



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:37 PM UTC

PDB ID : 3DBH / pdb\_00003dbh  
Title : Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190Ala-NEDD8Ala72Arg)  
Authors : Souphron, J.; Schulman, B.A.  
Deposited on : 2008-05-31  
Resolution : 2.85 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>.

---

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

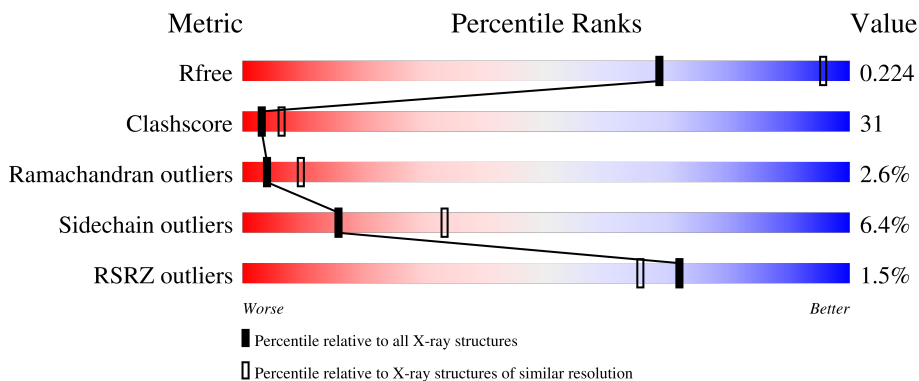
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

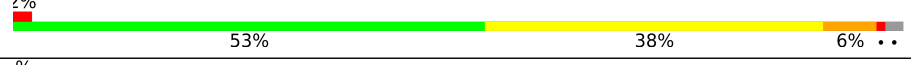

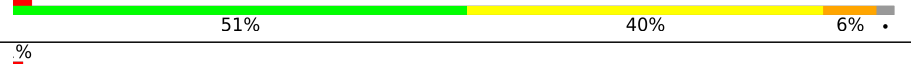

The reported resolution of this entry is 2.85 Å.

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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	 53% 40% 5% ..
1	C	531	 53% 38% 6% ..
1	E	531	 57% 36% 5% ..
1	G	531	 51% 40% 6% .
2	B	434	 49% 42% 8%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	D	434	<p>2% 48% 44% 7%</p>
2	F	434	<p>3% 47% 45% 7%</p>
2	H	434	<p>% 42% 43% 13%</p>
3	I	88	<p>% 53% 35% 9%</p>
3	J	88	<p>39% 41% 7% 14%</p>
3	K	88	<p>% 38% 41% 8% 14%</p>
3	L	88	<p>% 22% 56% 9% 14%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32578 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	523	4136	2618	705	798	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

*Continued on next page...*

*Continued from previous page...*

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	C	N	O	S	0	0	0
			3398	2172	574	635	17			
2	D	432	Total	C	N	O	S	0	0	0
			3402	2175	575	635	17			
2	F	431	Total	C	N	O	S	0	0	0
			3391	2169	573	632	17			
2	H	431	Total	C	N	O	S	0	0	0
			3383	2162	572	632	17			

There are 20 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	190	ALA	ARG	engineered mutation	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	190	ALA	ARG	engineered mutation	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	190	ALA	ARG	engineered mutation	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	190	ALA	ARG	engineered mutation	UNP Q8TBC4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	86	Total	C	N	O	S	0	0	0
			670	416	123	129	2			
3	J	76	Total	C	N	O	S	0	0	0
			606	381	107	116	2			
3	K	76	Total	C	N	O	S	0	0	0
			606	381	107	116	2			
3	L	76	Total	C	N	O	S	0	0	0
			606	381	107	116	2			

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	ARG	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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	172	ARG	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
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	ARG	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	ARG	ALA	engineered mutation	UNP Q15843

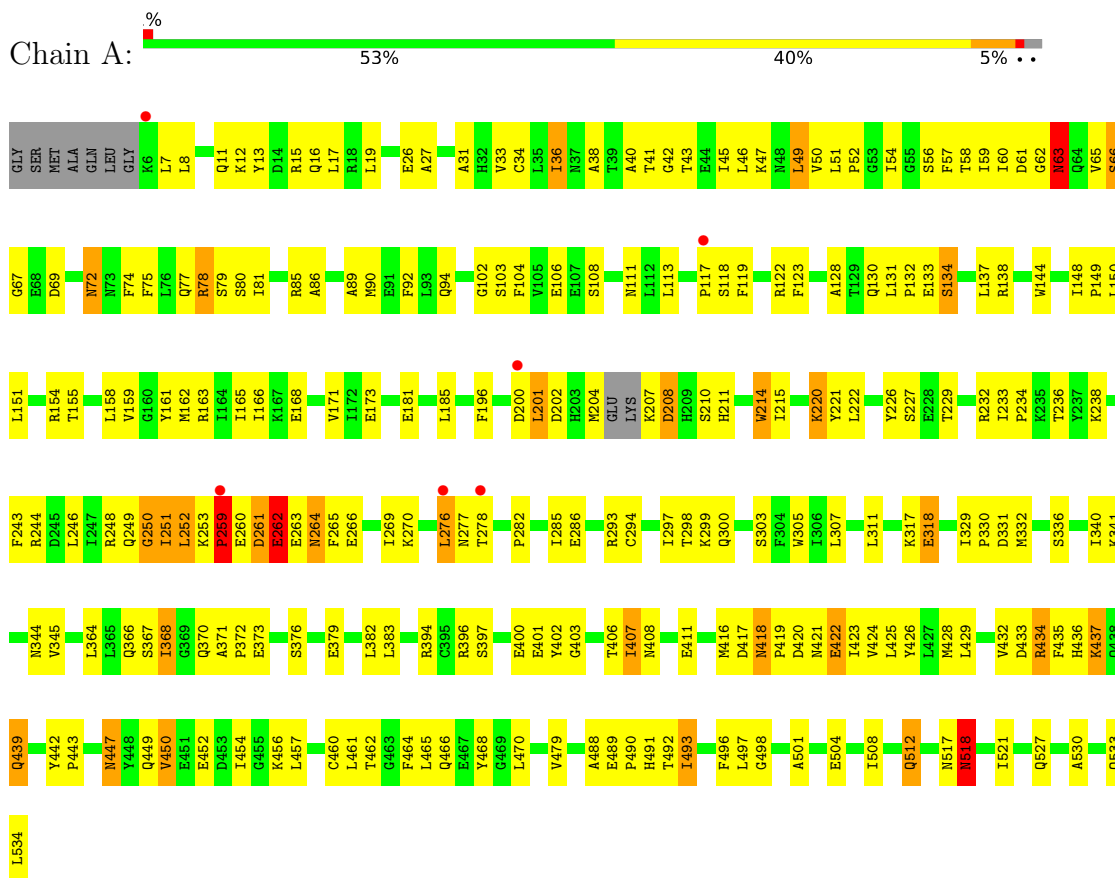
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

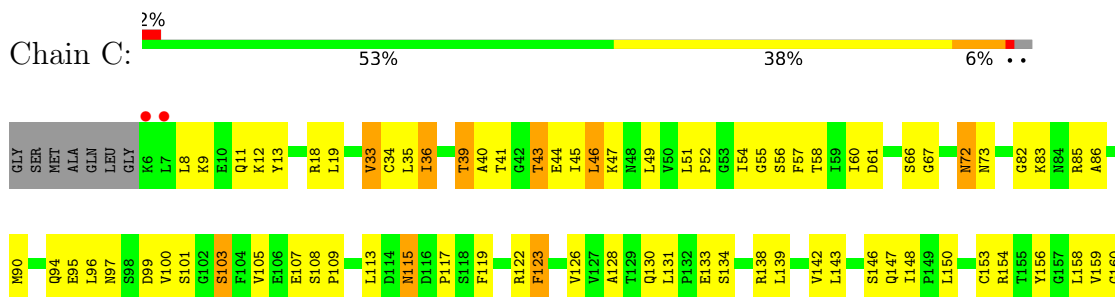
### 3 Residue-property plots [i](#)

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.

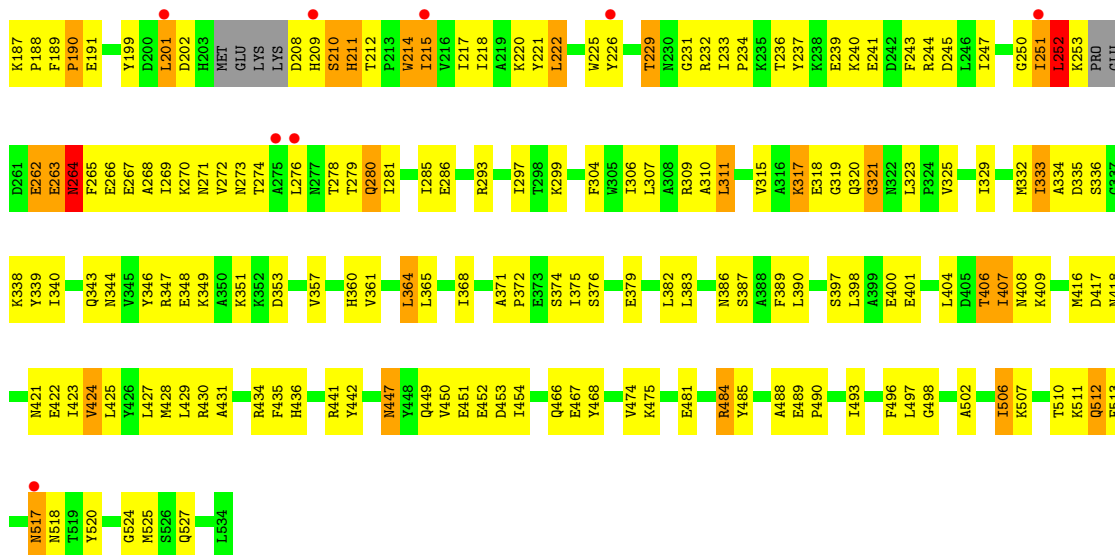
- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



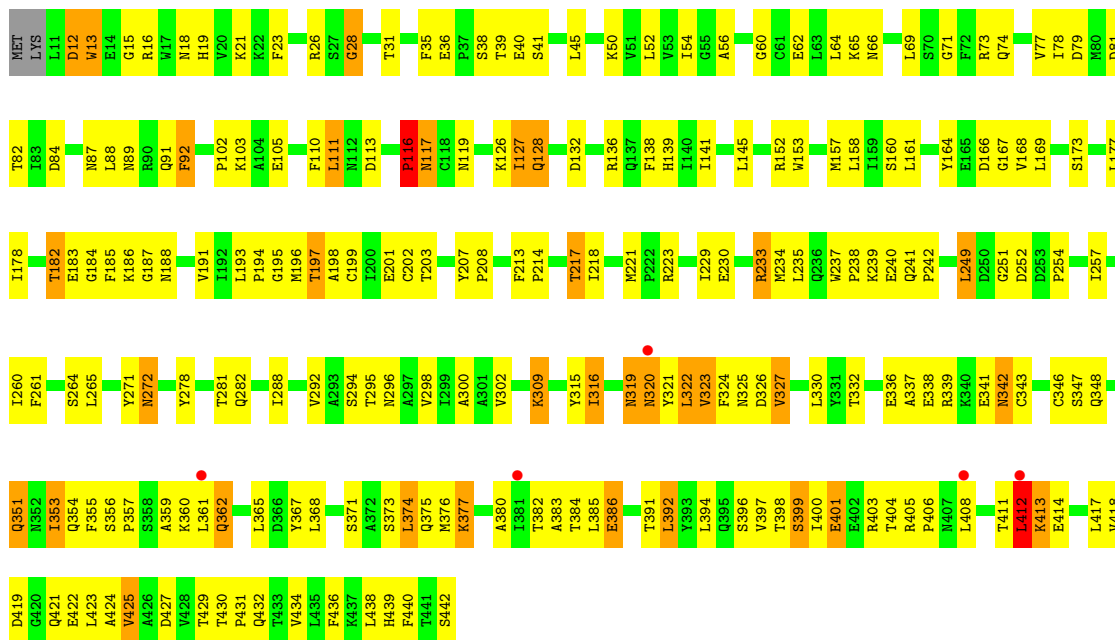
- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



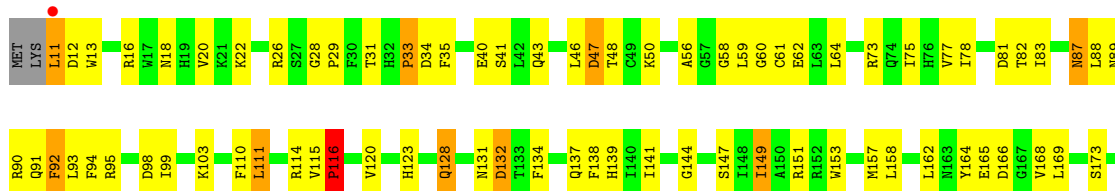




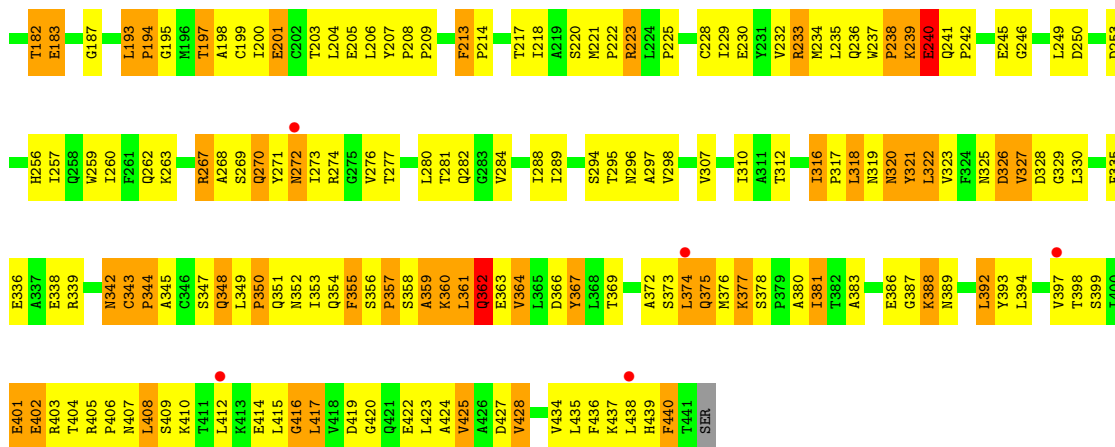
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



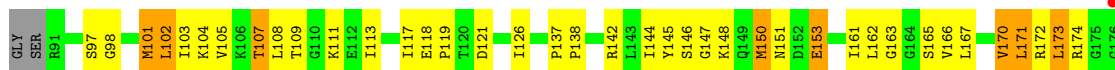
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



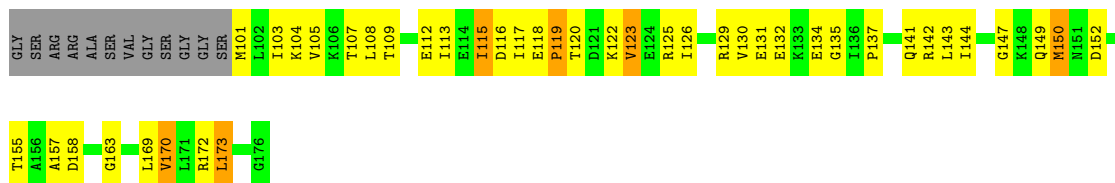
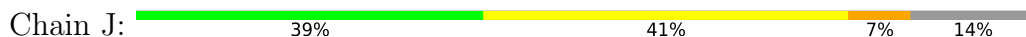




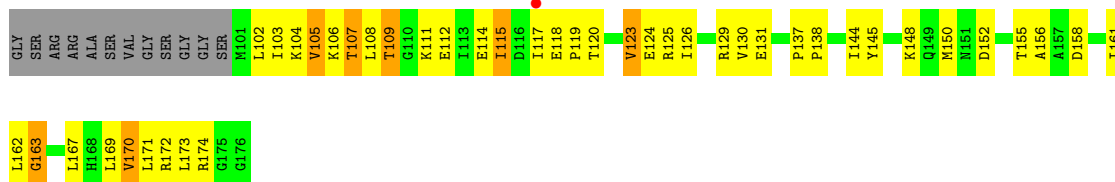
• Molecule 3: NEDD8



• Molecule 3: NEDD8



• Molecule 3: NEDD8



• Molecule 3: NEDD8



M151	D152	E153	K154	T155	A156	A157	D158	I161	L162	G163	G164	S165	V166	L167	H168	L169	V170	L171	R172	L173	R174	G175	G176
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.65Å 198.10Å 210.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-2.85) 88.6 (50.00-2.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.86Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.274 0.219 , 0.224	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.9	Xtrriage
Anisotropy	0.396	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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	0.53	0/4218	1.06	26/5706 (0.5%)
1	C	0.51	0/4203	1.02	22/5682 (0.4%)
1	E	0.59	0/4216	1.11	32/5704 (0.6%)
1	G	0.55	0/4191	1.02	24/5668 (0.4%)
2	B	0.57	0/3476	1.14	21/4731 (0.4%)
2	D	0.56	1/3480 (0.0%)	1.13	29/4735 (0.6%)
2	F	0.58	0/3469	1.11	23/4723 (0.5%)
2	H	0.57	1/3461 (0.0%)	1.13	30/4713 (0.6%)
3	I	0.53	0/675	1.17	5/899 (0.6%)
3	J	0.48	0/611	1.06	5/815 (0.6%)
3	K	0.49	0/611	1.16	3/815 (0.4%)
3	L	0.45	0/611	1.14	4/815 (0.5%)
All	All	0.55	2/33222 (0.0%)	1.09	224/45006 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	MET	SD-CE	5.27	1.92	1.79
2	D	388	LYS	CE-NZ	5.04	1.64	1.49

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	GLN	N-CA-C	13.14	125.69	111.36
2	D	13	TRP	N-CA-C	12.83	127.88	110.55
2	B	414	GLU	N-CA-C	-11.86	97.41	113.30
1	A	208	ASP	N-CA-C	-11.51	98.61	112.89
2	D	385	LEU	N-CA-C	10.76	123.09	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	230	0
1	C	4125	0	4065	216	0
1	E	4136	0	4065	221	0
1	G	4113	0	4058	247	0
2	B	3398	0	3377	242	0
2	D	3402	0	3388	233	0
2	F	3391	0	3372	274	0
2	H	3383	0	3351	314	0
3	I	670	0	707	41	0
3	J	606	0	643	47	0
3	K	606	0	643	45	0
3	L	606	0	643	62	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	32578	0	32392	2027	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 31.

The worst 5 of 2027 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	1.09	1.17
2:D:357:PRO:HA	2:D:412:LEU:HD12	1.22	1.15
2:F:419:ASP:HB2	2:F:438:LEU:HB2	1.29	1.13
2:F:241:GLN:HG2	2:F:245:GLU:HA	1.26	1.12
2:F:425:VAL:HB	2:F:434:VAL:HG13	1.31	1.10

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%)	442 (85%)	61 (12%)	15 (3%)	3	8
1	C	513/531 (97%)	448 (87%)	56 (11%)	9 (2%)	6	15
1	E	519/531 (98%)	465 (90%)	47 (9%)	7 (1%)	9	21
1	G	512/531 (96%)	437 (85%)	62 (12%)	13 (2%)	4	10
2	B	430/434 (99%)	373 (87%)	51 (12%)	6 (1%)	9	19
2	D	430/434 (99%)	366 (85%)	53 (12%)	11 (3%)	4	9
2	F	429/434 (99%)	359 (84%)	55 (13%)	15 (4%)	3	6
2	H	429/434 (99%)	347 (81%)	63 (15%)	19 (4%)	2	3
3	I	84/88 (96%)	76 (90%)	4 (5%)	4 (5%)	2	3
3	J	74/88 (84%)	67 (90%)	5 (7%)	2 (3%)	4	9
3	K	74/88 (84%)	66 (89%)	6 (8%)	2 (3%)	4	9
3	L	74/88 (84%)	64 (86%)	5 (7%)	5 (7%)	1	1
All	All	4086/4212 (97%)	3510 (86%)	468 (12%)	108 (3%)	4	9

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	450	VAL
2	B	116	PRO
1	C	263	GLU
1	C	422	GLU

### 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	45
1	C	451/462 (98%)	425 (94%)	26 (6%)	18	38
1	E	450/462 (97%)	420 (93%)	30 (7%)	15	31
1	G	450/462 (97%)	434 (96%)	16 (4%)	31	56
2	B	377/381 (99%)	350 (93%)	27 (7%)	13	28
2	D	378/381 (99%)	353 (93%)	25 (7%)	15	32
2	F	376/381 (99%)	345 (92%)	31 (8%)	10	23
2	H	374/381 (98%)	338 (90%)	36 (10%)	8	17
3	I	73/74 (99%)	67 (92%)	6 (8%)	10	23
3	J	67/74 (90%)	65 (97%)	2 (3%)	36	61
3	K	67/74 (90%)	61 (91%)	6 (9%)	9	19
3	L	67/74 (90%)	64 (96%)	3 (4%)	24	48
All	All	3582/3668 (98%)	3352 (94%)	230 (6%)	16	33

5 of 230 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	171	VAL
2	H	392	LEU
2	F	111	LEU
2	H	378	SER
2	H	213	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	354	GLN
2	H	125	ASN
2	F	407	ASN
1	G	277	ASN
2	H	325	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 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%)	-0.07	6 (1%) 78 73	49, 84, 116, 147	0
1	C	520/531 (97%)	0.11	10 (1%) 66 59	58, 89, 123, 157	0
1	E	523/531 (98%)	-0.11	6 (1%) 78 73	46, 71, 137, 158	0
1	G	518/531 (97%)	0.04	9 (1%) 69 63	49, 80, 143, 157	0
2	B	432/434 (99%)	-0.00	5 (1%) 76 71	47, 76, 116, 130	0
2	D	432/434 (99%)	0.12	7 (1%) 70 64	55, 92, 122, 143	0
2	F	431/434 (99%)	0.08	11 (2%) 57 48	50, 76, 124, 147	0
2	H	431/434 (99%)	0.22	5 (1%) 76 71	52, 83, 133, 152	0
3	I	86/88 (97%)	0.03	1 (1%) 76 71	61, 87, 106, 117	0
3	J	76/88 (86%)	0.15	0 100 100	75, 101, 119, 124	0
3	K	76/88 (86%)	0.04	1 (1%) 75 68	68, 91, 111, 121	0
3	L	76/88 (86%)	0.27	1 (1%) 75 68	75, 112, 132, 140	0
All	All	4123/4212 (97%)	0.05	62 (1%) 72 65	46, 84, 126, 158	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	3.4
2	D	11	LEU	3.4
2	D	388	LYS	3.3
1	A	276	LEU	3.3
2	F	419	ASP	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	0.04	79,79,79,79	0
4	ZN	F	4	1/1	0.99	0.04	74,74,74,74	0
4	ZN	H	2	1/1	0.99	0.05	84,84,84,84	0
4	ZN	D	3	1/1	1.00	0.03	93,93,93,93	0

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

There are no such residues in this entry.