wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 09:40 AM EDT

PDB ID	:	3DBL
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

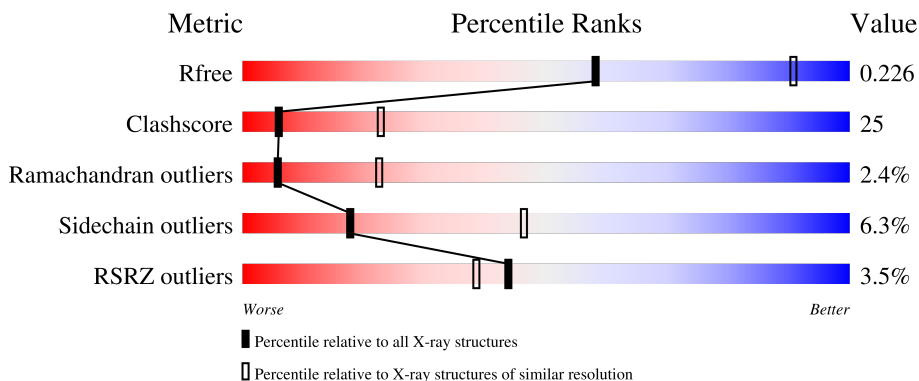|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	Percentile Ranks	Value
Rfree		0.226
Clashscore		25
Ramachandran outliers		2.4%
Sidechain outliers		6.3%
RSRZ outliers		3.5%

Worse ... *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 >=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 <=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	2% 60% 35% · ·
1	C	531	.% 60% 34% · ·
1	E	531	2% 60% 34% · ·
1	G	531	3% 59% 35% ·
2	B	434	4% 52% 41% 5% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	434	4% 57% 38% 5%
2	F	434	6% 52% 40% 6% ••
2	H	434	6% 49% 44% 6% •
3	I	88	60% 34% ••
3	J	88	3% 48% 33% 6% 14%
3	K	88	% 41% 40% 5% • 14%
3	L	88	6% 31% 51% 5% 14%

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
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	521	Total	C	N	O	S	0	0	0
			4119	2609	703	792	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

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
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
3	I	86	Total 668	C 415	N 121	O 130	S 2	0	0	0
3	J	76	Total 604	C 380	N 105	O 117	S 2	0	0	0
3	K	76	Total 604	C 380	N 105	O 117	S 2	0	0	0
3	L	76	Total 604	C 380	N 105	O 117	S 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

Continued on next page...

Continued from previous page...

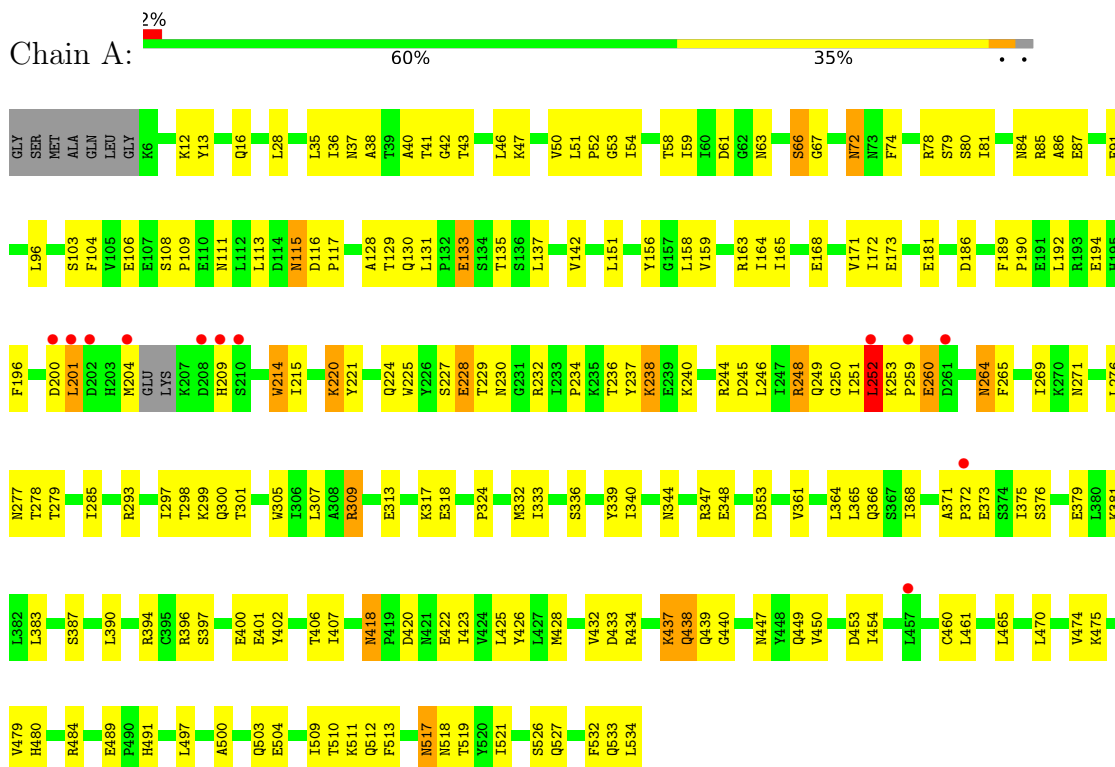| Chain	Residue	Modelled	Actual	Comment	Reference
K	94	SER	-	expression tag	UNP Q15843
K	95	VAL	-	expression tag	UNP Q15843
K	96	GLY	-	expression tag	UNP Q15843
K	97	SER	-	expression tag	UNP Q15843
K	98	GLY	-	expression tag	UNP Q15843
K	99	GLY	-	expression tag	UNP Q15843
K	100	SER	-	expression tag	UNP 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 (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain C:

V272 N273 T274 N277 T278 T279 S284 I288 R293 I297 T298 K299 Q300 T301 P302 I306 R309 A310 L311 K312 E313 F314 V315 A316 K317 E318 G327 P330 D331 M332 I333 L342 Q343 N344 V345 Y346 R347 E348 K349 A350 D353 V357 G358 N359 H360 V361

L364 L365 I368 G369 Q370 S376 E379 R391 S397 E400 I407 N408 K409 I413 N418 P419 D420 N421 E422 I423 V424 L425 Y426 L427 M428 L429 R430 R434 F435 H436 K437 Q438 R441 S446 N447 Y448 Q449 V450 D453 I454 G463 F464 L465 Q466 E467 Y468
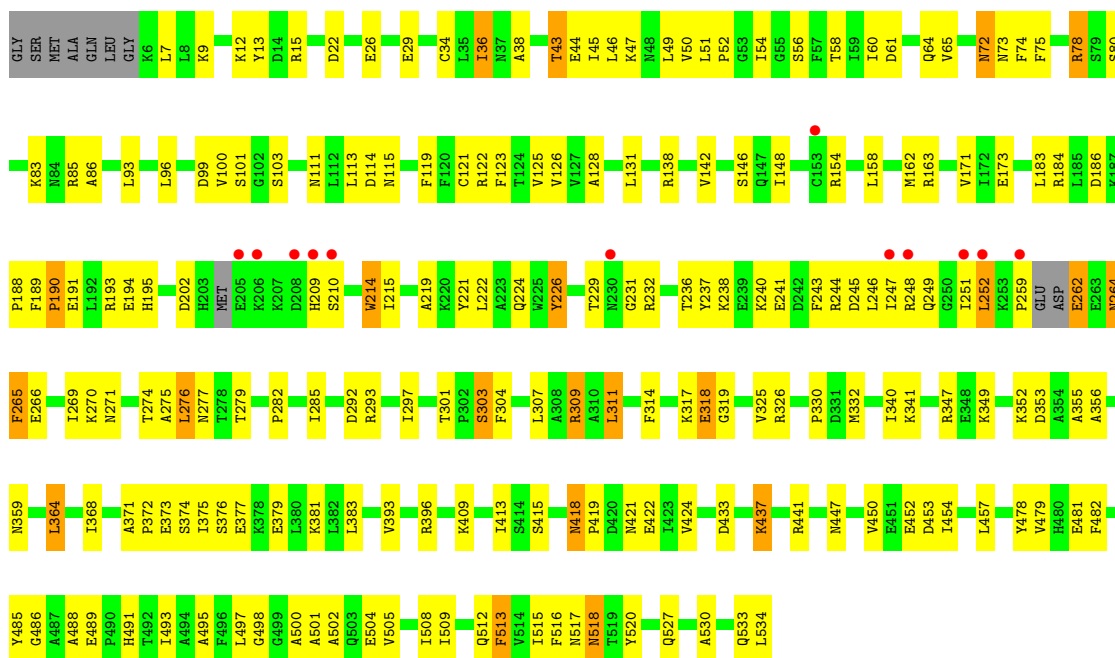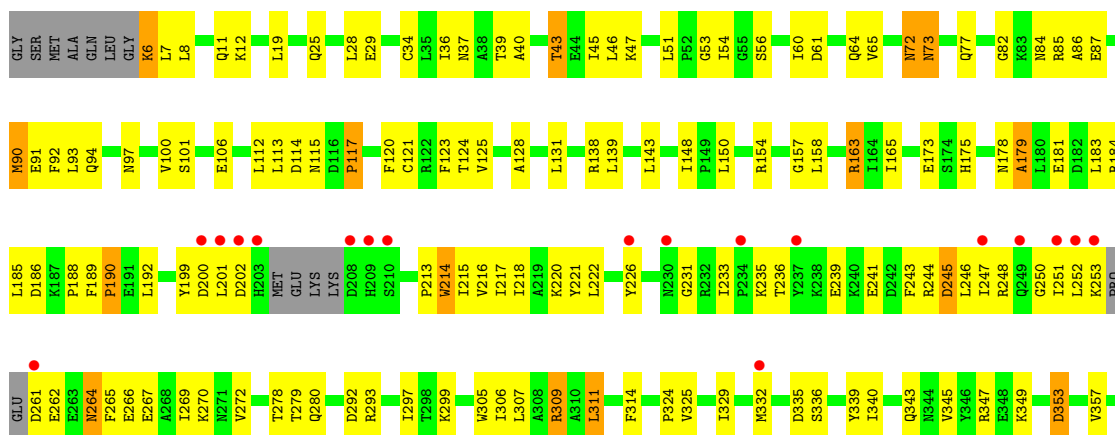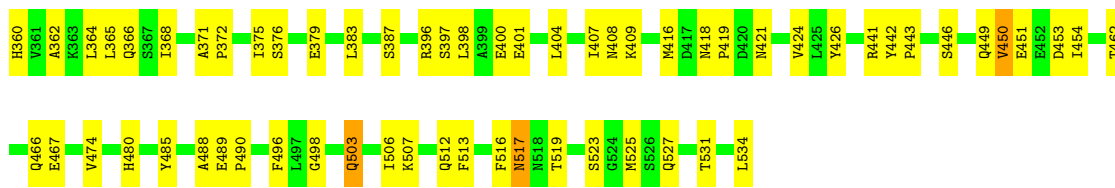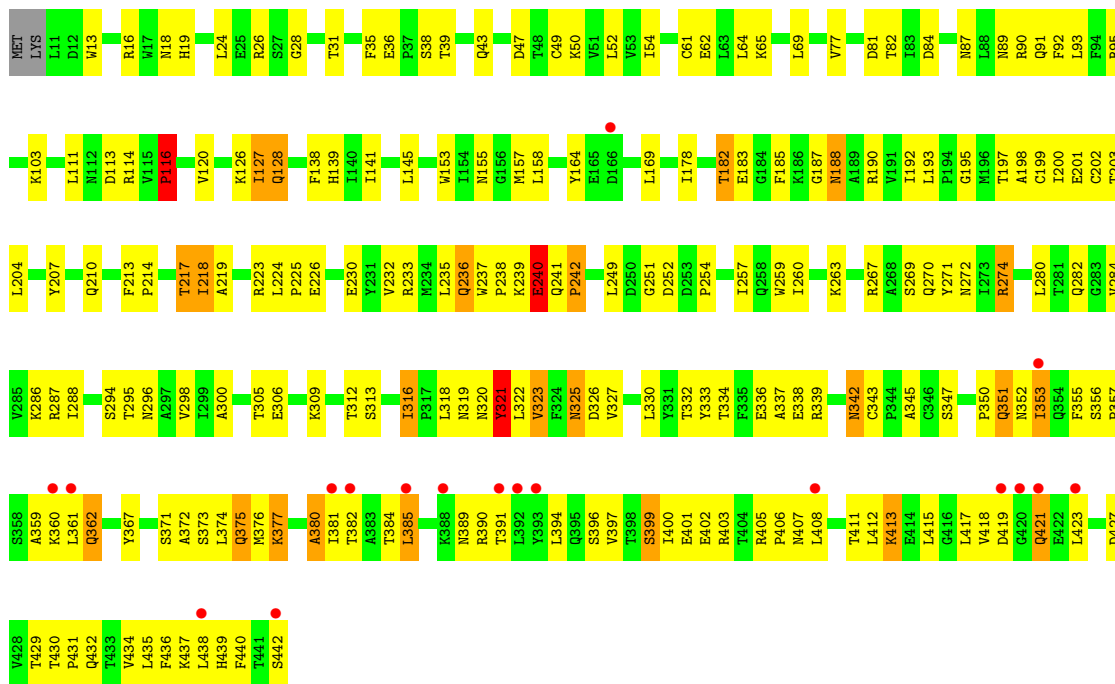
D476 V479 H480 E489 I493 L497 A500 Q503 E504 K507 I508 Q512 F513 N518 I521 M525 S526 Q527 T528 S529 A530 T531 Q533 L534

• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain E:

GLY SER MET ALA GLN LEU GLY K6 L7 L8 K9 K12 Y13 D14 R15 D22 E26 E29 C34 L35 I36 N37 A38 T43 E44 I45 L46 K47 N48 L49 V50 L51 P52 G53 I54 G55 S56 F57 T58 I59 I60 D61 Q64 V65 N72 N73 F74 F75 R78 S79 S80

K83 N84 R85 A86 L93 L96 D99 V100 S101 G102 S103 N111 L112 L113 D114 N115 F119 F120 C121 R122 F123 T124 V125 V126 V127 A128 L131 R138 V142 S146 Q147 I148 C153 R154 L158 M162 R163 V171 I172 E173 L183 R184 L185 D186 K187

P188 F189 P190 E191 L192 R193 E194 H195 D202 H203 MET E205 K206 K207 D208 H209 S210 W214 I215 A219 K220 Y221 L222 A223 Q224 W225 Y226 T229 N230 G231 R232 T236 Y237 K238 E239 K240 E241 D242 F243 R244 D245 L246 I247 R248 Q249 G250 I251 L252 K253 P259 GLU ASP E262 E263 N264

F265 E266 I269 K270 N271 T274 A275 L276 N277 T278 T279 P282 I285 D292 R293 I297 T301 P302 S303 F304 L307 A308 R309 A310 L311 F314 K317 E318 G319 V325 R326 P330 D331 M332 I340 K341 R347 E348 K349 K352 D353 A354 A355 A356

N359 L364 I368 A371 P372 E373 S374 I375 S376 E377 K378 E379 L380 K381 L382 L383 V393 R396 K409 I413 S414 S415 N418 P419 D420 N421 E422 I423 V424 D433 K437 R441 N447 V450 E451 E452 D453 I454 L457 Y478 V479 H480 E481 F482

Y485 G486 A487 A488 E489 P490 H491 T492 I493 A494 A495 F496 L497 G498 G499 A500 A501 A502 Q503 E504 V505 I508 I509 Q512 F513 V514 I515 F516 N517 N518 T519 Y520 Q527 A530 Q533 L534

• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain G:

GLY SER MET ALA GLN LEU GLY K6 L7 L8 Q11 K12 L19 Q25 L28 E29 C34 L35 I36 N37 A38 T39 A40 T43 E44 I45 L46 K47 L51 P52 G53 I54 G55 S56 I60 D61 Q64 V65 N72 N73 Q77 G82 K83 N84 R85 A86 E87

M90 E91 F92 L93 Q94 N97 V100 S101 E106 L112 L113 D114 N115 D116 P117 F120 C121 R122 F123 T124 V125 A128 L131 R138 L139 L143 I148 P149 G150 R154 G157 L158 R163 I164 I165 E173 S174 H175 N178 A179 L180 E181 D182 L183 R184

L185 D186 K187 P188 F189 P190 E191 L192 Y199 D200 L201 D202 H203 MET GLU LYS LYS D208 H209 S210 P213 W214 I215 V216 I217 I218 A219 K220 Y221 L222 Y226 N230 G231 I233 P234 K235 T236 Y237 K238 E239 K240 E241 D242 F243 R244 D245 L246 I247 R248 Q249 G250 I251 L252 K253 PRO

GLU D261 E262 E263 N264 F265 E266 E267 A268 I269 K270 N271 V272 V325 T278 T279 Q280 D292 R293 I297 T298 K299 W305 I306 L307 A308 R309 A310 L311 F314 P324 V325 I329 M332 D335 S336 Y339 I340 Q343 N344 V345 Y346 R347 E348 K349 D353 V357
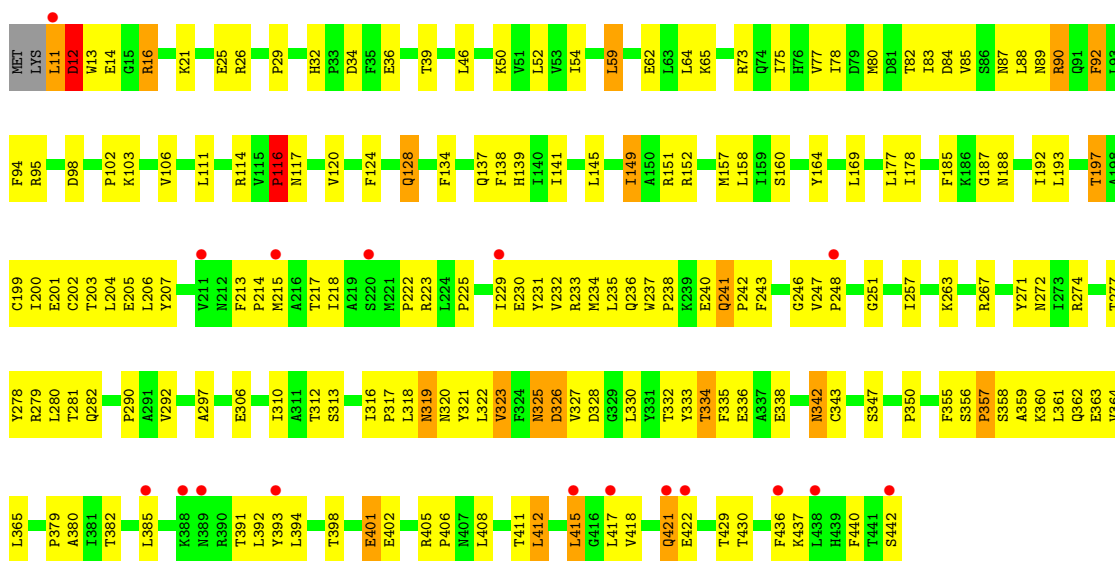
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain B:

• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain D:

• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain F:

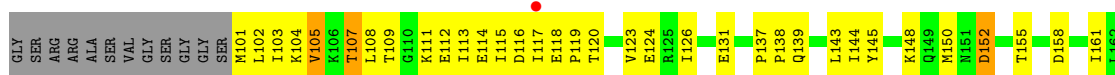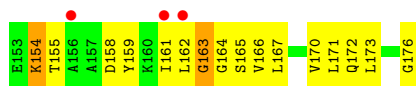• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain H:

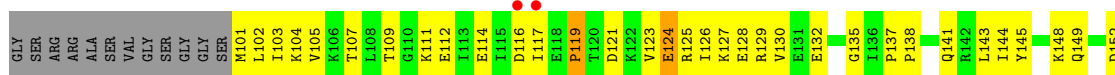• Molecule 3: NEDD8

Chain I:

60%   34%

GLY SER R91 M101 L102 I103 K104 V105 K106 T107 L108 T109 E112 I113 I117 E118 K122 V123 E124 R125 I126 E134 Q139 R142 G147 K148 D152 T155 A156 I161 L162 G163 G164 S165 V166 V170 L171 Q172 L173 R174 G175 G176

• Molecule 3: NEDD8

3%

Chain J:

48%   33%   6%   14%

GLY SER ARG ARG ALA SER VAL GLY SER GLY SER M101 L102 V105 L108 I113 E114 I115 D116 I117 E118 P119 T120 V123 E124 R125 R129 V130 P138 Q139 Q140 Q141 R142 L143 I144 K148 Q149 M150 N151 D152 E153 K154 T155 A156 A157 D158 I161 L162 G163 L167

V170 L171 Q172 L173 G176

• Molecule 3: NEDD8

%

Chain K:

41%   40%   5%   14%

GLY SER ARG ARG ALA SER VAL GLY SER GLY SER M101 L102 I103 K104 V105 K106 T107 L108 T109 G110 K111 E112 I113 E114 I115 D116 I117 E118 P119 T120 V123 E124 R125 I126 E131 P137 P138 Q139 L143 I144 Y145 K148 Q149 M150 N151 D152 T155 D158 I161 L162

G163 L167 V170 L171 Q172 L173 G176

• Molecule 3: NEDD8

6%

Chain L:

31%   51%   5%   14%

GLY SER ARG ARG ALA SER VAL GLY SER GLY SER M101 L102 I103 K104 V105 K106 T107 L108 T109 G110 K111 E112 I113 E114 I115 D116 I117 E118 P119 T120 D121 K122 V123 E124 R125 I126 K127 E128 R129 V130 E131 E132 G135 I136 P137 P138 Q141 R142 L143 I144 Y145 K148 Q149 D152

E153 K154 T155 A156 A157 D158 Y159 K160 I161 L162 G163 G164 S165 V166 L167 V170 L171 Q172 L173 G176

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.12Å 198.95Å 210.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.99 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-2.90) 92.7 (48.99-2.91)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.274 0.227 , 0.226	Depositor DCC
R_{free} test set	5854 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32577	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage'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.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.67	0/5706
1	C	0.41	0/4203	0.62	0/5682
1	E	0.45	0/4198	0.66	0/5678
1	G	0.43	0/4191	0.64	0/5668
2	B	0.47	1/3482 (0.0%)	0.71	2/4738 (0.0%)
2	D	0.44	0/3486	0.67	1/4742 (0.0%)
2	F	0.51	1/3475 (0.0%)	0.75	3/4730 (0.1%)
2	H	0.46	0/3467	0.71	2/4720 (0.0%)
3	I	0.44	0/673	0.68	0/897
3	J	0.42	0/609	0.70	0/813
3	K	0.48	0/609	0.75	1/813 (0.1%)
3	L	0.38	0/609	0.67	0/813
All	All	0.45	2/33220 (0.0%)	0.68	9/45000 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	380	ALA	CA-CB	-9.09	1.33	1.52
2	B	380	ALA	CA-CB	-5.91	1.40	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	165	GLU	N-CA-C	-8.34	88.48	111.00
2	B	240	GLU	N-CA-C	-7.18	91.61	111.00
2	D	12	ASP	N-CA-C	-7.13	91.75	111.00
3	K	173	LEU	CA-CB-CG	-7.12	98.91	115.30
2	H	321	TYR	N-CA-C	5.93	127.03	111.00

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	177	0
1	C	4125	0	4065	181	0
1	E	4119	0	4054	201	0
1	G	4113	0	4058	171	0
2	B	3404	0	3385	202	0
2	D	3408	0	3396	176	0
2	F	3397	0	3380	234	0
2	H	3389	0	3359	238	0
3	I	668	0	702	36	0
3	J	604	0	638	37	0
3	K	604	0	638	40	0
3	L	604	0	638	53	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	1615	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 25.

The worst 5 of 1615 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)
3:J:143:LEU:HB3	3:J:150:MET:HE3	1.26	1.15
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
1:E:184:ARG:HH12	1:E:325:VAL:HG22	1.11	1.07

There are no symmetry-related clashes.

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	518/531 (98%)	451 (87%)	54 (10%)	13 (2%)	5	21
1	C	513/531 (97%)	452 (88%)	52 (10%)	9 (2%)	8	29
1	E	515/531 (97%)	464 (90%)	42 (8%)	9 (2%)	9	31
1	G	512/531 (96%)	447 (87%)	56 (11%)	9 (2%)	8	29
2	B	430/434 (99%)	376 (87%)	46 (11%)	8 (2%)	8	28
2	D	430/434 (99%)	370 (86%)	50 (12%)	10 (2%)	6	23
2	F	429/434 (99%)	360 (84%)	55 (13%)	14 (3%)	4	15
2	H	429/434 (99%)	355 (83%)	60 (14%)	14 (3%)	4	15
3	I	84/88 (96%)	78 (93%)	4 (5%)	2 (2%)	6	22
3	J	74/88 (84%)	70 (95%)	1 (1%)	3 (4%)	3	11
3	K	74/88 (84%)	65 (88%)	6 (8%)	3 (4%)	3	11
3	L	74/88 (84%)	65 (88%)	5 (7%)	4 (5%)	2	6
All	All	4082/4212 (97%)	3553 (87%)	431 (11%)	98 (2%)	6	22

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 ⓘ

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%)	426 (94%)	26 (6%)	20	50
1	C	451/462 (98%)	424 (94%)	27 (6%)	19	49
1	E	448/462 (97%)	420 (94%)	28 (6%)	18	46
1	G	450/462 (97%)	429 (95%)	21 (5%)	26	59
2	B	378/382 (99%)	350 (93%)	28 (7%)	13	38
2	D	379/382 (99%)	354 (93%)	25 (7%)	16	44
2	F	377/382 (99%)	346 (92%)	31 (8%)	11	32
2	H	375/382 (98%)	351 (94%)	24 (6%)	17	45
3	I	73/74 (99%)	67 (92%)	6 (8%)	11	32
3	J	67/74 (90%)	62 (92%)	5 (8%)	13	37
3	K	67/74 (90%)	63 (94%)	4 (6%)	19	49
3	L	67/74 (90%)	66 (98%)	1 (2%)	65	87
All	All	3584/3672 (98%)	3358 (94%)	226 (6%)	18	46

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	171	LEU
2	H	348	GLN
1	E	517	ASN
2	H	321	TYR
1	G	516	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	343	GLN
2	H	439	HIS
1	G	436	HIS
2	H	262	GLN
1	C	447	ASN

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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

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 ⓘ

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 ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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	522/531 (98%)	0.05	12 (2%)	60	58	33, 67, 99, 122	0
1	C	520/531 (97%)	0.07	5 (0%)	82	82	41, 68, 102, 130	0
1	E	521/531 (98%)	0.11	12 (2%)	60	58	32, 56, 116, 134	0
1	G	518/531 (97%)	0.14	18 (3%)	44	38	34, 64, 124, 137	0
2	B	432/434 (99%)	0.16	18 (4%)	36	32	36, 59, 109, 117	0
2	D	432/434 (99%)	0.27	17 (3%)	39	35	40, 70, 109, 117	0
2	F	431/434 (99%)	0.39	28 (6%)	18	14	37, 61, 116, 124	0
2	H	431/434 (99%)	0.29	26 (6%)	21	18	37, 69, 116, 122	0
3	I	86/88 (97%)	-0.05	0	100	100	47, 68, 93, 97	0
3	J	76/88 (86%)	0.34	3 (3%)	39	35	58, 77, 96, 98	0
3	K	76/88 (86%)	0.12	1 (1%)	77	77	56, 73, 90, 91	0
3	L	76/88 (86%)	0.53	5 (6%)	18	14	67, 93, 115, 121	0
All	All	4121/4212 (97%)	0.18	145 (3%)	44	38	32, 66, 113, 137	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	408	LEU	5.5
2	F	441	THR	5.3
2	H	360	LYS	5.2
1	C	259	PRO	5.1
1	G	201	LEU	5.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	ZN	F	4	1/1	0.97	0.18	62,62,62,62	0
4	ZN	D	3	1/1	0.99	0.19	74,74,74,74	0
4	ZN	B	1	1/1	0.99	0.16	65,65,65,65	0
4	ZN	H	2	1/1	0.99	0.17	80,80,80,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.