

# Integrative Structure Validation Report ?

April 09, 2025 - 04:21 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	8ZZT
PDB-Dev ID	PDBDEV_00000029
Structure Title	Complex of UbchH5c, RNF168-RING domain and the nucleosome
Structure Authors	Horn V; Uckelmann M; Zhang H; Eerland J; Aarsman I; le Paige UB; Davidovich C; Sixma TK; van Ingen H
Deposited on	2019-02-18

*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)*

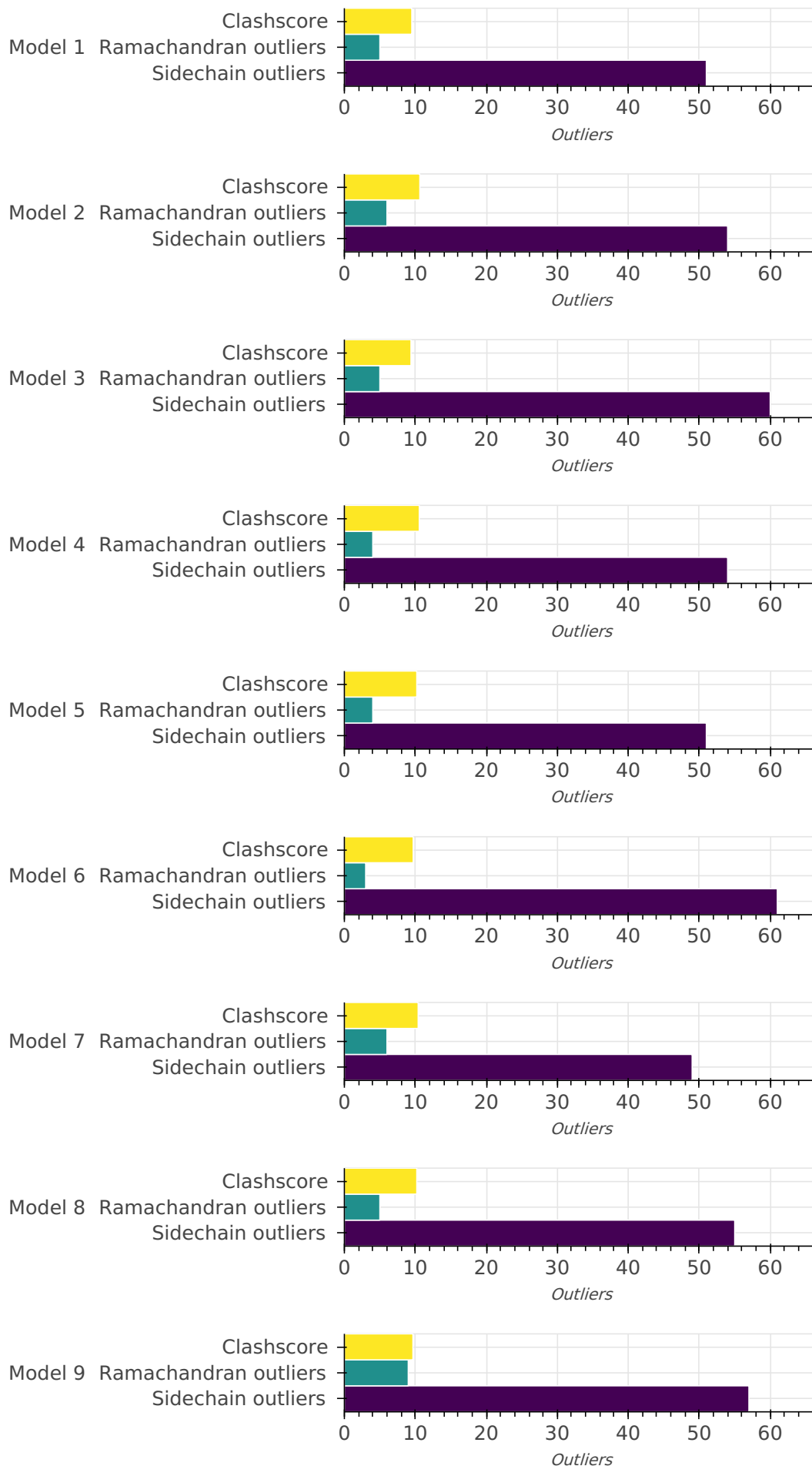
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

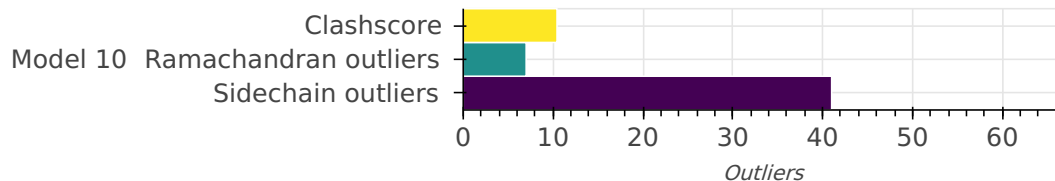
*List of references used to build this report is available [here](#).*

## 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 10 model(s). A total of 3 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	1-10	1	H3	A	99	-	1-99	100.00 / 100.00	Atomic
				E					
		2	H4	B	80	-	1-80	100.00 / 100.00	Atomic
				F					
		3	H2A N18S mutant	C	107	-	1-107	100.00 / 100.00	Atomic
				G					
		4	H2B S121A mutant	D	95	-	1-95	100.00 / 100.00	Atomic
				H					
		5	DNA strand 1	I	147	-	1-147	100.00 / 100.00	Atomic
		6	DNA strand 2	J	147	-	1-147	100.00 / 100.00	Atomic
		7	RNF168 RING domain	K	91	-	1-91	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
		8	Ubch5c	L	153	-	1-153	100.00 / 100.00	Atomic

### Datasets used for modeling ?

*There are 3 unique datasets used to build the models in this entry.*

ID	Dataset type	Database name	Data access code
1	Integrative model	PDB	<a href="#">8ZZS</a>
2	Experimental model	PDB	<a href="#">1X23</a>
3	Other	Not available	<a href="#">10.1038/s41467-019-09756-z</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	None	None	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="#">HADDOCK</a>	2.20	molecular docking	<a href="http://haddock.science.uu.nl/services/HADDOCK/">http://haddock.science.uu.nl/services/HADDOCK/</a>

### Data quality ?

### 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 no bond angle outliers.

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	9.50	244
2	10.63	273
3	9.38	241
4	10.55	271
5	10.20	262
6	9.70	249
7	10.40	267
8	10.20	262
9	9.66	248
10	10.44	268

There are 2585 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)
K:50:PRO:HB3	L:101:PRO:HD2	1.11	8	7
I:88:DG:H4'	I:89:DC:H5'	0.93	5	6
B:65:VAL:HG21	B:79:GLY:HA3	0.90	10	5
J:88:DG:H4'	J:89:DC:H5'	0.90	9	8
I:58:DG:H4'	I:59:DG:H5'	0.88	4	7
A:49:GLN:HA	I:50:DC:H5''	0.85	2	7
L:41:ALA:HB3	L:58:LEU:HB2	0.84	1	10
L:100:SER:HB3	L:103:LEU:HG	0.84	2	4
A:81:VAL:HB	B:22:LYS:HD3	0.84	6	1
J:103:DA:H2'	J:104:DG:C8	0.83	9	9
B:56:ARG:HD3	J:102:DC:H3'	0.82	2	5
C:44:TYR:HB2	D:83:GLU:HG3	0.82	4	2
D:9:ILE:HD11	J:122:DG:H5''	0.82	7	3
E:30:PRO:HD3	I:91:DT:H5''	0.81	7	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
L:100:SER:HB2	L:103:LEU:HG	0.81	4	6
K:39:GLN:HA	K:43:GLU:HB2	0.81	1	1
J:31:DG:H2'	J:32:DT:C6	0.81	2	7
B:22:LYS:HB2	G:102:LEU:HD22	0.81	6	1
I:55:DA:H1'	I:56:DA:C8	0.81	5	9
B:25:SER:HA	J:81:DT:H5''	0.80	7	7
E:80:ARG:HD3	J:71:DG:H3'	0.78	3	5
L:81:HIS:HE1	L:116:LEU:HA	0.78	3	2
H:7:TYR:HA	H:10:TYR:HD2	0.78	5	8
F:10:PRO:HG2	J:61:DA:H2'	0.77	1	5
J:79:DG:H1'	J:80:DC:C5	0.77	8	7
I:8:DT:H2'	I:9:DC:C6	0.77	3	3
L:41:ALA:HB2	L:60:ILE:HD11	0.77	3	3
D:90:LYS:HG2	L:97:SER:HB2	0.77	7	3
J:58:DG:H4'	J:59:DG:H5'	0.76	8	3
A:67:LEU:HA	A:95:ARG:HH22	0.76	6	5
B:12:ILE:HA	B:15:LEU:HD12	0.76	4	7
D:34:SER:HB2	F:76:TYR:HB3	0.76	3	3
L:11:ARG:HD3	L:67:PRO:HG3	0.76	8	1
J:32:DT:H3'	J:33:DG:C8	0.76	4	3
J:121:DT:H4'	J:122:DG:H5'	0.75	10	1
C:4:ARG:HG3	I:31:DG:H5'	0.75	2	2
J:31:DG:H3'	J:32:DT:H71	0.75	9	1
J:33:DG:H5''	J:34:DT:H71	0.75	7	2
I:45:DT:H2'	I:46:DG:C8	0.75	4	9
I:49:DC:H4'	I:50:DC:OP1	0.74	6	9
J:9:DC:H2'	J:10:DC:C6	0.74	1	1
I:88:DG:H1'	I:89:DC:C5	0.74	2	8
J:74:DT:H2'	J:75:DT:C6	0.74	8	8
L:5:GLU:HB3	L:64:THR:HG23	0.74	7	1
I:47:DC:H2'	I:48:DT:C6	0.74	3	8
C:3:SER:HA	I:31:DG:H5'	0.73	7	5
I:131:DT:H4'	I:132:DG:OP3	0.73	8	6
J:32:DT:H3'	J:33:DG:H8	0.73	4	2
I:77:DC:H4'	I:78:DA:OP1	0.73	1	3

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
L:69:LYS:HD2	L:70:PRO:HD2	0.73	7	2
E:5:TYR:HA	J:145:DG:H5''	0.73	6	1
K:16:ILE:HG21	L:68:PHE:CE1	0.72	3	5
I:28:DA:H2'	I:29:DA:O4'	0.72	2	7
E:27:ARG:NH2	J:60:DC:H5'	0.72	7	3
L:3:SER:HB3	L:6:PHE:HB2	0.72	9	2
I:60:DC:H2'	I:61:DA:C8	0.72	8	9
A:29:LEU:HB3	J:91:DT:H5''	0.72	8	7
C:88:THR:HG21	E:62:ALA:HB1	0.72	8	1
J:10:DC:H2'	J:11:DA:C8	0.72	3	6
L:26:GLN:HB3	L:44:MET:HB2	0.72	1	7
C:4:ARG:HA	C:7:ARG:HD3	0.72	10	2
J:49:DC:H4'	J:50:DC:OP3	0.71	5	8
I:99:DG:H4'	I:100:DA:OP3	0.71	10	6
E:43:LYS:HB3	E:46:LEU:HD11	0.71	8	8
J:40:DG:H4'	J:41:DA:OP3	0.71	2	2
D:7:TYR:HA	D:10:TYR:HD2	0.71	4	6
J:88:DG:H1'	J:89:DC:C5	0.71	8	7
J:14:DT:H1'	J:15:DG:C8	0.71	8	3
J:57:DA:H2'	J:57:DA:OP3	0.70	4	1
J:11:DA:H2'	J:12:DC:O4'	0.70	3	8
I:139:DG:H2'	I:140:DA:C8	0.70	1	1
E:70:ASP:HA	E:73:LEU:HD12	0.70	10	1
D:5:GLU:HA	J:123:DG:H5''	0.70	10	6
E:26:ILE:HB	E:57:GLN:HE22	0.70	7	1
E:25:LEU:HD22	F:14:ARG:HB3	0.70	4	10
J:42:DA:H2'	J:43:DA:C8	0.69	6	4
J:57:DA:H4'	J:58:DG:OP1	0.69	4	3
E:68:PHE:HE2	F:15:LEU:HB3	0.69	5	1
J:16:DC:H4'	J:17:DA:OP1	0.69	8	5
I:72:DG:H2'	I:73:DA:C8	0.69	1	4
E:51:SER:HB2	F:61:ALA:HB2	0.69	6	4
B:76:TYR:HB3	H:31:ILE:HG23	0.69	3	3
J:60:DC:H2'	J:61:DA:C8	0.69	9	5
L:91:CYS:SG	L:125:LEU:HG	0.69	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
H:68:VAL:HG13	H:72:LEU:HD12	0.68	2	9
A:29:LEU:HD23	J:91:DT:H5''	0.68	6	5
J:77:DC:H2'	J:77:DC:OP1	0.68	5	4
J:77:DC:H4'	J:78:DA:OP3	0.68	7	3
J:124:DT:H2'	J:125:DA:C8	0.68	10	3
I:67:DA:H1'	I:68:DG:N7	0.68	2	7
I:99:DG:H1'	I:100:DA:C8	0.68	7	7
C:31:GLY:HA2	J:112:DA:H5'	0.68	3	2
J:38:DT:H2'	J:38:DT:OP1	0.68	6	7
I:36:DT:H2'	I:37:DT:C6	0.68	5	3
L:39:TRP:HB2	L:60:ILE:HB	0.68	7	4
G:28:GLU:HB3	H:57:SER:HB2	0.68	9	4
J:34:DT:H4'	J:35:DA:OP1	0.67	1	4
I:88:DG:H1'	I:89:DC:C6	0.67	7	8
C:2:LYS:HG2	C:7:ARG:HG3	0.67	1	1
I:14:DT:H2'	I:14:DT:OP1	0.67	10	5

### 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	986	940	41	5
2	986	929	51	6
3	986	943	38	5
4	986	943	39	4
5	986	945	37	4
6	986	941	42	3
7	986	938	42	6
8	986	941	40	5
9	986	940	37	9
10	986	937	42	7

There are 17 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
C	105	LYS	10
G	106	LYS	10



Chain	Res	Type	Models (Total)
E	7	PRO	4
H	73	PRO	4
H	74	GLY	4
A	7	PRO	3
C	106	LYS	3
D	2	LYS	3
L	124	PRO	3
K	7	PRO	2
K	43	GLU	2
A	45	ASP	1
D	73	PRO	1
K	16	ILE	1
K	40	SER	1
K	46	SER	1
L	99	TRP	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	853	743	59	51
2	853	735	64	54
3	853	736	57	60
4	853	740	59	54
5	853	728	74	51
6	853	737	55	61
7	853	749	55	49
8	853	721	77	55
9	853	741	55	57
10	853	744	68	41

*There are 159 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100 rows.*

Chain	Res	Type	Models (Total)
C	85	SER	10
G	63	THR	10

Chain	Res	Type	Models (Total)
K	57	SER	10
L	106	SER	10
L	113	CYS	10
A	51	SER	9
D	61	SER	9
E	44	THR	9
E	45	ASP	9
G	85	SER	9
H	61	SER	9
K	41	THR	9
B	74	THR	8
C	6	SER	8
D	26	SER	8
E	51	SER	8
F	51	THR	8
F	74	THR	8
L	27	CYS	8
A	44	THR	7
C	5	SER	7
C	82	LYS	7
D	93	SER	7
E	22	THR	7
G	3	SER	7
K	58	SER	7
L	81	HIS	7
A	22	THR	6
B	51	THR	6
E	13	ARG	6
L	13	ASN	6
L	28	SER	6
L	34	ASP	6
L	75	PHE	6
L	97	SER	6
A	40	GLN	5
B	46	ASP	5

Chain	Res	Type	Models (Total)
C	3	SER	5
C	88	THR	5
D	22	THR	5
E	9	THR	5
E	23	GLU	5
H	6	SER	5
H	93	SER	5
K	1	LEU	5
K	10	SER	5
L	18	ASP	5
L	93	ASP	5
A	32	GLN	4
A	50	SER	4
C	63	THR	4
G	5	SER	4
K	47	LEU	4
L	3	SER	4
L	64	THR	4
L	76	THR	4
L	89	SER	4
L	146	GLU	4
A	3	HIS	3
A	28	LYS	3
D	15	LEU	3
D	21	ASP	3
E	27	ARG	3
E	50	SER	3
G	55	ASN	3
H	22	THR	3
H	57	SER	3
K	8	SER	3
K	34	CYS	3
K	89	ARG	3
L	32	VAL	3
L	86	SER	3

Chain	Res	Type	Models (Total)
L	87	ASN	3
L	104	THR	3
A	21	SER	2
A	41	ASP	2
B	23	ARG	2
C	25	ASN	2
G	25	ASN	2
G	88	THR	2
H	21	ASP	2
H	65	GLN	2
K	14	CYS	2
K	29	CYS	2
K	40	SER	2
K	46	SER	2
K	52	CYS	2
K	68	SER	2
L	42	THR	2
L	48	ASP	2
L	59	THR	2
L	61	HIS	2
L	114	SER	2
L	118	ASP	2
L	138	ASP	2
L	153	MET	2
A	48	PHE	1
A	56	LEU	1
B	2	ASP	1
B	12	ILE	1

Fit of model to data used for modeling ?

Fit of model to data used for validation ?

Validation for this section is under development.

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### *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.*