



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:42 AM UTC

PDB ID : 2ONI / pdb_00002oni
Title : Catalytic Domain of the Human NEDD4-like E3 Ligase
Authors : Walker, J.R.; Avvakumov, G.V.; Xue, S.; Butler-Cole, C.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2007-01-24
Resolution : 2.20 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

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
Mogul : 2022.3.0, CSD as543be (2022)
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

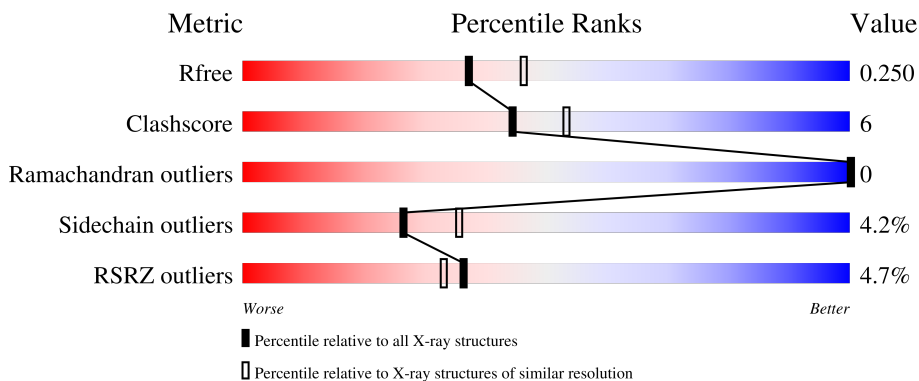
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

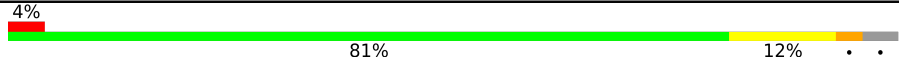
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	392	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3269 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-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	377	3149	2040	521	569	5	14	8	3	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	556	MSE	-	cloning artifact	UNP Q96PU5
A	557	HIS	-	cloning artifact	UNP Q96PU5
A	558	HIS	-	cloning artifact	UNP Q96PU5
A	559	HIS	-	cloning artifact	UNP Q96PU5
A	560	HIS	-	cloning artifact	UNP Q96PU5
A	561	HIS	-	cloning artifact	UNP Q96PU5
A	562	HIS	-	cloning artifact	UNP Q96PU5
A	563	SER	-	cloning artifact	UNP Q96PU5
A	564	SER	-	cloning artifact	UNP Q96PU5
A	565	GLY	-	cloning artifact	UNP Q96PU5
A	566	ARG	-	cloning artifact	UNP Q96PU5
A	567	GLU	-	cloning artifact	UNP Q96PU5
A	568	ASN	-	cloning artifact	UNP Q96PU5
A	569	LEU	-	cloning artifact	UNP Q96PU5
A	570	TYR	-	cloning artifact	UNP Q96PU5
A	571	PHE	-	cloning artifact	UNP Q96PU5
A	572	GLN	-	cloning artifact	UNP Q96PU5
A	573	GLY	-	cloning artifact	UNP Q96PU5
A	600	MSE	MET	modified residue	UNP Q96PU5
A	616	MSE	MET	modified residue	UNP Q96PU5
A	655	MSE	MET	modified residue	UNP Q96PU5
A	718	MSE	MET	modified residue	UNP Q96PU5
A	719	MSE	MET	modified residue	UNP Q96PU5
A	729	MSE	MET	modified residue	UNP Q96PU5
A	754	MSE	MET	modified residue	UNP Q96PU5
A	778	MSE	MET	modified residue	UNP Q96PU5
A	804	MSE	MET	modified residue	UNP Q96PU5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	832	MSE	MET	modified residue	UNP Q96PU5
A	870	MSE	MET	modified residue	UNP Q96PU5
A	890	MSE	MET	modified residue	UNP Q96PU5
A	943	MSE	MET	modified residue	UNP Q96PU5

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

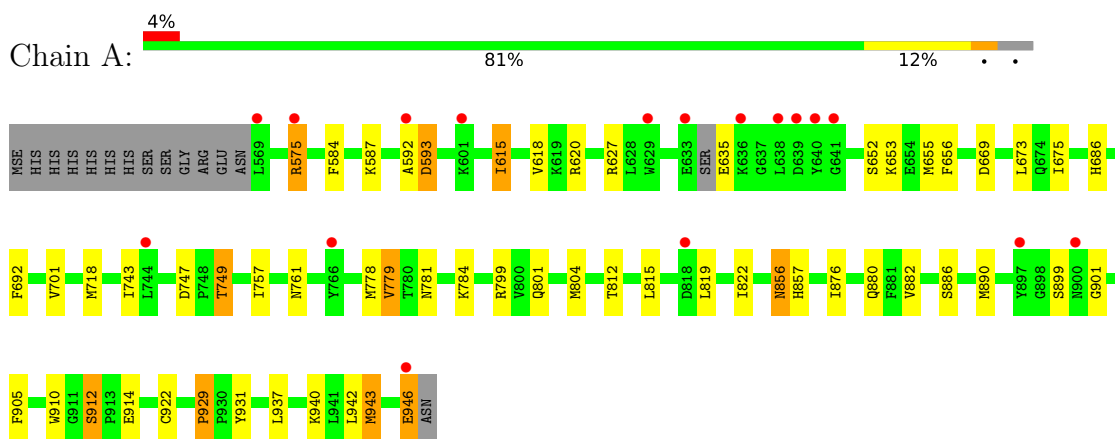
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	119	Total O 119 119	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: E3 ubiquitin-protein ligase NEDD4-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	103.06Å 103.06Å 182.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.28 – 2.20 28.28 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.28-2.20) 99.5 (28.28-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.259 0.202 , 0.250	Depositor DCC
R_{free} test set	1534 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3269	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA

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	0.96	0/3220	1.02	7/4331 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	901	GLY	CA-C-N	5.63	125.96	119.93
1	A	901	GLY	C-N-CA	5.63	125.96	119.93
1	A	686	HIS	N-CA-C	5.28	117.72	111.33
1	A	929	PRO	N-CA-C	5.21	115.47	110.47
1	A	779	VAL	CB-CA-C	5.21	117.27	110.96
1	A	592	ALA	N-CA-C	-5.12	106.88	113.02
1	A	749	THR	N-CA-C	5.05	117.44	111.33

There are no chirality outliers.

There are no planarity outliers.

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	3149	0	3027	37	0
2	A	1	0	0	0	0
3	A	119	0	0	1	0
All	All	3269	0	3027	37	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 6.

All (37) 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:931:TYR:CE1	1:A:940:LYS:HD2	2.08	0.88
1:A:761:ASN:HD21	1:A:799:ARG:HH22	1.34	0.74
1:A:669:ASP:HB2	1:A:880:GLN:HE21	1.55	0.71
1:A:593:ASP:HB3	1:A:620:ARG:HH22	1.60	0.66
1:A:718:MSE:HE3	1:A:801:GLN:HE21	1.63	0.62
1:A:743:ILE:O	1:A:784:LYS:HE2	2.01	0.61
1:A:819:LEU:O	1:A:822:ILE:HG12	2.00	0.60
1:A:718:MSE:HE3	1:A:801:GLN:NE2	2.17	0.59
1:A:882:VAL:HG11	1:A:905:PHE:CE1	2.39	0.57
1:A:669:ASP:HB2	1:A:880:GLN:NE2	2.18	0.57
1:A:747:ASP:OD1	1:A:749:THR:HG23	2.06	0.55
1:A:856:ASN:C	1:A:856:ASN:HD22	2.16	0.54
1:A:912:SER:OG	1:A:914:GLU:HG2	2.08	0.52
1:A:575[B]:ARG:NH1	3:A:69:HOH:O	2.40	0.51
1:A:615:ILE:HG13	1:A:692:PHE:HE1	1.77	0.50
1:A:942:LEU:O	1:A:946:GLU:HG3	2.12	0.50
1:A:675:ILE:CD1	1:A:804:MSE:HE2	2.42	0.49
1:A:876:ILE:CG2	1:A:886:SER:HB2	2.43	0.48
1:A:675:ILE:HD11	1:A:804:MSE:HE2	1.94	0.48
1:A:781:ASN:HA	1:A:784:LYS:HD3	1.96	0.48
1:A:856:ASN:C	1:A:856:ASN:ND2	2.71	0.47
1:A:653:LYS:HE2	1:A:890:MSE:O	2.15	0.46
1:A:876:ILE:HG23	1:A:886:SER:HB2	1.98	0.46
1:A:856:ASN:HD22	1:A:857:HIS:N	2.14	0.45
1:A:812:THR:HA	1:A:815:LEU:O	2.17	0.45
1:A:761:ASN:HD21	1:A:799:ARG:NH2	2.07	0.44
1:A:931:TYR:CZ	1:A:940:LYS:HD2	2.50	0.44
1:A:937:LEU:HD23	1:A:937:LEU:C	2.43	0.43
1:A:584:PHE:HB2	1:A:822:ILE:HD11	2.01	0.43
1:A:656:PHE:HB3	1:A:673:LEU:HD13	2.01	0.43
1:A:943:MSE:HE3	1:A:943:MSE:HB2	1.93	0.43
1:A:718:MSE:HE2	1:A:804:MSE:HG2	2.02	0.42
1:A:652:SER:HA	1:A:655:MSE:HE2	2.02	0.41
1:A:701:VAL:HB	1:A:815:LEU:HD11	2.03	0.41
1:A:910:TRP:O	1:A:929:PRO:HA	2.21	0.40
1:A:819:LEU:HD23	1:A:819:LEU:HA	1.94	0.40
1:A:899:SER:HB2	1:A:922:CYS:HB2	2.03	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	376/392 (96%)	369 (98%)	7 (2%)	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	335/343 (98%)	319 (95%)	16 (5%)	23 30

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575[A]	ARG
1	A	575[B]	ARG
1	A	587	LYS
1	A	593	ASP
1	A	615	ILE
1	A	618	VAL
1	A	627	ARG
1	A	635	GLU
1	A	757	ILE
1	A	778[A]	MSE

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Mol	Chain	Res	Type
1	A	778[B]	MSE
1	A	779	VAL
1	A	856	ASN
1	A	912	SER
1	A	943	MSE
1	A	946	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	605	ASN
1	A	727	ASN
1	A	761	ASN
1	A	764	GLN
1	A	798	ASN
1	A	801	GLN
1	A	856	ASN
1	A	880	GLN
1	A	909	GLN
1	A	920	HIS

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 1 ligands modelled in this entry, 1 is 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 [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, 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	364/392 (92%)	0.20	17 (4%) 36 33	23, 48, 73, 104	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	LEU	4.4
1	A	744	LEU	3.0
1	A	639	ASP	2.9
1	A	629	TRP	2.9
1	A	900	ASN	2.9
1	A	592	ALA	2.8
1	A	766	TYR	2.7
1	A	638	LEU	2.7
1	A	633	GLU	2.6
1	A	636	LYS	2.4
1	A	640	TYR	2.3
1	A	946	GLU	2.2
1	A	641	GLY	2.2
1	A	601[A]	LYS	2.2
1	A	818	ASP	2.2
1	A	575[A]	ARG	2.1
1	A	897	TYR	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 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, 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(\AA^2)	Q<0.9
2	NA	A	1000	1/1	0.80	0.14	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.