



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 10:17 PM UTC

PDB ID : 3DBL / pdb\_00003dbl  
Title : Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190wt-NEDD8Ala72Gln)  
Authors : Souphron, J.; Schulman, B.A.  
Deposited on : 2008-06-01  
Resolution : 2.90 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](mailto: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>.

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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

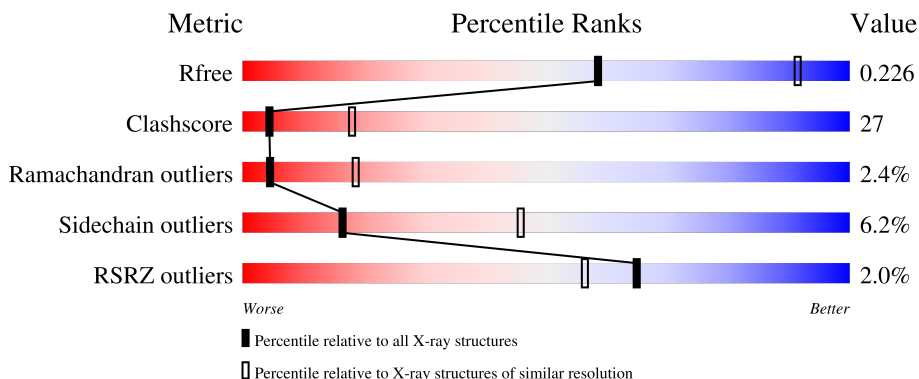
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




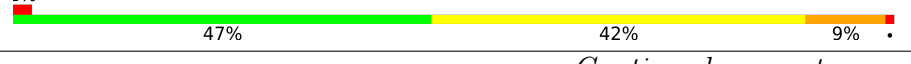
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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  $\geq 3$ , 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	531	
1	C	531	
1	E	531	
1	G	531	
2	B	434	

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Mol	Chain	Length	Quality of chain
2	D	434	<p>3% 53% 42% . .</p>
2	F	434	<p>3% 50% 42% 6% ..</p>
2	H	434	<p>3% 45% 47% 7% ..</p>
3	I	88	<p>3% 53% 39% 6% .</p>
3	J	88	<p>2% 43% 35% 8% 14%</p>
3	K	88	<p>2% 39% 34% 14% 14%</p>
3	L	88	<p>5% 25% 55% 7% 14%</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 32577 atoms, of which 0 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 NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	522	4138	2621	704	797	16	0	0	0
1	C	520	4125	2612	702	795	16	0	0	0
1	E	521	4119	2609	703	792	15	0	0	0
1	G	518	4113	2605	700	793	15	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q13564
A	0	SER	-	expression tag	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLU	deletion	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLY	deletion	UNP Q13564
A	?	-	ALA	deletion	UNP Q13564
C	-1	GLY	-	expression tag	UNP Q13564
C	0	SER	-	expression tag	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLU	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLY	deletion	UNP Q13564
C	?	-	ALA	deletion	UNP Q13564
E	-1	GLY	-	expression tag	UNP Q13564
E	0	SER	-	expression tag	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLU	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLY	deletion	UNP Q13564
E	?	-	ALA	deletion	UNP Q13564

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q13564
G	0	SER	-	expression tag	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLU	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLY	deletion	UNP Q13564
G	?	-	ALA	deletion	UNP Q13564

- Molecule 2 is a protein called NEDD8-activating enzyme E1 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	432	Total 3404	C 2175	N 577	O 635	S 17	0	0	0
2	D	432	Total 3408	C 2178	N 578	O 635	S 17	0	0	0
2	F	431	Total 3397	C 2172	N 576	O 632	S 17	0	0	0
2	H	431	Total 3389	C 2165	N 575	O 632	S 17	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP Q8TBC4
B	10	LYS	-	expression tag	UNP Q8TBC4
B	11	LEU	-	expression tag	UNP Q8TBC4
B	216	ALA	CYS	engineered mutation	UNP Q8TBC4
D	9	MET	-	expression tag	UNP Q8TBC4
D	10	LYS	-	expression tag	UNP Q8TBC4
D	11	LEU	-	expression tag	UNP Q8TBC4
D	216	ALA	CYS	engineered mutation	UNP Q8TBC4
F	9	MET	-	expression tag	UNP Q8TBC4
F	10	LYS	-	expression tag	UNP Q8TBC4
F	11	LEU	-	expression tag	UNP Q8TBC4
F	216	ALA	CYS	engineered mutation	UNP Q8TBC4
H	9	MET	-	expression tag	UNP Q8TBC4
H	10	LYS	-	expression tag	UNP Q8TBC4
H	11	LEU	-	expression tag	UNP Q8TBC4
H	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	86	668	415	121	130	2	0	0	0
3	J	76	604	380	105	117	2	0	0	0
3	K	76	604	380	105	117	2	0	0	0
3	L	76	604	380	105	117	2	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	89	GLY	-	expression tag	UNP Q15843
I	90	SER	-	expression tag	UNP Q15843
I	91	ARG	-	expression tag	UNP Q15843
I	92	ARG	-	expression tag	UNP Q15843
I	93	ALA	-	expression tag	UNP Q15843
I	94	SER	-	expression tag	UNP Q15843
I	95	VAL	-	expression tag	UNP Q15843
I	96	GLY	-	expression tag	UNP Q15843
I	97	SER	-	expression tag	UNP Q15843
I	98	GLY	-	expression tag	UNP Q15843
I	99	GLY	-	expression tag	UNP Q15843
I	100	SER	-	expression tag	UNP Q15843
I	172	GLN	ALA	engineered mutation	UNP Q15843
J	89	GLY	-	expression tag	UNP Q15843
J	90	SER	-	expression tag	UNP Q15843
J	91	ARG	-	expression tag	UNP Q15843
J	92	ARG	-	expression tag	UNP Q15843
J	93	ALA	-	expression tag	UNP Q15843
J	94	SER	-	expression tag	UNP Q15843
J	95	VAL	-	expression tag	UNP Q15843
J	96	GLY	-	expression tag	UNP Q15843
J	97	SER	-	expression tag	UNP Q15843
J	98	GLY	-	expression tag	UNP Q15843
J	99	GLY	-	expression tag	UNP Q15843
J	100	SER	-	expression tag	UNP Q15843
J	172	GLN	ALA	engineered mutation	UNP Q15843
K	89	GLY	-	expression tag	UNP Q15843
K	90	SER	-	expression tag	UNP Q15843
K	91	ARG	-	expression tag	UNP Q15843
K	92	ARG	-	expression tag	UNP Q15843
K	93	ALA	-	expression tag	UNP Q15843

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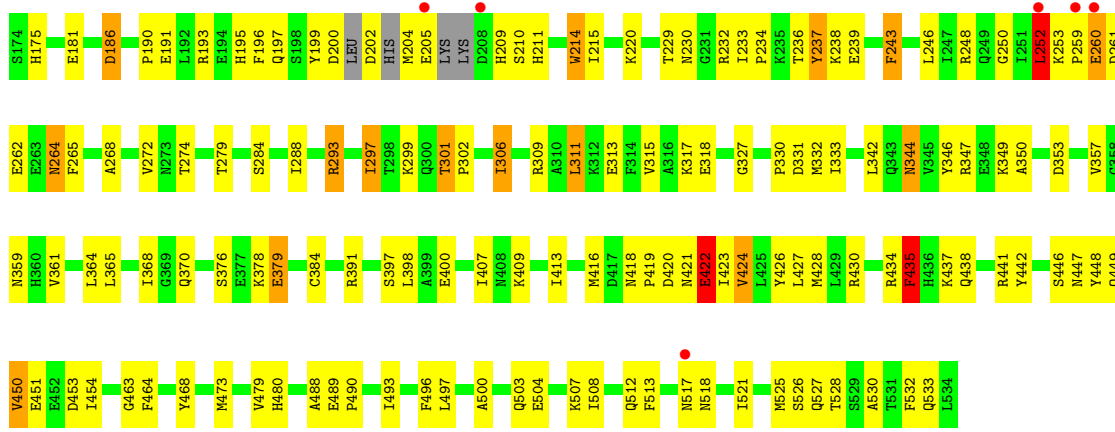
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Chain	Residue	Modelled	Actual	Comment	Reference
K	94	SER	-	expression tag	UNP Q15843
K	95	VAL	-	expression tag	UNP Q15843
K	96	GLY	-	expression tag	UNP Q15843
K	97	SER	-	expression tag	UNP Q15843
K	98	GLY	-	expression tag	UNP Q15843
K	99	GLY	-	expression tag	UNP Q15843
K	100	SER	-	expression tag	UNP Q15843
K	172	GLN	ALA	engineered mutation	UNP Q15843
L	89	GLY	-	expression tag	UNP Q15843
L	90	SER	-	expression tag	UNP Q15843
L	91	ARG	-	expression tag	UNP Q15843
L	92	ARG	-	expression tag	UNP Q15843
L	93	ALA	-	expression tag	UNP Q15843
L	94	SER	-	expression tag	UNP Q15843
L	95	VAL	-	expression tag	UNP Q15843
L	96	GLY	-	expression tag	UNP Q15843
L	97	SER	-	expression tag	UNP Q15843
L	98	GLY	-	expression tag	UNP Q15843
L	99	GLY	-	expression tag	UNP Q15843
L	100	SER	-	expression tag	UNP Q15843
L	172	GLN	ALA	engineered mutation	UNP Q15843

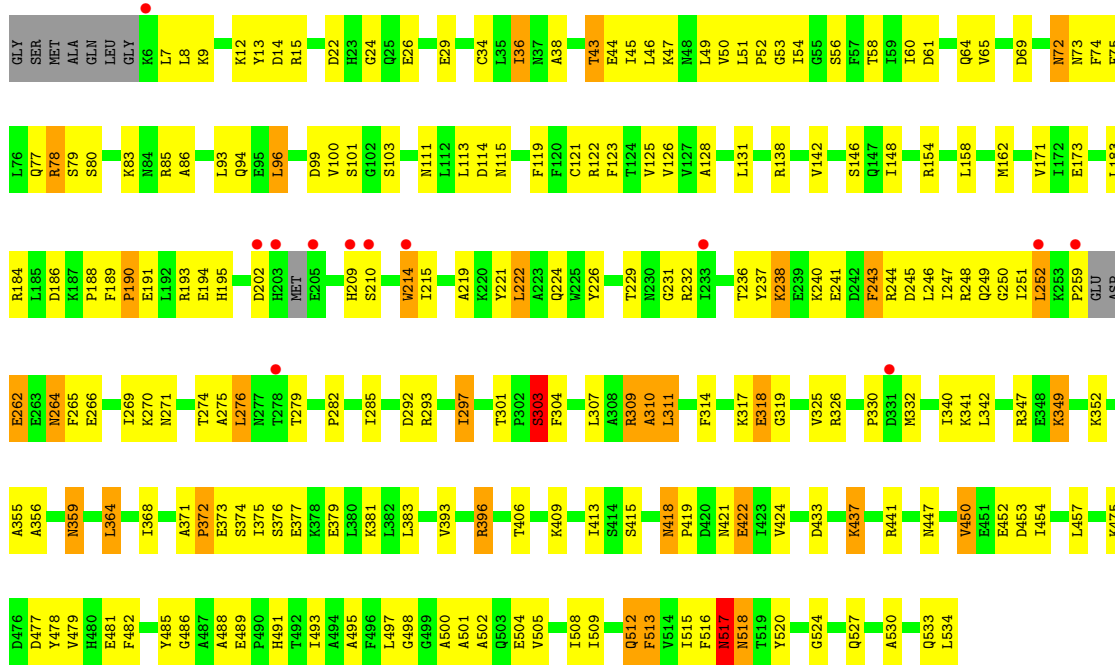
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

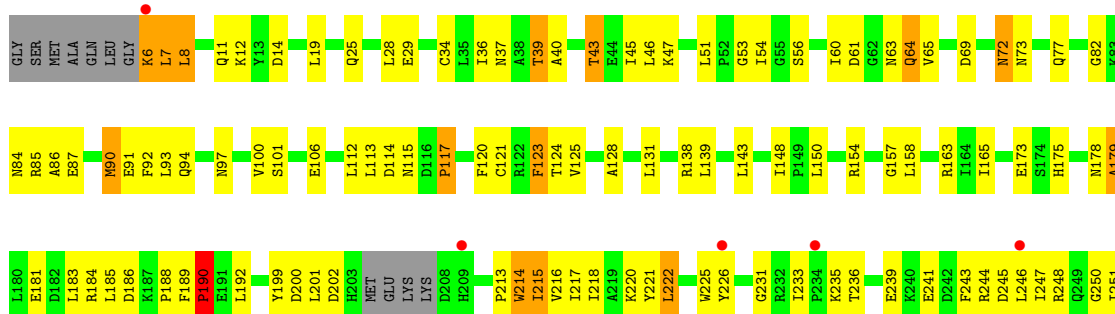


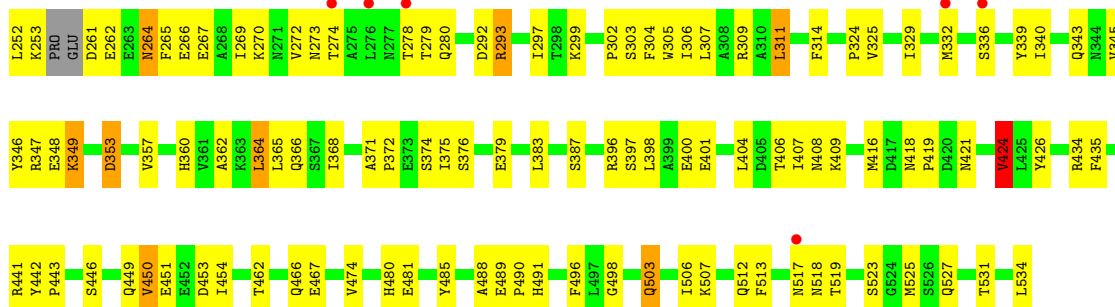


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

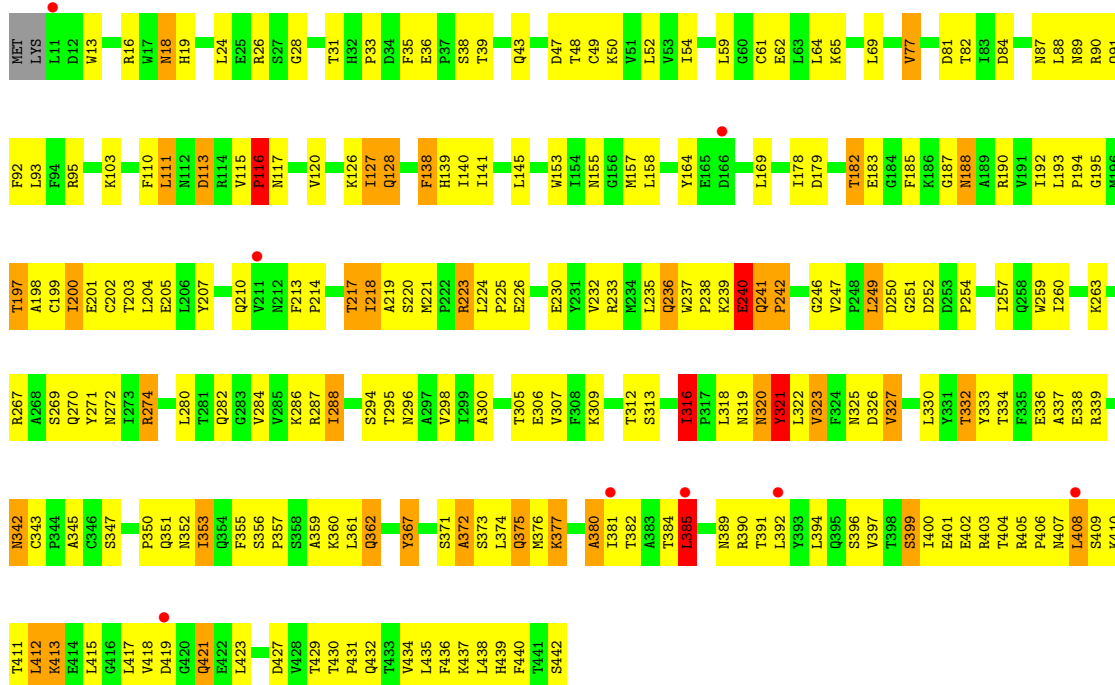


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

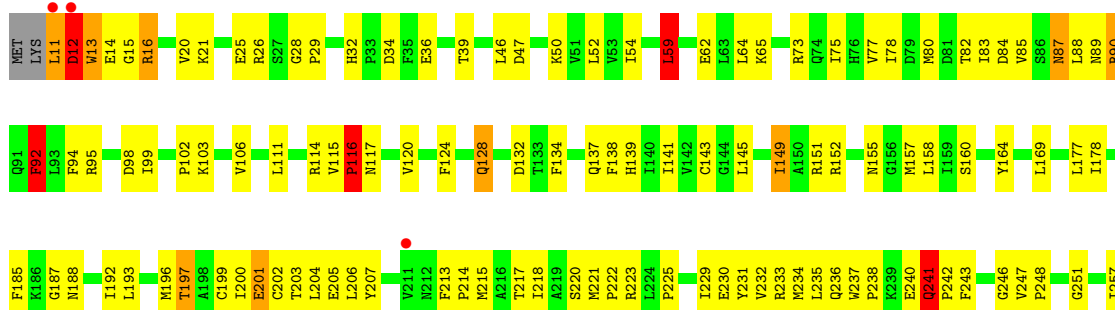




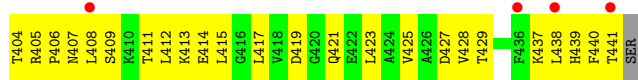
● Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



● Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



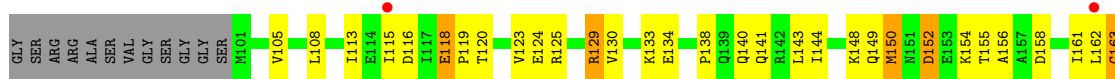
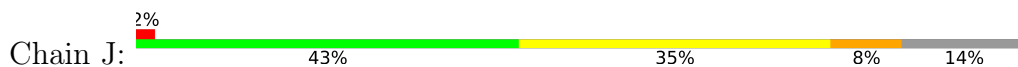




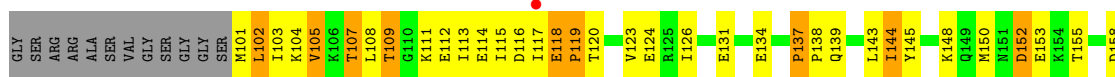
• Molecule 3: NEDD8



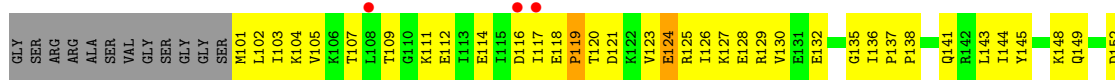
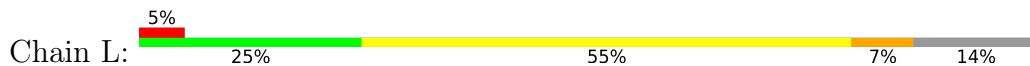
• Molecule 3: NEDD8



• Molecule 3: NEDD8



• Molecule 3: NEDD8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.12Å 198.95Å 210.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-2.90) 92.6 (50.00-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.91Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.274 0.227 , 0.226	Depositor DCC
$R_{free}$ test set	5854 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.52	0/4218	1.03	24/5706 (0.4%)
1	C	0.50	0/4203	1.01	20/5682 (0.4%)
1	E	0.54	0/4198	1.02	22/5678 (0.4%)
1	G	0.50	0/4191	1.01	14/5668 (0.2%)
2	B	0.58	1/3482 (0.0%)	1.12	25/4738 (0.5%)
2	D	0.54	0/3486	1.07	25/4742 (0.5%)
2	F	0.63	1/3475 (0.0%)	1.15	21/4730 (0.4%)
2	H	0.58	1/3467 (0.0%)	1.10	24/4720 (0.5%)
3	I	0.54	0/673	0.99	2/897 (0.2%)
3	J	0.49	0/609	1.05	5/813 (0.6%)
3	K	0.54	0/609	1.15	7/813 (0.9%)
3	L	0.49	0/609	1.06	5/813 (0.6%)
All	All	0.54	3/33220 (0.0%)	1.06	194/45000 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	380	ALA	CA-CB	-13.00	1.33	1.53
2	B	380	ALA	CA-CB	-7.94	1.40	1.53
2	H	380	ALA	CA-CB	-6.18	1.42	1.53

The worst 5 of 194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	165	GLU	N-CA-C	-14.32	88.48	109.96
2	F	321	TYR	N-CA-C	13.24	126.70	110.41
2	H	321	TYR	N-CA-C	12.50	127.03	110.53
2	B	321	TYR	N-CA-C	12.21	126.42	110.43
1	C	517	ASN	N-CA-C	11.71	124.12	111.36

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	A	4138	0	4080	193	0
1	C	4125	0	4065	200	0
1	E	4119	0	4054	212	0
1	G	4113	0	4058	184	0
2	B	3404	0	3385	218	0
2	D	3408	0	3396	186	0
2	F	3397	0	3380	245	0
2	H	3389	0	3359	250	0
3	I	668	0	702	40	0
3	J	604	0	638	38	0
3	K	604	0	638	40	0
3	L	604	0	638	55	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	32577	0	32393	1728	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 27.

The worst 5 of 1728 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:149:ILE:H	2:D:149:ILE:HD12	1.01	1.14
2:H:359:ALA:HB3	2:H:412:LEU:HD11	1.26	1.13
2:F:149:ILE:HD12	2:F:149:ILE:H	1.15	1.11
3:J:150:MET:HE1	3:J:167:LEU:HD13	1.33	1.08
1:E:184:ARG:HH12	1:E:325:VAL:HG22	1.11	1.07

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	518/531 (98%)	451 (87%)	54 (10%)	13 (2%)	4	17
1	C	513/531 (97%)	452 (88%)	52 (10%)	9 (2%)	6	25
1	E	515/531 (97%)	464 (90%)	42 (8%)	9 (2%)	7	26
1	G	512/531 (96%)	447 (87%)	56 (11%)	9 (2%)	6	25
2	B	430/434 (99%)	376 (87%)	46 (11%)	8 (2%)	6	23
2	D	430/434 (99%)	370 (86%)	50 (12%)	10 (2%)	5	19
2	F	429/434 (99%)	360 (84%)	55 (13%)	14 (3%)	3	13
2	H	429/434 (99%)	355 (83%)	60 (14%)	14 (3%)	3	13
3	I	84/88 (96%)	78 (93%)	4 (5%)	2 (2%)	4	18
3	J	74/88 (84%)	70 (95%)	1 (1%)	3 (4%)	2	9
3	K	74/88 (84%)	65 (88%)	6 (8%)	3 (4%)	2	9
3	L	74/88 (84%)	65 (88%)	5 (7%)	4 (5%)	1	5
All	All	4082/4212 (97%)	3553 (87%)	431 (11%)	98 (2%)	4	18

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	LEU
1	C	252	LEU
2	D	116	PRO
2	D	204	LEU
1	E	202	ASP

### 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	452/462 (98%)	430 (95%)	22 (5%)	22	54
1	C	451/462 (98%)	429 (95%)	22 (5%)	22	54
1	E	448/462 (97%)	421 (94%)	27 (6%)	17	47
1	G	450/462 (97%)	430 (96%)	20 (4%)	25	59
2	B	378/382 (99%)	346 (92%)	32 (8%)	10	31
2	D	379/382 (99%)	357 (94%)	22 (6%)	18	49
2	F	377/382 (99%)	347 (92%)	30 (8%)	11	34
2	H	375/382 (98%)	351 (94%)	24 (6%)	16	44
3	I	73/74 (99%)	66 (90%)	7 (10%)	8	26
3	J	67/74 (90%)	62 (92%)	5 (8%)	12	37
3	K	67/74 (90%)	59 (88%)	8 (12%)	5	16
3	L	67/74 (90%)	65 (97%)	2 (3%)	36	70
All	All	3584/3672 (98%)	3363 (94%)	221 (6%)	16	46

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	171	VAL
2	F	118	CYS
3	L	119	PRO
2	H	114	ARG
1	E	292	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	342	ASN
2	H	131	ASN
2	F	395	GLN
1	G	343	GLN
2	H	320	ASN

### 5.3.3 RNA

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 4 ligands modelled in this entry, 4 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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	522/531 (98%)	0.06	4 (0%) 82 77	33, 67, 99, 122	0
1	C	520/531 (97%)	0.11	10 (1%) 66 58	41, 68, 102, 130	0
1	E	521/531 (98%)	-0.01	12 (2%) 61 52	32, 56, 116, 134	0
1	G	518/531 (97%)	0.15	11 (2%) 63 54	34, 64, 124, 137	0
2	B	432/434 (99%)	0.06	8 (1%) 66 58	36, 59, 109, 117	0
2	D	432/434 (99%)	0.19	5 (1%) 76 69	40, 70, 109, 117	0
2	F	431/434 (99%)	0.24	11 (2%) 57 48	37, 61, 116, 124	0
2	H	431/434 (99%)	0.35	11 (2%) 57 48	37, 69, 116, 122	0
3	I	86/88 (97%)	0.14	3 (3%) 47 38	47, 68, 93, 97	0
3	J	76/88 (86%)	0.31	2 (2%) 57 48	58, 77, 96, 98	0
3	K	76/88 (86%)	0.22	2 (2%) 57 48	56, 73, 90, 91	0
3	L	76/88 (86%)	0.64	4 (5%) 32 25	67, 93, 115, 121	0
All	All	4121/4212 (97%)	0.15	83 (2%) 65 56	32, 66, 113, 137	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	176	GLY	3.8
2	B	211	VAL	3.7
3	L	116	ASP	3.6
1	E	203	HIS	3.4
3	K	117	ILE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ZN	B	1	1/1	0.99	0.05	65,65,65,65	0
4	ZN	D	3	1/1	0.99	0.06	74,74,74,74	0
4	ZN	F	4	1/1	0.99	0.04	62,62,62,62	0
4	ZN	H	2	1/1	0.99	0.05	80,80,80,80	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.