



wwPDB X-ray Structure Validation Summary Report ⓘ

May 6, 2025 – 04:31 PM JST

PDB ID : 9LHJ / pdb_00009lhj
Title : UBE2N/UBE2V2 complexed with a covalent inhibitor
Authors : Li, S.; Wu, X.; Zhou, L.; Lu, X.
Deposited on : 2025-01-12
Resolution : 1.68 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

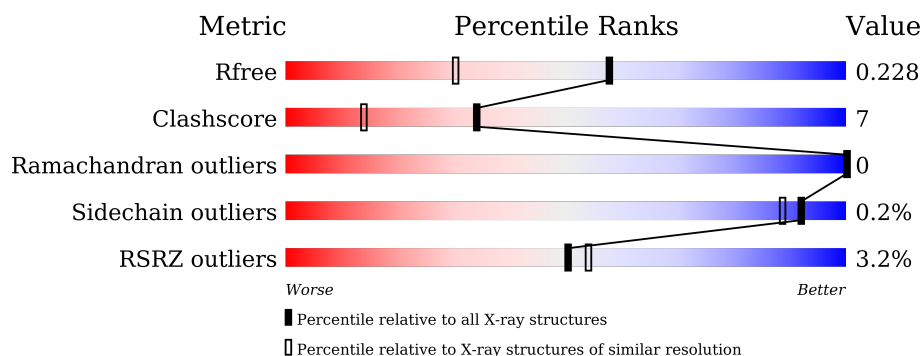
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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}	164625	8422 (1.70-1.66)
Clashscore	180529	1005 (1.68-1.68)
Ramachandran outliers	177936	9065 (1.70-1.66)
Sidechain outliers	177891	9064 (1.70-1.66)
RSRZ outliers	164620	8421 (1.70-1.66)

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	152	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	152	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>•</div> </div> </div>
2	C	145	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div> </div>
2	D	145	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5324 atoms, of which 64 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 Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	146	Total	C	F	H	N	O	S	0	0	0
			1234	773	1	32	208	216	4			
1	B	147	Total	C	F	H	N	O	S	0	0	0
			1241	778	1	32	209	217	4			

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 variant 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	7	0
			1158	724	205	220	9			
2	D	138	Total	C	N	O	S	0	0	0
			1099	691	192	208	8			

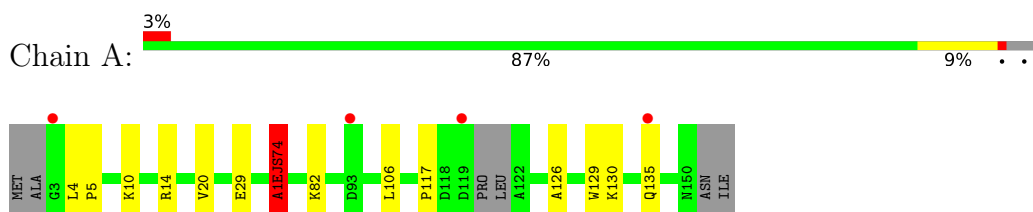
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	193	Total	O	0	0
			193	193		
3	C	163	Total	O	0	0
			163	163		
3	D	123	Total	O	0	0
			123	123		

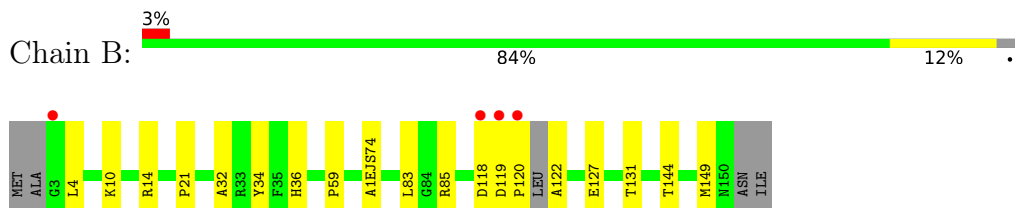
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

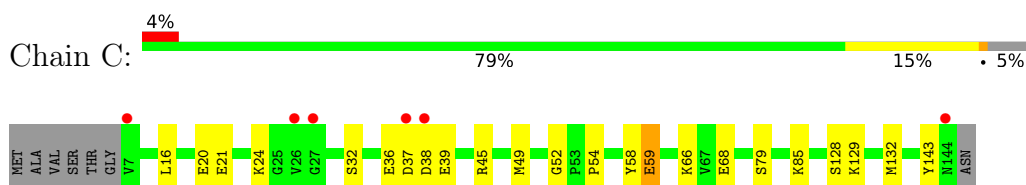
- Molecule 1: Ubiquitin-conjugating enzyme E2 N



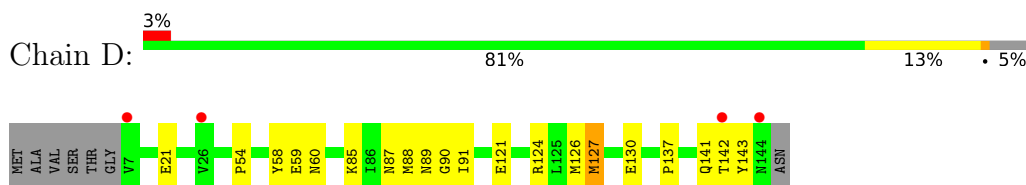
- Molecule 1: Ubiquitin-conjugating enzyme E2 N



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.41Å 71.60Å 68.56Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	35.80 – 1.68 35.80 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.80-1.68) 100.0 (35.80-1.68)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.68Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.182 , 0.228 0.182 , 0.228	Depositor DCC
R_{free} test set	3638 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5324	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6915e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1EJS

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	0.31	0/1181	0.52	0/1605
1	B	0.39	0/1189	0.57	0/1617
2	C	0.36	0/1181	0.54	0/1595
2	D	0.34	0/1122	0.59	1/1518 (0.1%)
All	All	0.35	0/4673	0.55	1/6335 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	127	MET	N-CA-CB	-5.34	102.07	110.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	74	A1EJS	Mainchain

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	A	1202	32	1159	17	0
1	B	1209	32	1166	17	0
2	C	1158	0	1153	17	0
2	D	1099	0	1102	21	0
3	A	113	0	0	1	0
3	B	193	0	0	4	2
3	C	163	0	0	1	2
3	D	123	0	0	2	0
All	All	5260	64	4580	69	2

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 7.

The worst 5 of 69 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:D:54:PRO:HA	2:D:59:GLU:HG3	1.42	0.98
2:C:21:GLU:HA	2:C:24:LYS:HE3	1.52	0.89
1:A:106:LEU:HD13	2:D:89:ASN:HD21	1.45	0.82
1:B:127:GLU:O	1:B:131:THR:HG23	1.80	0.80
2:C:21:GLU:HA	2:C:24:LYS:CE	2.13	0.79

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:353:HOH:O	3:C:333:HOH:O[2_555]	1.95	0.25
3:B:217:HOH:O	3:C:350:HOH:O[2_655]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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	141/152 (93%)	139 (99%)	2 (1%)	0	100	100
1	B	142/152 (93%)	138 (97%)	4 (3%)	0	100	100
2	C	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
2	D	136/145 (94%)	133 (98%)	3 (2%)	0	100	100
All	All	562/594 (95%)	551 (98%)	11 (2%)	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 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	123/128 (96%)	123 (100%)	0	100	100
1	B	124/128 (97%)	124 (100%)	0	100	100
2	C	131/129 (102%)	130 (99%)	1 (1%)	79	70
2	D	124/129 (96%)	124 (100%)	0	100	100
All	All	502/514 (98%)	501 (100%)	1 (0%)	92	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	59	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such

sidechains are listed below:

Mol	Chain	Res	Type
2	D	89	ASN
2	D	110	GLN
2	D	141	GLN
1	B	135	GLN
1	A	43	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	A1EJS	B	74	1	49,52,53	2.09	12 (24%)	61,72,74	1.56	9 (14%)
1	A1EJS	A	74	1	49,52,53	2.09	13 (26%)	61,72,74	1.72	12 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A1EJS	B	74	1	-	9/32/49/51	0/5/5/5
1	A1EJS	A	74	1	-	7/32/49/51	0/5/5/5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	A1EJS	C20-N23	6.14	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	A1EJS	C20-N23	5.99	1.43	1.34
1	B	74	A1EJS	C10-C13	5.81	1.52	1.41
1	A	74	A1EJS	C10-C13	5.51	1.51	1.41
1	A	74	A1EJS	C10-NZ	4.93	1.44	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	A1EJS	C35-N23-C20	-5.78	115.19	123.28
1	A	74	A1EJS	C17-C18-N19	-5.44	116.49	121.64
1	B	74	A1EJS	C17-C18-N19	-4.87	117.04	121.64
1	B	74	A1EJS	C35-N23-C20	-3.93	117.78	123.28
1	B	74	A1EJS	C27-C26-C25	3.71	123.02	118.81

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	74	A1EJS	C10-C13-N16-C17
1	A	74	A1EJS	O-C-CA-CB
1	B	74	A1EJS	C10-C13-N16-C17
1	B	74	A1EJS	C13-C10-NZ-CE
1	B	74	A1EJS	C11-C10-NZ-CE

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	74	A1EJS	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

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	145/152 (95%)	0.12	4 (2%) 55 58	14, 24, 41, 57	0
1	B	146/152 (96%)	-0.15	4 (2%) 56 59	12, 19, 35, 48	0
2	C	138/145 (95%)	-0.06	6 (4%) 40 44	9, 20, 41, 60	7 (5%)
2	D	138/145 (95%)	0.23	4 (2%) 54 57	14, 24, 41, 59	0
All	All	567/594 (95%)	0.03	18 (3%) 50 54	9, 22, 41, 60	7 (1%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	26	VAL	3.4
2	D	142	THR	3.2
2	D	26	VAL	3.1
2	C	27	GLY	2.8
1	A	135	GLN	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	A1EJS	B	74	48/49	0.92	0.10	12,25,40,46	0
1	A1EJS	A	74	48/49	0.93	0.09	16,26,44,55	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.