	CB-CG-CD2	4.39	125.49	131.20	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	0.32	16

There are 16 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:191:ARG:HD3	A:256:THR:HG21	0.55	1	1
A:531:GLN:HE21	A:549:TRP:CG	0.55	1	1
C:1112:VAL:HG22	C:1132:LEU:HD12	0.51	1	1
A:245:LYS:HE2	A:249:GLU:OE2	0.47	1	1
B:264:MET:HE1	B:298:TYR:CD1	0.46	1	1
C:1108:MET:O	C:1112:VAL:HG23	0.45	1	1
C:682:MET:HE2	C:694:LEU:HD22	0.44	1	1
E:52:VAL:CG1	E:80:LEU:HD11	0.42	1	1
C:1005:GLU:HG3	C:1039:MET:SD	0.42	1	1
E:373:ARG:HG3	E:507:MET:HE2	0.42	1	1
C:582:LYS:HE2	C:584:MET:SD	0.41	1	1
E:14:ARG:HA	E:15:PRO:HD3	0.41	1	1
F:124:ASP:HA	F:125:PRO:HD3	0.41	1	1
A:531:GLN:HE21	A:549:TRP:CD1	0.41	1	1
E:1:GLY:HA3	E:2:PRO:HD3	0.41	1	1
C:495:GLU:HA	C:496:PRO:HD3	0.40	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	3106	2964	122	20

*There are 20 unique backbone outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	14	PRO	1
A	28	PHE	1
A	383	ASN	1
A	425	GLY	1
B	123	LYS	1
B	275	ASP	1
C	39	ASN	1
C	567	ILE	1
E	2	PRO	1
E	10	GLN	1
E	11	PRO	1
E	12	SER	1
E	15	PRO	1
E	33	ASP	1
E	37	GLY	1
E	355	ASP	1
F	122	ASN	1
F	125	PRO	1
F	128	PRO	1
F	131	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	2761	2668	63	30

*There are 30 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	59	ILE	1



Chain	Res	Type	Models (Total)
A	73	LEU	1
A	374	PHE	1
A	419	LEU	1
A	700	TYR	1
B	178	ASN	1
B	258	ASN	1
B	373	HIS	1
C	4	MET	1
C	128	ASP	1
C	416	LEU	1
C	536	GLU	1
C	764	LEU	1
C	898	THR	1
C	973	ASN	1
C	1035	THR	1
E	23	THR	1
E	27	THR	1
E	80	LEU	1
E	103	LEU	1
E	113	HIS	1
E	209	ASP	1
E	295	ARG	1
E	313	ASP	1
E	346	ASP	1
E	602	TYR	1
E	610	THR	1
F	99	THR	1
F	126	THR	1
F	135	ARG	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 1534 crosslinking restraints combined in 1534 restraint groups.

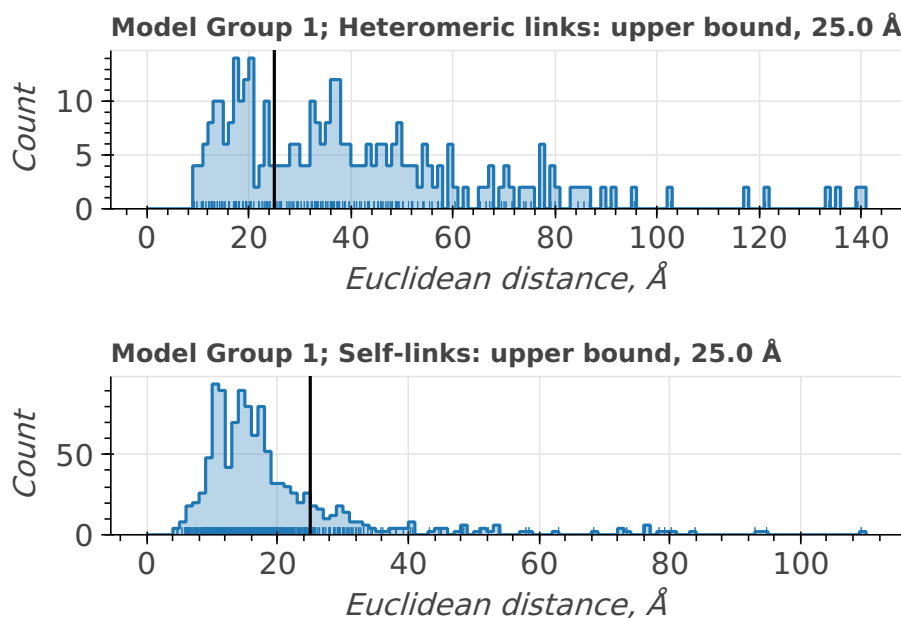
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
SDA	GLU	CA	SER	CA	upper bound	25.0	30
SDA	CYS	CA	LYS	CA	upper bound	25.0	8
SDA	LEU	CA	LYS	CA	upper bound	25.0	66
SDA	GLU	CA	LYS	CA	upper bound	25.0	218
SDA	PHE	CA	THR	CA	upper bound	25.0	4
SDA	ASN	CA	LYS	CA	upper bound	25.0	34
SDA	LYS	CA	TYR	CA	upper bound	25.0	118
SDA	ASP	CA	THR	CA	upper bound	25.0	20
SDA	LEU	CA	TYR	CA	upper bound	25.0	16
SDA	CYS	CA	SER	CA	upper bound	25.0	4
SDA	LEU	CA	THR	CA	upper bound	25.0	16
SDA	LYS	CA	VAL	CA	upper bound	25.0	68
SDA	HIS	CA	LYS	CA	upper bound	25.0	64
SDA	ILE	CA	LYS	CA	upper bound	25.0	44
SDA	LYS	CA	TRP	CA	upper bound	25.0	6
SDA	ASP	CA	TYR	CA	upper bound	25.0	16
SDA	GLY	CA	TYR	CA	upper bound	25.0	16
SDA	GLN	CA	THR	CA	upper bound	25.0	8
SDA	LYS	CA	THR	CA	upper bound	25.0	34
SDA	ASP	CA	LYS	CA	upper bound	25.0	106
SDA	LYS	CA	LYS	CA	upper bound	25.0	56
SDA	ALA	CA	LYS	CA	upper bound	25.0	86
SDA	MET	CA	SER	CA	upper bound	25.0	8
SDA	GLU	CA	THR	CA	upper bound	25.0	34
SDA	GLU	CA	TYR	CA	upper bound	25.0	26
SDA	SER	CA	TYR	CA	upper bound	25.0	8
SDA	THR	CA	VAL	CA	upper bound	25.0	12
SDA	SER	CA	SER	CA	upper bound	25.0	4
SDA	ILE	CA	TYR	CA	upper bound	25.0	14
SDA	LEU	CA	SER	CA	upper bound	25.0	20
SDA	LYS	CA	SER	CA	upper bound	25.0	32

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
SDA	SER	CA	THR	CA	upper bound	25.0	4
SDA	ILE	CA	SER	CA	upper bound	25.0	10
SDA	HIS	CA	SER	CA	upper bound	25.0	8
SDA	SER	CA	VAL	CA	upper bound	25.0	12
SDA	ALA	CA	GLU	CA	upper bound	25.0	8
SDA	ALA	CA	THR	CA	upper bound	25.0	16
SDA	ALA	CA	GLY	CA	upper bound	25.0	6
SDA	THR	CA	TYR	CA	upper bound	25.0	10
SDA	GLY	CA	LYS	CA	upper bound	25.0	40
SDA	LYS	CA	PRO	CA	upper bound	25.0	12
SDA	ALA	CA	ILE	CA	upper bound	25.0	2
SDA	ALA	CA	MET	CA	upper bound	25.0	2
SDA	ALA	CA	TYR	CA	upper bound	25.0	12
SDA	GLY	CA	THR	CA	upper bound	25.0	8
SDA	ARG	CA	SER	CA	upper bound	25.0	4
SDA	GLU	CA	GLY	CA	upper bound	25.0	10
SDA	GLY	CA	GLY	CA	upper bound	25.0	2
SDA	GLN	CA	LYS	CA	upper bound	25.0	30
SDA	LYS	CA	MET	CA	upper bound	25.0	10
SDA	LYS	CA	PHE	CA	upper bound	25.0	26
SDA	HIS	CA	TYR	CA	upper bound	25.0	4
SDA	ASP	CA	SER	CA	upper bound	25.0	4
SDA	CYS	CA	THR	CA	upper bound	25.0	4
SDA	ALA	CA	SER	CA	upper bound	25.0	12
SDA	ARG	CA	LYS	CA	upper bound	25.0	4
SDA	PRO	CA	SER	CA	upper bound	25.0	2
SDA	PHE	CA	SER	CA	upper bound	25.0	8
SDA	PRO	CA	TYR	CA	upper bound	25.0	2
SDA	MET	CA	THR	CA	upper bound	25.0	4
SDA	ASN	CA	TYR	CA	upper bound	25.0	2
SDA	MET	CA	TYR	CA	upper bound	25.0	2
SDA	ASN	CA	SER	CA	upper bound	25.0	2
SDA	ARG	CA	TYR	CA	upper bound	25.0	2
SDA	ILE	CA	THR	CA	upper bound	25.0	4
SDA	GLN	CA	SER	CA	upper bound	25.0	4

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
SDA	CYS	CA	GLY	CA	upper bound	25.0	8
SDA	THR	CA	THR	CA	upper bound	25.0	2
SDA	CYS	CA	TYR	CA	upper bound	25.0	2
SDA	GLN	CA	TYR	CA	upper bound	25.0	10
SDA	TYR	CA	TYR	CA	upper bound	25.0	6
SDA	GLY	CA	PHE	CA	upper bound	25.0	2
SDA	GLY	CA	LEU	CA	upper bound	25.0	2
SDA	GLY	CA	SER	CA	upper bound	25.0	2
SDA	TYR	CA	VAL	CA	upper bound	25.0	2
SDA	PHE	CA	TYR	CA	upper bound	25.0	2
SDA	SER	CA	TRP	CA	upper bound	25.0	2
SDA	ALA	CA	PRO	CA	upper bound	25.0	2
SDA	HIS	CA	THR	CA	upper bound	25.0	2
SDA	ALA	CA	ALA	CA	upper bound	25.0	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

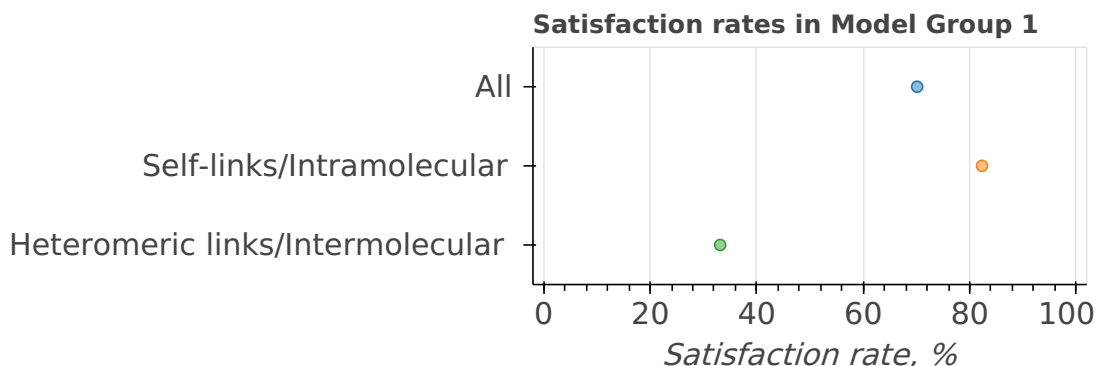
*Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of*

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=1534)
1	1	1	1/1	All	70.14	29.86	1534
				Self-links/ Intramolecular	82.32	17.68	1154
				Heteromeric links/ Intermolecular	33.16	66.84	380

#### 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.*