



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:03 PM GMT

PDB ID : 4BE8  
Title : NEDD4 HECT A889F structure  
Authors : Maspero, E.; Valentini, E.; Mari, S.; Cecatiello, V.; Polo, S.; Pasqualato, S.  
Deposited on : 2013-03-06  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

---

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

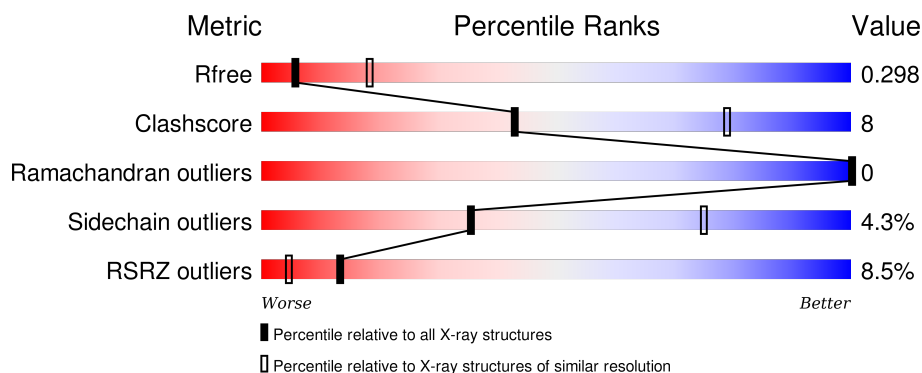
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	385	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3124 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 E3 UBIQUITIN-PROTEIN LIGASE NEDD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			3121	2023	525	559	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	515	GLY	-	EXPRESSION TAG	UNP P46934
A	516	PRO	-	EXPRESSION TAG	UNP P46934
A	517	LEU	-	EXPRESSION TAG	UNP P46934
A	518	GLY	-	EXPRESSION TAG	UNP P46934
A	626	ILE	LEU	ENGINEERED MUTATION	UNP P46934
A	.	-	CYS	DELETION	UNP P46934
A	628	PRO	GLU	ENGINEERED MUTATION	UNP P46934
A	777	SER	CYS	ENGINEERED MUTATION	UNP P46934
A	888	PHE	ALA	ENGINEERED MUTATION	UNP P46934

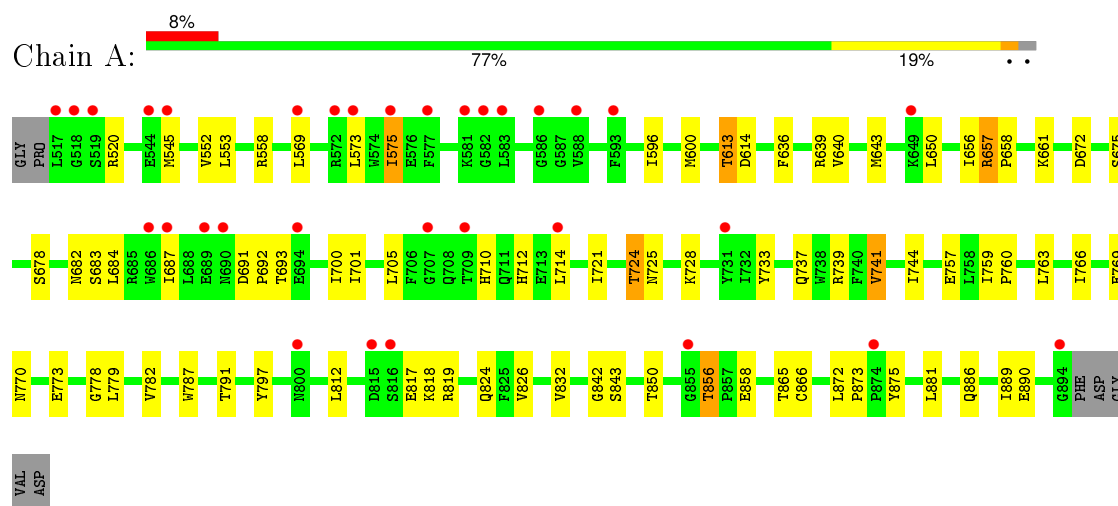
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		

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

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: E3 UBIQUITIN-PROTEIN LIGASE NEDD4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.55Å 100.55Å 96.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.58 – 3.00 44.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.58-3.00) 99.3 (44.58-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.246 , 0.295 0.240 , 0.298	Depositor DCC
$R_{free}$ test set	581 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.8	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 94.8	EDS
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 11622 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3124	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.26	0/3207	0.43	0/4331

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	710	HIS	Peptide

### 5.2 Too-close contacts [i](#)

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	3121	0	2997	50	0
2	A	3	0	0	0	0
All	All	3124	0	2997	50	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 8.

All (50) 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)
1:A:656:ILE:HG12	1:A:658:PRO:HD2	1.54	0.88
1:A:658:PRO:HG3	1:A:672:ASP:HB3	1.70	0.73
1:A:700:ILE:HG13	1:A:712:HIS:O	1.92	0.68
1:A:573:LEU:HB3	1:A:575:ILE:HD11	1.79	0.65
1:A:818:LYS:NZ	1:A:890:GLU:OE2	2.30	0.64
1:A:856:THR:OG1	1:A:858:GLU:OE1	2.16	0.62
1:A:657:ARG:NH2	1:A:773:GLU:OE1	2.28	0.62
1:A:600:MET:HE1	1:A:640:VAL:HG11	1.81	0.61
1:A:683:SER:HB3	1:A:705:LEU:HG	1.82	0.60
1:A:678:SER:O	1:A:682:ASN:ND2	2.35	0.60
1:A:773:GLU:OE1	1:A:824:GLN:NE2	2.34	0.59
1:A:552:VAL:HG22	1:A:596:ILE:HD13	1.86	0.57
1:A:700:ILE:HG12	1:A:701:ILE:N	2.20	0.57
1:A:700:ILE:HG13	1:A:712:HIS:C	2.25	0.56
1:A:760:PRO:HB2	1:A:763:LEU:HB2	1.86	0.56
1:A:545:MET:HG3	1:A:575:ILE:HG23	1.88	0.55
1:A:787:TRP:O	1:A:791:THR:OG1	2.21	0.54
1:A:639:ARG:NE	1:A:757:GLU:OE1	2.40	0.54
1:A:739:ARG:O	1:A:739:ARG:NH1	2.36	0.54
1:A:886:GLN:HA	1:A:889:ILE:HG12	1.92	0.51
1:A:614:ASP:HB3	1:A:842:GLY:HA2	1.92	0.51
1:A:691:ASP:OD2	1:A:693:THR:OG1	2.17	0.51
1:A:600:MET:CE	1:A:640:VAL:HG11	2.40	0.51
1:A:737:GLN:HA	1:A:741:VAL:HG22	1.92	0.50
1:A:656:ILE:HG13	1:A:675:SER:HB2	1.95	0.48
1:A:650:LEU:HD11	1:A:778:GLY:HA3	1.96	0.48
1:A:843:SER:HB2	1:A:866:CYS:HB2	1.96	0.47
1:A:520:ARG:NH2	1:A:817:GLU:OE2	2.31	0.46
1:A:636:PHE:O	1:A:640:VAL:HG12	2.15	0.45
1:A:724:THR:OG1	1:A:725:ASN:N	2.49	0.45
1:A:875:TYR:CD2	1:A:881:LEU:HA	2.51	0.45
1:A:657:ARG:HB3	1:A:658:PRO:HD3	1.99	0.45
1:A:650:LEU:HA	1:A:650:LEU:HD12	1.69	0.44
1:A:733:TYR:O	1:A:737:GLN:HG2	2.18	0.44
1:A:763:LEU:O	1:A:766:ILE:HG22	2.17	0.44
1:A:520:ARG:NH1	1:A:890:GLU:OE2	2.45	0.43
1:A:684:LEU:HA	1:A:687:ILE:HG22	2.01	0.42
1:A:553:LEU:HA	1:A:596:ILE:HD11	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:HD13	1:A:643:MET:HE2	2.01	0.42
1:A:691:ASP:HA	1:A:692:PRO:HD3	1.76	0.42
1:A:613:THR:HA	1:A:614:ASP:HA	1.43	0.41
1:A:759:ILE:HA	1:A:760:PRO:HD3	1.92	0.41
1:A:650:LEU:HD11	1:A:778:GLY:CA	2.50	0.41
1:A:770:ASN:N	1:A:770:ASN:OD1	2.52	0.41
1:A:558:ARG:H	1:A:558:ARG:HG2	1.66	0.41
1:A:872:LEU:HA	1:A:873:PRO:HD3	1.82	0.41
1:A:826:VAL:O	1:A:865:THR:HA	2.21	0.41
1:A:687:ILE:O	1:A:728:LYS:HE2	2.20	0.40
1:A:812:LEU:O	1:A:819:ARG:NH2	2.54	0.40
1:A:661:LYS:NZ	1:A:769:GLU:OE2	2.55	0.40

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	376/385 (98%)	364 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	325/345 (94%)	311 (96%)	14 (4%)	35 75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	ILE
1	A	613	THR
1	A	657	ARG
1	A	714	LEU
1	A	721	ILE
1	A	724	THR
1	A	741	VAL
1	A	744	ILE
1	A	779	LEU
1	A	782	VAL
1	A	797	TYR
1	A	832	VAL
1	A	850	THR
1	A	856	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	378/385 (98%)	0.57	32 (8%) 13 5	97, 133, 187, 210	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	LEU	4.3
1	A	582	GLY	4.0
1	A	517	LEU	3.6
1	A	707	GLY	3.5
1	A	577	PHE	3.5
1	A	686	TRP	3.4
1	A	588	VAL	3.2
1	A	575	ILE	3.2
1	A	649	LYS	3.1
1	A	714	LEU	3.1
1	A	709	THR	2.9
1	A	545	MET	2.9
1	A	569	LEU	2.8
1	A	518	GLY	2.8
1	A	581	LYS	2.7
1	A	894	GLY	2.7
1	A	689	GLU	2.7
1	A	874	PRO	2.7
1	A	694	GLU	2.6
1	A	572	ARG	2.6
1	A	855	GLY	2.5
1	A	815	ASP	2.4
1	A	519	SER	2.4
1	A	690	ASN	2.3
1	A	544	GLU	2.3
1	A	573	LEU	2.3
1	A	731	TYR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	816	SER	2.3
1	A	593	PHE	2.3
1	A	687	ILE	2.2
1	A	586	GLY	2.2
1	A	800	ASN	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.