



wwPDB EM Validation Summary Report ⓘ

Apr 9, 2025 – 03:17 PM JST

PDB ID : 9IPU / pdb_00009ipu
EMDB ID : EMD-60781
Title : cryo-EM structure of the RNF168(1-193)/UbcH5c-Ub ubiquitylation module bound to H1.0-K63-Ub3 modified chromosome
Authors : Ai, H.S.; Deng, Z.H.; Liu, L.
Deposited on : 2024-07-11
Resolution : 4.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

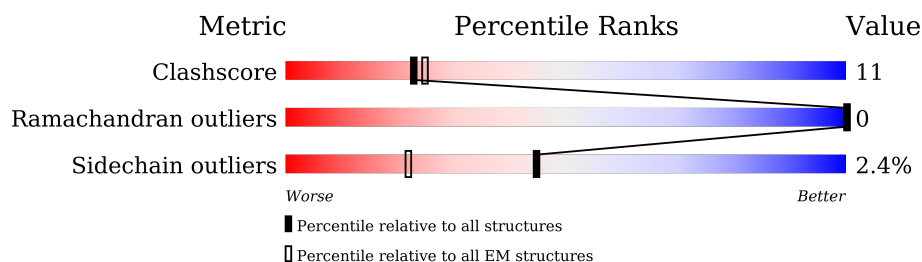
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	I	194	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	129	
4	G	129	
5	D	125	
5	H	125	

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Mol	Chain	Length	Quality of chain
6	K	147	 72%28%
7	L	193	 33%9%57%
8	M	75	 61%20%19%
9	J	171	 56%38%6%
10	N	171	 58%38%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15750 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H1.0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	72	Total	C	N	O	S	0	0
			526	327	97	100	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	82	CYS	LYS	conflict	UNP P07305

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	98	Total	C	N	O	S	0	0
			810	511	157	140	2		
2	E	97	Total	C	N	O	S	0	0
			801	505	155	139	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	CYS	conflict	UNP Q71DI3
E	110	SER	CYS	conflict	UNP Q71DI3

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	83	Total	C	N	O	S	0	0
			668	422	132	113	1		
3	F	83	Total	C	N	O	S	0	0
			662	419	129	113	1		

- Molecule 4 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	109	Total	C	N	O	S	0	0
			833	523	164	145	1		
4	G	109	Total	C	N	O	S	0	0
			833	523	164	145	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	CYS	LYS	conflict	UNP P04908
G	15	CYS	LYS	conflict	UNP P04908

- Molecule 5 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	94	Total	C	N	O	S	0	0
			735	461	134	138	2		
5	H	94	Total	C	N	O	S	0	0
			735	461	134	138	2		

- Molecule 6 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	147	Total	C	N	O	S	0	0
			1125	726	187	207	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	21	SER	CYS	conflict	UNP P61077
K	107	SER	CYS	conflict	UNP P61077
K	111	SER	CYS	conflict	UNP P61077

- Molecule 7 is a protein called E3 ubiquitin-protein ligase RNF168.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	83	Total	C	N	O	S	0	0
			641	404	115	112	10		

- Molecule 8 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	61	Total	C	N	O	S	0	0
			407	251	68	87	1		

- Molecule 9 is a DNA chain called DNA (171-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	170	Total	C	N	O	P	0	0
			3488	1653	645	1020	170		

- Molecule 10 is a DNA chain called DNA (171-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	170	Total	C	N	O	P	0	0
			3484	1652	643	1019	170		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	L	2	Total	Zn	0
			2	2	

GLY

- Molecule 3: Histone H4

Chain F:  61% 21% 19%



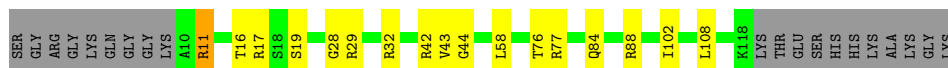
- Molecule 4: Histone H2A type 1-B/E

Chain C:  72% 12% 16%



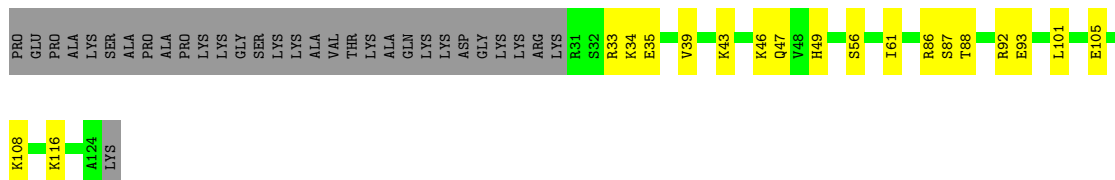
- Molecule 4: Histone H2A type 1-B/E

Chain G:  71% 12% 16%



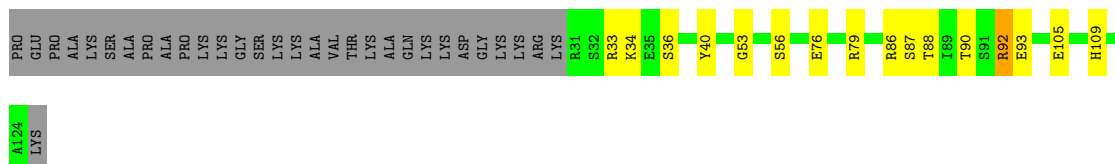
- Molecule 5: Histone H2B type 1-K

Chain D:  60% 15% 25%



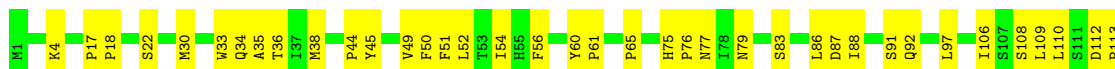
- Molecule 5: Histone H2B type 1-K

Chain H:  62% 12% 25%



- Molecule 6: Ubiquitin-conjugating enzyme E2 D3

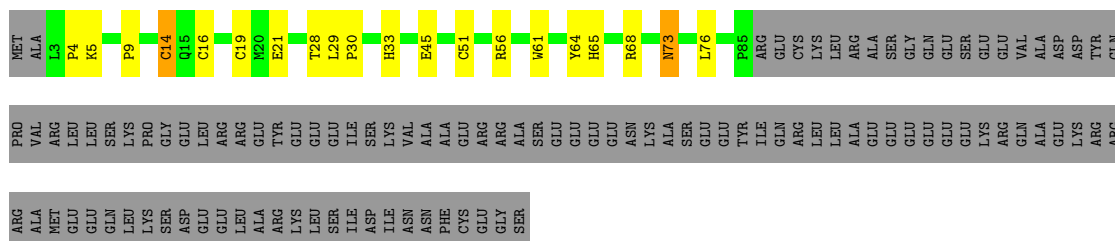
Chain K:  72% 28%





• Molecule 7: E3 ubiquitin-protein ligase RNF168

Chain L: 33% 9% 57%



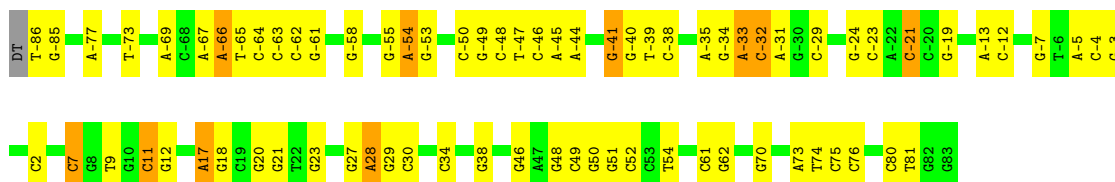
• Molecule 8: Ubiquitin

Chain M: 61% 20% 19%



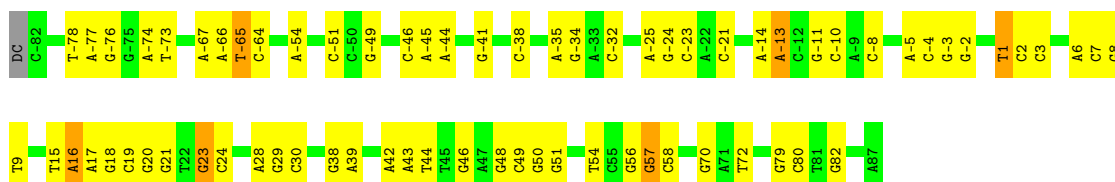
• Molecule 9: DNA (171-MER)

Chain J: 56% 38% 6%



• Molecule 10: DNA (171-MER)

Chain N: 58% 38% 4%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36240	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	I	0.59	0/532	0.79	1/716 (0.1%)
2	A	0.34	0/822	0.55	0/1102
2	E	0.33	0/813	0.55	0/1090
3	B	0.35	0/675	0.58	0/903
3	F	0.35	0/669	0.58	0/896
4	C	0.32	0/843	0.53	0/1139
4	G	0.30	0/843	0.52	0/1139
5	D	0.34	0/746	0.48	0/1003
5	H	0.32	0/746	0.48	0/1003
6	K	0.27	0/1160	0.43	0/1589
7	L	0.25	0/658	0.53	0/902
8	M	0.25	0/409	0.42	0/556
9	J	0.82	6/3913 (0.2%)	1.32	28/6038 (0.5%)
10	N	0.81	6/3908 (0.2%)	1.30	28/6029 (0.5%)
All	All	0.61	12/16737 (0.1%)	1.00	57/24105 (0.2%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	79	DG	C3'-O3'	-7.20	1.34	1.44
10	N	-78	DT	C1'-N1	6.26	1.57	1.49
10	N	-77	DA	C3'-O3'	5.98	1.51	1.44
10	N	82	DG	C3'-O3'	-5.94	1.36	1.44
9	J	-69	DA	C3'-O3'	-5.92	1.36	1.44

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	21	DG	O4'-C1'-N9	9.69	114.78	108.00
10	N	54	DT	P-O3'-C3'	8.00	129.30	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	54	DT	P-O3'-C3'	7.60	128.82	119.70
9	J	-58	DG	P-O3'-C3'	7.58	128.79	119.70
10	N	-2	DG	O4'-C1'-N9	7.39	113.17	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	526	0	524	4	0
2	A	810	0	851	45	0
2	E	801	0	839	48	0
3	B	668	0	719	21	0
3	F	662	0	708	20	0
4	C	833	0	883	23	0
4	G	833	0	883	21	0
5	D	735	0	756	31	0
5	H	735	0	756	36	0
6	K	1125	0	1079	31	0
7	L	641	0	613	15	0
8	M	407	0	325	9	0
9	J	3488	0	1908	96	0
10	N	3484	0	1908	105	0
11	L	2	0	0	0	0
All	All	15750	0	12752	314	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 314 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:49:ARG:HH12	10:N:-66:DA:C5'	1.11	1.59
2:E:49:ARG:NH1	10:N:-66:DA:H5''	1.12	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:ARG:NH1	9:J:-66:DA:H5''	1.08	1.39
2:A:45:THR:HG21	10:N:70:DG:OP1	1.30	1.27
2:A:49:ARG:CZ	9:J:-66:DA:H5''	1.64	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	70/194 (36%)	69 (99%)	1 (1%)	0	100	100
2	A	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
2	E	95/135 (70%)	93 (98%)	2 (2%)	0	100	100
3	B	81/102 (79%)	75 (93%)	6 (7%)	0	100	100
3	F	81/102 (79%)	79 (98%)	2 (2%)	0	100	100
4	C	107/129 (83%)	104 (97%)	3 (3%)	0	100	100
4	G	107/129 (83%)	107 (100%)	0	0	100	100
5	D	92/125 (74%)	91 (99%)	1 (1%)	0	100	100
5	H	92/125 (74%)	89 (97%)	3 (3%)	0	100	100
6	K	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
7	L	81/193 (42%)	71 (88%)	10 (12%)	0	100	100
8	M	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
All	All	1100/1591 (69%)	1060 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	54/158 (34%)	54 (100%)	0	100	100
2	A	86/110 (78%)	83 (96%)	3 (4%)	31	53
2	E	85/110 (77%)	83 (98%)	2 (2%)	44	64
3	B	69/78 (88%)	63 (91%)	6 (9%)	8	26
3	F	68/78 (87%)	66 (97%)	2 (3%)	37	58
4	C	84/99 (85%)	82 (98%)	2 (2%)	44	64
4	G	84/99 (85%)	83 (99%)	1 (1%)	67	79
5	D	80/104 (77%)	78 (98%)	2 (2%)	42	63
5	H	80/104 (77%)	79 (99%)	1 (1%)	65	77
6	K	120/132 (91%)	119 (99%)	1 (1%)	79	85
7	L	74/176 (42%)	72 (97%)	2 (3%)	40	60
8	M	35/68 (52%)	35 (100%)	0	100	100
All	All	919/1316 (70%)	897 (98%)	22 (2%)	45	64

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	129	ARG
4	G	11	ARG
3	F	67	ARG
5	H	92	ARG
3	B	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	68	GLN
8	M	25	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.