



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:07 AM GMT

PDB ID : 3DBH  
Title : Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APBP1-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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

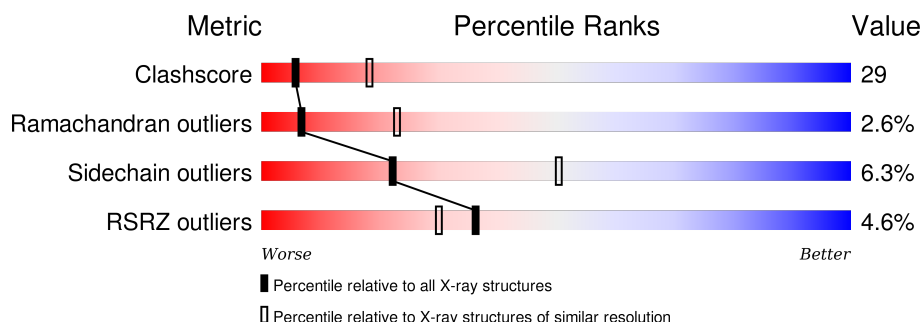
# 1 Overall quality at a glance

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))
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>39%</div> <div>..</div> </div> </div>
1	C	531	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>5%</div> <div>.</div> </div> </div>
1	E	531	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div>...</div> </div> </div>
1	G	531	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>37%</div> <div>5%</div> <div>.</div> </div> </div>
2	B	434	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>42%</div> <div>5%</div> </div> </div>
2	D	434	<div> <div>8%</div> <div> <div></div> <div>52%</div> <div>42%</div> <div>5%</div> </div> </div>
2	F	434	<div> <div>6%</div> <div> <div></div> <div>51%</div> <div>42%</div> <div>6%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	434	<div><div></div><div>7%</div><div>45%</div><div>44%</div><div>10%</div><div></div></div>
3	I	88	<div><div></div><div>56%</div><div>38%</div><div>5%</div><div></div></div>
3	J	88	<div><div></div><div>6%</div><div>40%</div><div>44%</div><div></div><div>14%</div></div>
3	K	88	<div><div></div><div>2%</div><div>39%</div><div>43%</div><div>5%</div><div>14%</div></div>
3	L	88	<div><div></div><div>5%</div><div>26%</div><div>55%</div><div>6%</div><div>14%</div></div>

## 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
1	A	522	Total	C	N	O	S	0	0	0
			4138	2621	704	797	16			
1	C	520	Total	C	N	O	S	0	0	0
			4125	2612	702	795	16			
1	E	523	Total	C	N	O	S	0	0	0
			4136	2618	705	798	15			
1	G	518	Total	C	N	O	S	0	0	0
			4113	2605	700	793	15			

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
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	UNP Q8TBC4
B	216	ALA	CYS	ENGINEERED	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	UNP Q8TBC4
D	216	ALA	CYS	ENGINEERED	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	UNP Q8TBC4
F	216	ALA	CYS	ENGINEERED	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	UNP Q8TBC4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ALA	CYS	ENGINEERED	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	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

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

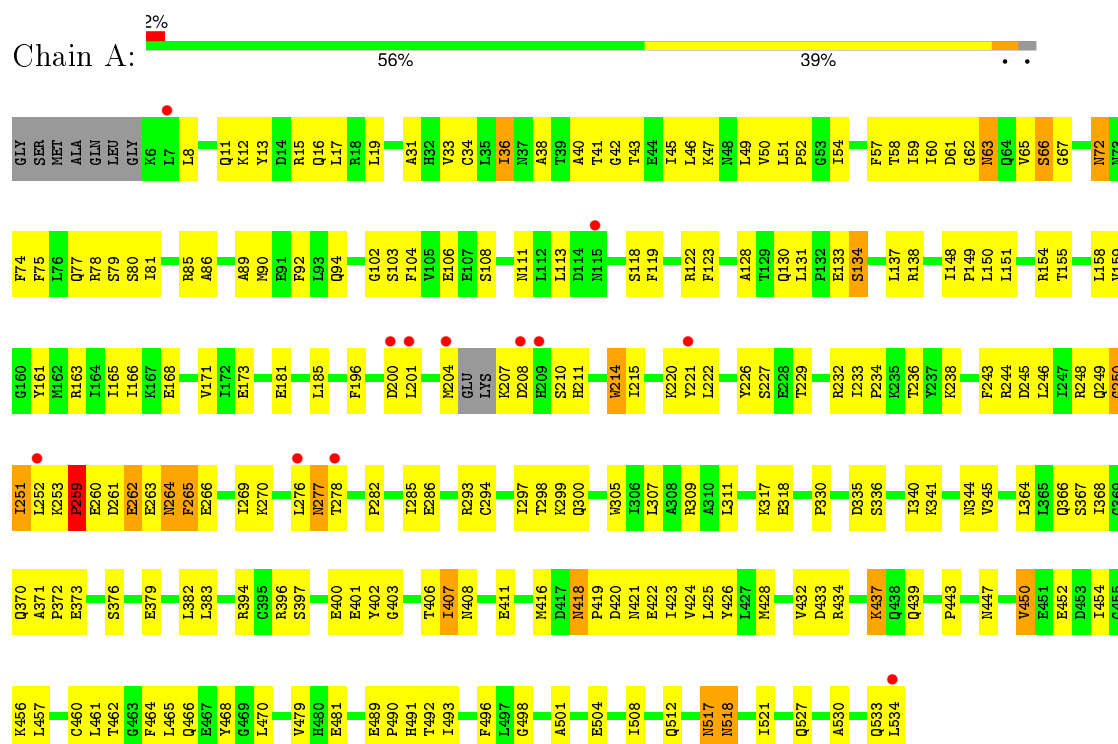
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

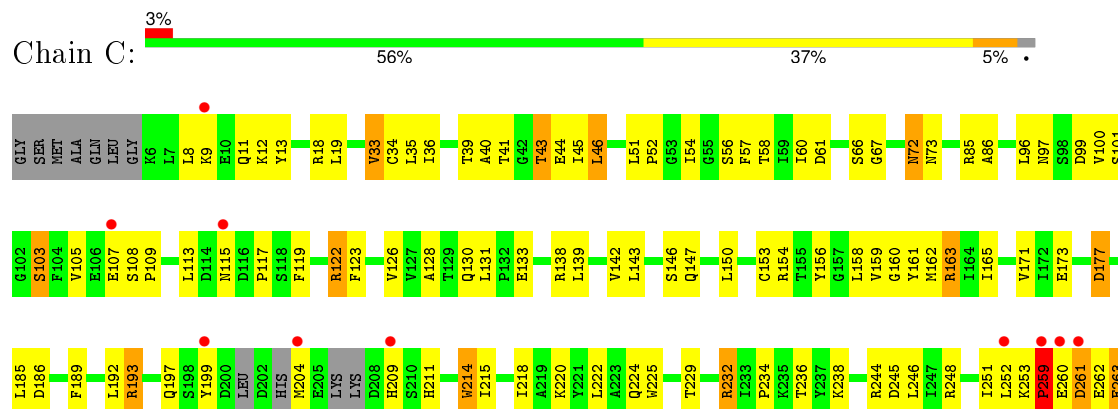
### 3 Residue-property plots

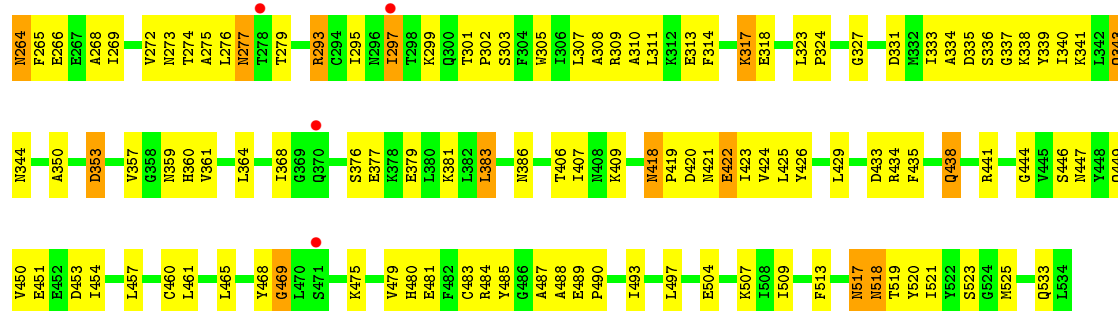
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

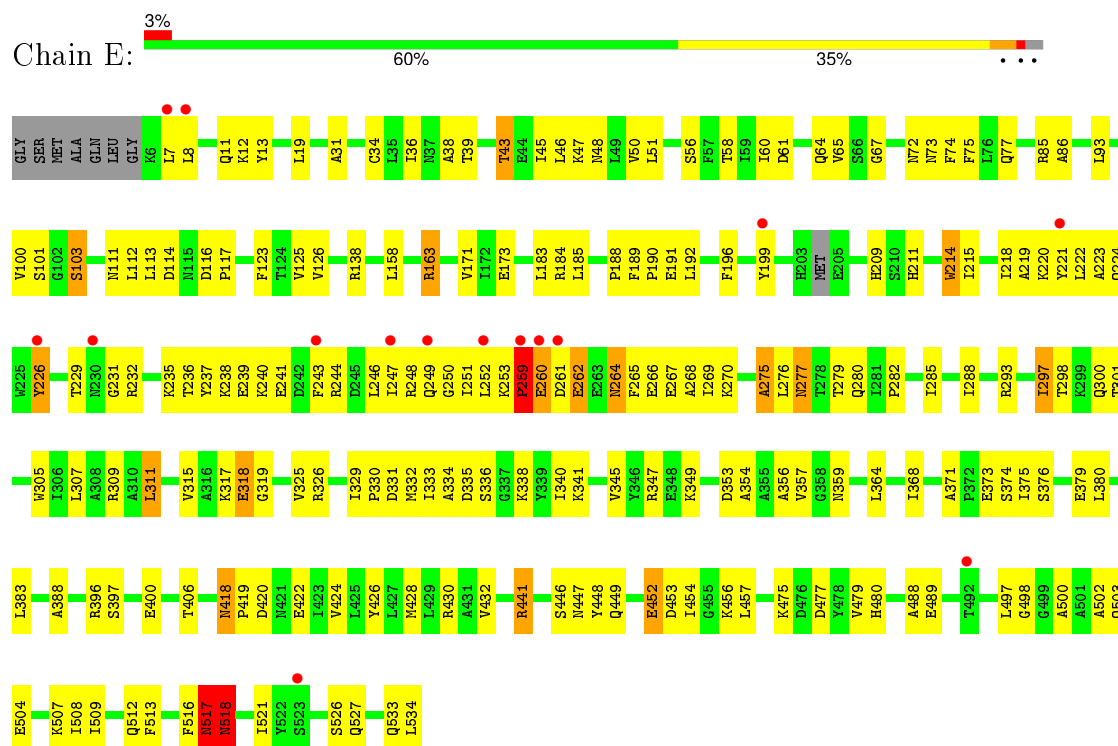


- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

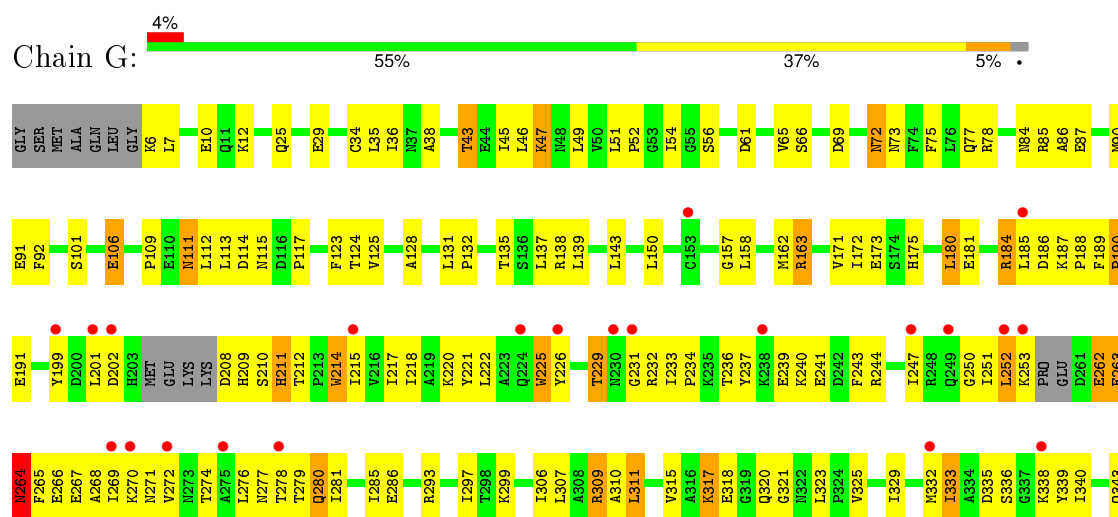


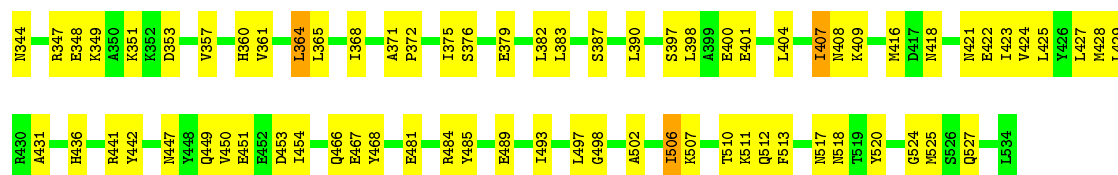


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

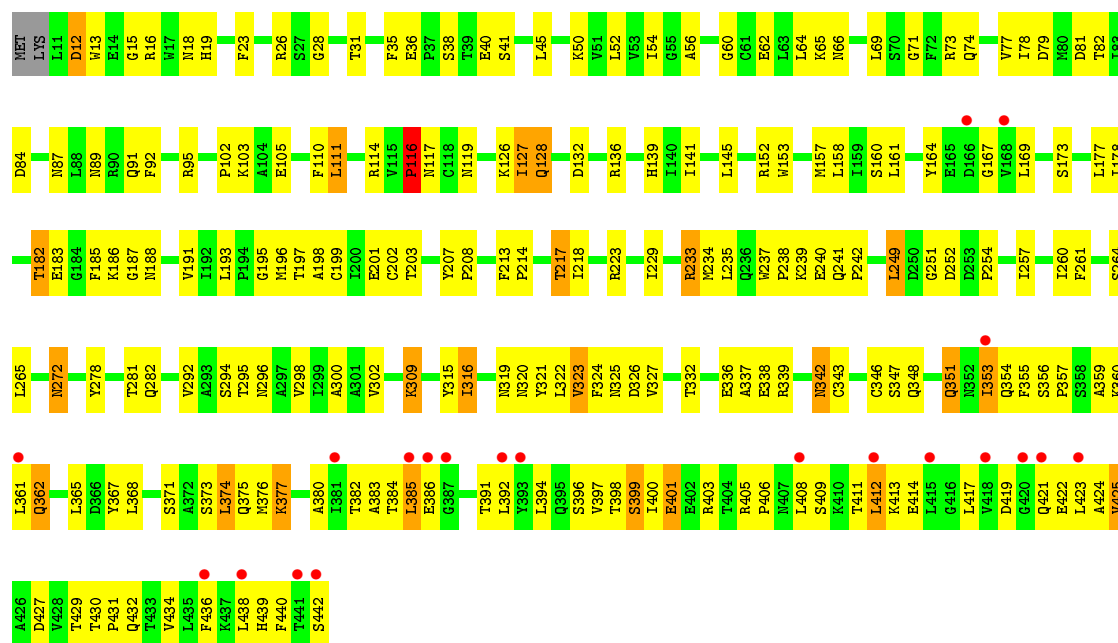


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

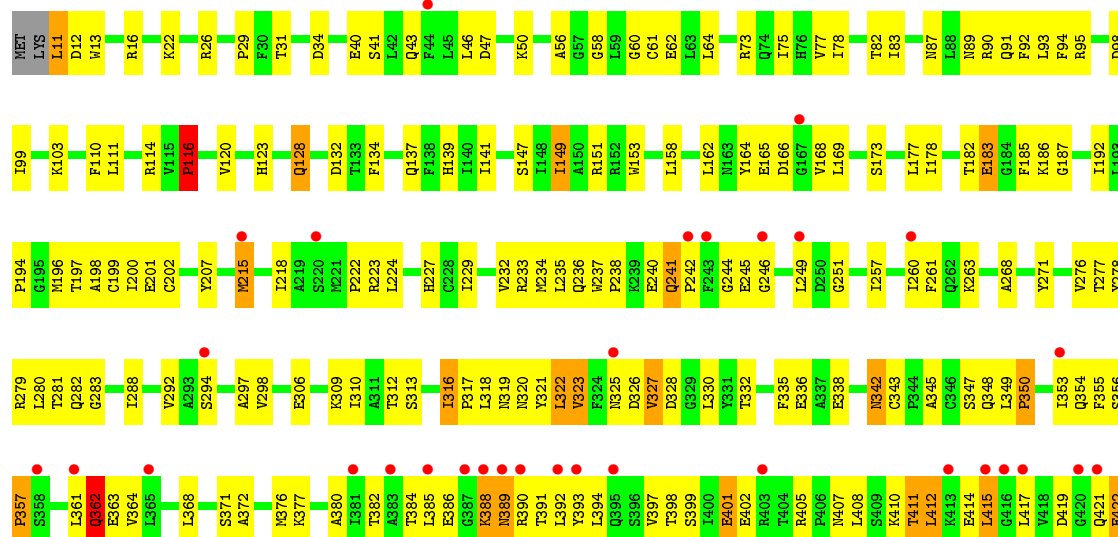




• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



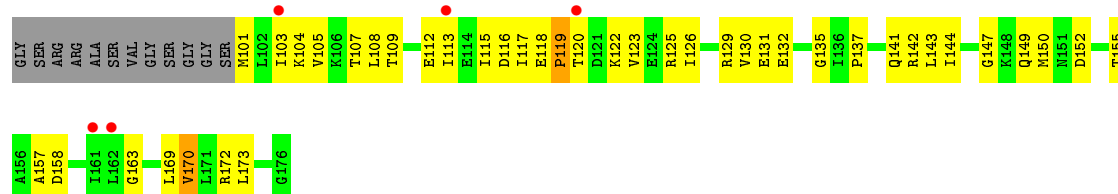


Chain I: 



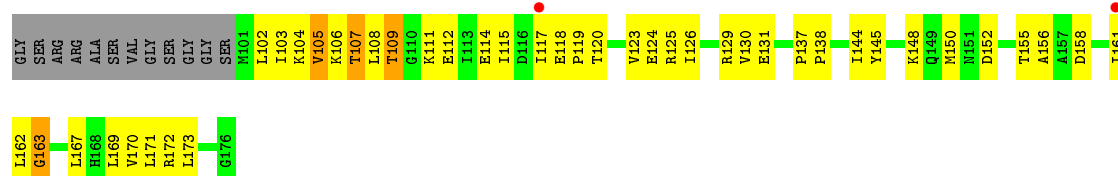
• Molecule 3: NEDD8

Chain J: 



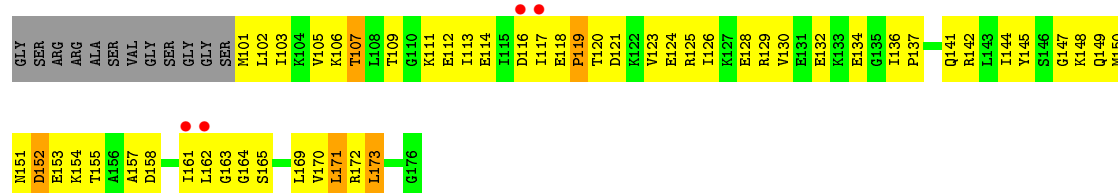
• Molecule 3: NEDD8

Chain K: 



• Molecule 3: NEDD8

Chain L: 



## 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 49.43 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-2.85) 88.6 (49.43-2.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.274 0.225 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	70.9	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 57.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 127296 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	A	0.43	0/4218	0.69	0/5706
1	C	0.41	0/4203	0.65	1/5682 (0.0%)
1	E	0.47	0/4216	0.71	2/5704 (0.0%)
1	G	0.45	0/4191	0.68	1/5668 (0.0%)
2	B	0.46	0/3476	0.76	5/4731 (0.1%)
2	D	0.47	1/3480 (0.0%)	0.72	4/4735 (0.1%)
2	F	0.48	0/3469	0.75	4/4723 (0.1%)
2	H	0.47	1/3461 (0.0%)	0.72	1/4713 (0.0%)
3	I	0.44	0/675	0.78	0/899
3	J	0.37	0/611	0.71	0/815
3	K	0.38	0/611	0.76	1/815 (0.1%)
3	L	0.36	0/611	0.72	0/815
All	All	0.45	2/33222 (0.0%)	0.71	19/45006 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	388	LYS	CE-NZ	6.17	1.64	1.49
2	H	143	CYS	CB-SG	-5.08	1.73	1.81

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	420	GLY	N-CA-C	-9.28	89.91	113.10
2	B	12	ASP	N-CA-C	-8.11	89.11	111.00
2	B	241	GLN	N-CA-C	-7.56	90.58	111.00
2	D	12	ASP	N-CA-C	-6.68	92.95	111.00
2	B	385	LEU	CA-CB-CG	-6.61	100.09	115.30

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	210	0
1	C	4125	0	4065	196	0
1	E	4136	0	4065	206	0
1	G	4113	0	4058	223	0
2	B	3398	0	3377	225	0
2	D	3402	0	3388	216	0
2	F	3391	0	3372	260	0
2	H	3383	0	3351	301	0
3	I	670	0	707	38	0
3	J	606	0	643	42	0
3	K	606	0	643	43	0
3	L	606	0	643	58	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	1878	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 29.

The worst 5 of 1878 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%)	6	20
1	C	513/531 (97%)	448 (87%)	56 (11%)	9 (2%)	11	33
1	E	519/531 (98%)	465 (90%)	47 (9%)	7 (1%)	15	42
1	G	512/531 (96%)	437 (85%)	62 (12%)	13 (2%)	7	24
2	B	430/434 (99%)	373 (87%)	51 (12%)	6 (1%)	14	40
2	D	430/434 (99%)	366 (85%)	53 (12%)	11 (3%)	7	23
2	F	429/434 (99%)	359 (84%)	55 (13%)	15 (4%)	4	16
2	H	429/434 (99%)	347 (81%)	63 (15%)	19 (4%)	3	10
3	I	84/88 (96%)	76 (90%)	4 (5%)	4 (5%)	3	9
3	J	74/88 (84%)	67 (90%)	5 (7%)	2 (3%)	6	22
3	K	74/88 (84%)	66 (89%)	6 (8%)	2 (3%)	6	22
3	L	74/88 (84%)	64 (86%)	5 (7%)	5 (7%)	1	3
All	All	4086/4212 (97%)	3510 (86%)	468 (12%)	108 (3%)	7	23

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%)	431 (95%)	21 (5%)	33	66
1	C	451/462 (98%)	424 (94%)	27 (6%)	24	53
1	E	450/462 (97%)	421 (94%)	29 (6%)	22	50
1	G	450/462 (97%)	430 (96%)	20 (4%)	35	68
2	B	377/381 (99%)	351 (93%)	26 (7%)	19	45
2	D	378/381 (99%)	354 (94%)	24 (6%)	22	50
2	F	376/381 (99%)	347 (92%)	29 (8%)	16	39
2	H	374/381 (98%)	338 (90%)	36 (10%)	10	28
3	I	73/74 (99%)	67 (92%)	6 (8%)	14	36
3	J	67/74 (90%)	65 (97%)	2 (3%)	48	80
3	K	67/74 (90%)	63 (94%)	4 (6%)	24	53
3	L	67/74 (90%)	64 (96%)	3 (4%)	34	67
All	All	3582/3668 (98%)	3355 (94%)	227 (6%)	22	50

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	422	GLU
1	E	422	GLU
2	H	342	ASN
3	J	170	VAL
1	E	226	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	375	GLN
1	E	277	ASN
2	H	272	ASN
2	D	432	GLN
1	E	115	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 carbohydrates 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%)	0.05	12 (2%) 64 59	49, 84, 116, 147	0
1	C	520/531 (97%)	0.13	14 (2%) 58 52	58, 89, 123, 157	0
1	E	523/531 (98%)	0.10	15 (2%) 55 49	46, 71, 137, 158	0
1	G	518/531 (97%)	0.20	22 (4%) 40 33	49, 80, 143, 157	0
2	B	432/434 (99%)	0.21	21 (4%) 33 27	47, 76, 116, 130	0
2	D	432/434 (99%)	0.41	36 (8%) 14 9	55, 93, 122, 143	0
2	F	431/434 (99%)	0.37	28 (6%) 22 16	50, 76, 124, 147	0
2	H	431/434 (99%)	0.35	32 (7%) 17 12	52, 83, 133, 152	0
3	I	86/88 (97%)	0.02	0 100 100	61, 87, 106, 117	0
3	J	76/88 (86%)	0.44	5 (6%) 22 16	75, 101, 119, 124	0
3	K	76/88 (86%)	0.18	2 (2%) 59 54	68, 91, 111, 121	0
3	L	76/88 (86%)	0.47	4 (5%) 30 24	75, 112, 132, 140	0
All	All	4123/4212 (97%)	0.22	191 (4%) 36 30	46, 84, 126, 158	0

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	385	LEU	6.7
1	E	252	LEU	5.8
1	C	259	PRO	5.8
2	F	385	LEU	5.6
1	C	260	GLU	5.3

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	D	3	1/1	0.99	0.17	1.25	93,93,93,93	0
4	ZN	H	2	1/1	0.97	0.16	0.51	84,84,84,84	0
4	ZN	F	4	1/1	0.96	0.19	0.33	74,74,74,74	0
4	ZN	B	1	1/1	0.98	0.16	0.04	79,79,79,79	0

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

There are no such residues in this entry.