



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:38 PM UTC

PDB ID : 8UQC / pdb_00008uqc
Title : Crystal structure of RNF168 (RING)-UbcH5c fused to H2A-H2B via a 20-residue linker (crystallization condition 2)
Authors : Hu, Q.; Botuyan, M.V.; Mer, G.
Deposited on : 2023-10-23
Resolution : 2.61 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

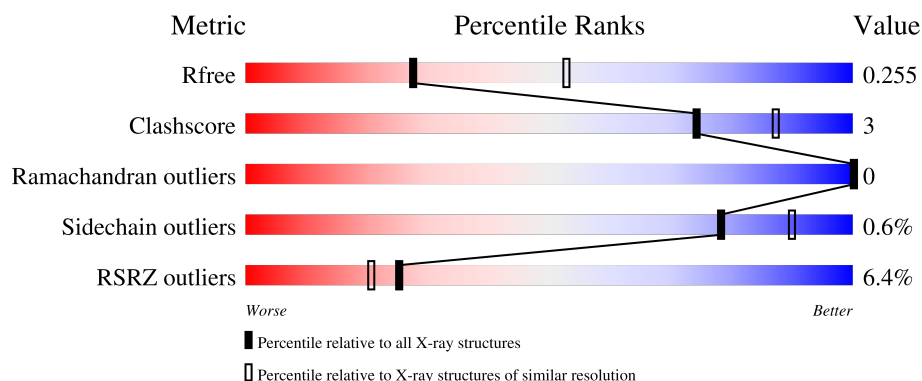
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	6% 85% 8% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6639 atoms, of which 3321 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 E3 ubiquitin-protein ligase RNF168, Ubiquitin-conjugating enzyme E2 D3, Histone H2B type 2-E, Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	420	Total	C	H	N	O	S	81	1	0
			6614	2078	3321	595	601	19			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8IYW5
A	0	HIS	-	expression tag	UNP Q8IYW5
A	95	SER	-	linker	UNP Q8IYW5
A	96	GLY	-	linker	UNP Q8IYW5
A	97	SER	-	linker	UNP Q8IYW5
A	98	GLY	-	linker	UNP Q8IYW5
A	99	SER	-	linker	UNP Q8IYW5
A	100	GLY	-	linker	UNP Q8IYW5
A	101	SER	-	linker	UNP Q8IYW5
A	1085	LYS	CYS	engineered mutation	UNP P61077
A	1148	GLY	-	linker	UNP P61077
A	1149	GLY	-	linker	UNP P61077
A	1150	SER	-	linker	UNP P61077
A	1151	GLY	-	linker	UNP P61077
A	1152	GLY	-	linker	UNP P61077
A	1153	GLY	-	linker	UNP P61077
A	1154	SER	-	linker	UNP P61077
A	1155	GLY	-	linker	UNP P61077
A	1156	GLY	-	linker	UNP P61077
A	1157	SER	-	linker	UNP P61077
A	1158	GLY	-	linker	UNP P61077
A	1159	GLY	-	linker	UNP P61077
A	1160	SER	-	linker	UNP P61077
A	1161	GLY	-	linker	UNP P61077
A	1162	GLY	-	linker	UNP P61077
A	1163	SER	-	linker	UNP P61077

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1164	GLY	-	linker	UNP P61077
A	1165	SER	-	linker	UNP P61077
A	1166	GLY	-	linker	UNP P61077
A	1167	SER	-	linker	UNP P61077
A	3011	SER	-	linker	UNP Q16778

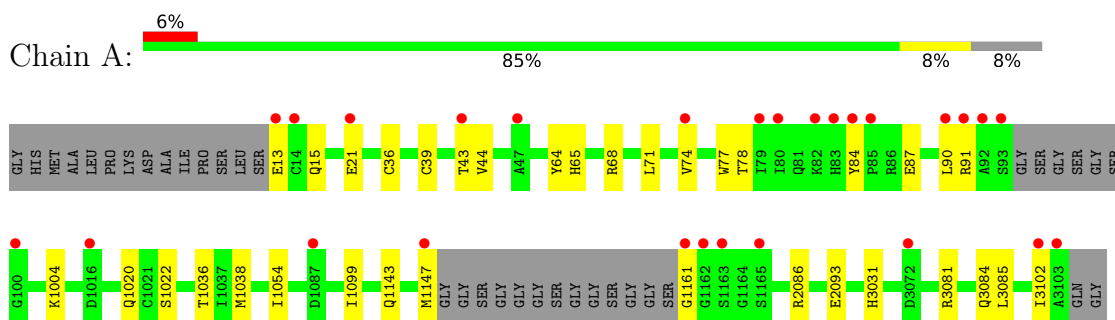
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		

- Molecule 1: E3 ubiquitin-protein ligase RNF168, Ubiquitin-conjugating enzyme E2 D3, Histone H2B type 2-E, Histone H2A type 1-B/E



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.98Å 101.98Å 86.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.94 – 2.61 43.94 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.94-2.61) 99.9 (43.94-2.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.252 0.228 , 0.255	Depositor DCC
R_{free} test set	1620 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6639	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.21	1/3366 (0.0%)	0.30	0/4558

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3031	HIS	ND1-CE1	-6.04	1.26	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	3293	3321	3321	20	0
2	A	2	0	0	0	0
3	A	23	0	0	0	0
All	All	3318	3321	3321	20	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 3.

The worst 5 of 20 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)
1:A:13:GLU:N	1:A:13:GLU:OE1	2.15	0.80
1:A:74:VAL:O	1:A:78:THR:HG23	1.93	0.68
1:A:1020:GLN:HA	1:A:1038:MET:HE3	1.85	0.58
1:A:43:THR:HG23	1:A:44:VAL:HG23	1.89	0.53
1:A:1022:SER:OG	1:A:1036:THR:OG1	2.29	0.51

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	415/455 (91%)	405 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	361/383 (94%)	359 (99%)	2 (1%)	78	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	TRP
1	A	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1046	GLN
1	A	1143	GLN
1	A	3084	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	420/455 (92%)	0.31	27 (6%) 25 21	14, 43, 87, 115	9 (2%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3103	ALA	6.0
1	A	80	ILE	5.0
1	A	82	LYS	4.0
1	A	13	GLU	3.6
1	A	1161	GLY	3.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	4001	1/1	0.99	0.04	45,45,45,45	0
2	ZN	A	4002	1/1	0.99	0.03	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.