



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2021 – 05:02 pm BST

PDB ID : 7NMZ  
Title : Structure of 14-3-3 eta in complex with Nedd4-2(335-455) containing two 14-3-3 binding motifs Ser342 and Ser448  
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Deposited on : 2021-02-23  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.22  
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) : 2.22

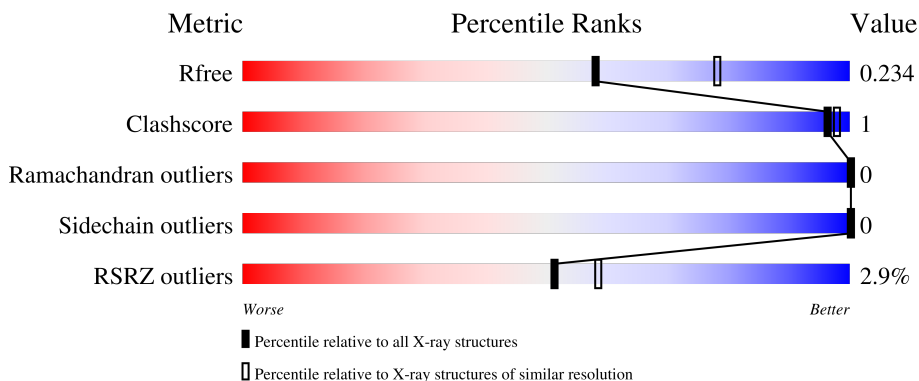
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	AA	236	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%, grey 97%);"></div> <div style="margin-left: 10px;"> <p>97%</p> </div> </div>
1	BA	236	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 95%, grey 95%);"></div> <div style="margin-left: 10px;"> <p>95%</p> </div> </div>
2	C	125	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 15%, yellow 15%, green 83%, grey 83%);"></div> <div style="margin-left: 10px;"> <p>83%</p> </div> </div>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3907 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 14-3-3 protein eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	236	1816	1142	309	356	9	0	0	0
1	BA	230	1766	1111	304	342	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1	GLY	-	expression tag	UNP Q04917
AA	2	HIS	-	expression tag	UNP Q04917
BA	1	GLY	-	expression tag	UNP Q04917
BA	2	HIS	-	expression tag	UNP Q04917

- Molecule 2 is a protein called E3 ubiquitin-protein ligase NEDD4-like.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	C	21	136	77	21	35	2	1	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	331	GLY	-	expression tag	UNP Q96PU5
C	332	ALA	-	expression tag	UNP Q96PU5
C	333	MET	-	expression tag	UNP Q96PU5
C	334	GLY	-	expression tag	UNP Q96PU5
C	367	ALA	THR	engineered mutation	UNP Q96PU5

- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	AA	106	Total 106	O 106	0	0
3	BA	78	Total 78	O 78	0	0
3	C	5	Total 5	O 5	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.86Å 58.95Å 106.76Å 90.00° 90.69° 90.00°	Depositor
Resolution (Å)	32.69 – 2.30 47.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.69-2.30) 99.9 (47.37-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.199 , 0.235 0.199 , 0.234	Depositor DCC
$R_{free}$ test set	1641 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: SEP

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	AA	0.27	0/1843	0.43	0/2495
1	BA	0.26	0/1789	0.42	0/2414
2	C	0.22	0/114	0.45	0/152
All	All	0.26	0/3746	0.42	0/5061

There are no bond length outliers.

There are no bond angle outliers.

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	AA	1816	0	1727	4	0
1	BA	1766	0	1702	3	0
2	C	136	0	106	0	0
3	AA	106	0	0	0	0
3	BA	78	0	0	0	0
3	C	5	0	0	0	0
All	All	3907	0	3535	7	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 1.

All (7) 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:AA:25:MET:HG2	1:AA:50:ALA:HB2	1.78	0.64
1:BA:25:MET:HG2	1:BA:50:ALA:HB2	1.93	0.50
1:BA:134:ARG:HG3	1:BA:188:ILE:HG13	1.94	0.48
1:AA:235:TRP:O	1:AA:236:THR:HG23	2.16	0.45
1:BA:89:GLU:O	1:BA:93:LYS:HG3	2.17	0.45
1:AA:167:MET:HE2	1:AA:173:ILE:HB	2.00	0.42
1:AA:214:ASN:HD21	1:AA:216:ASP:HB2	1.87	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	AA	234/236 (99%)	232 (99%)	2 (1%)	0	100	100
1	BA	226/236 (96%)	223 (99%)	3 (1%)	0	100	100
2	C	15/125 (12%)	14 (93%)	1 (7%)	0	100	100
All	All	475/597 (80%)	469 (99%)	6 (1%)	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	AA	183/206 (89%)	183 (100%)	0	100	100
1	BA	177/206 (86%)	177 (100%)	0	100	100
2	C	12/100 (12%)	12 (100%)	0	100	100
All	All	372/512 (73%)	372 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	146	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SEP	C	342	2	8,9,10	1.51	1 (12%)	8,12,14	1.84	2 (25%)
2	SEP	C	448	2	8,9,10	1.54	1 (12%)	8,12,14	1.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	C	342	2	-	0/5/8/10	-
2	SEP	C	448	2	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	448	SEP	P-O1P	3.31	1.61	1.50
2	C	342	SEP	P-O1P	3.21	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	342	SEP	OG-CB-CA	4.00	112.04	108.14
2	C	342	SEP	P-OG-CB	-2.52	111.37	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	AA	236/236 (100%)	-0.09	3 (1%) 77 81	22, 36, 72, 91	0
1	BA	230/236 (97%)	-0.02	3 (1%) 77 81	24, 46, 74, 88	0
2	C	19/125 (15%)	1.86	8 (42%) 0 0	44, 62, 86, 87	0
All	All	485/597 (81%)	0.02	14 (2%) 51 58	22, 42, 75, 91	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	452	VAL	4.5
2	C	453	THR	4.0
1	AA	74	ALA	3.7
2	C	444	PRO	3.7
2	C	451	THR	3.3
1	AA	73	MET	3.2
2	C	454	LEU	3.1
2	C	450	PRO	2.7
1	BA	117	PHE	2.7
1	BA	116	ASP	2.6
1	BA	236	THR	2.4
2	C	447	LEU	2.2
1	AA	190	ASN	2.1
2	C	338	LEU	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
2	SEP	C	342	10/11	0.98	0.13	29,36,43,49	0
2	SEP	C	448	10/11	0.98	0.13	24,29,36,44	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.