



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4Q7M  
Title : Structure of NBD288-Avi of TM287/288  
Authors : Bukowska, M.A.; Hohl, M.; Gruetter, M.G.; Seeger, M.A.  
Deposited on : 2014-04-25  
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  
<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

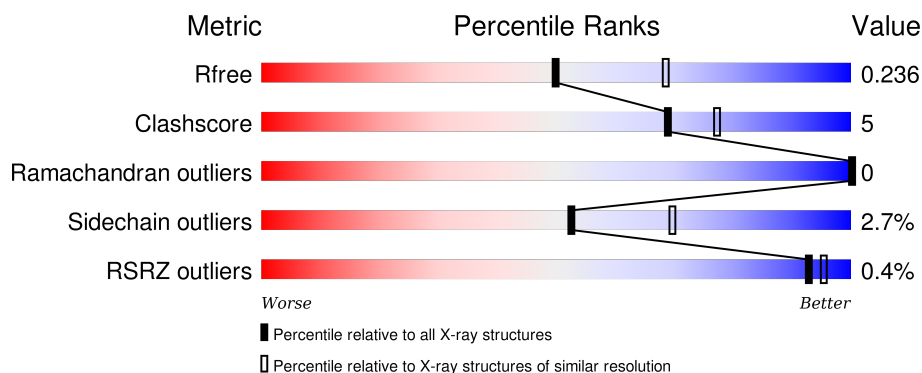
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	B	271	 83% 10% • 6%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2164 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 Uncharacterized ABC transporter ATP-binding protein TM\_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	255	Total	C	N	O	S	0	1	0
			2036	1298	346	388	4			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	351	MET	-	INITIATING METHIONINE	UNP Q9WYC4
B	352	SER	-	EXPRESSION TAG	UNP Q9WYC4
B	599	ALA	-	EXPRESSION TAG	UNP Q9WYC4
B	600	ALA	-	EXPRESSION TAG	UNP Q9WYC4
B	601	GLY	-	EXPRESSION TAG	UNP Q9WYC4
B	602	LEU	-	EXPRESSION TAG	UNP Q9WYC4
B	603	ASN	-	EXPRESSION TAG	UNP Q9WYC4
B	604	ASP	-	EXPRESSION TAG	UNP Q9WYC4
B	605	ILE	-	EXPRESSION TAG	UNP Q9WYC4
B	606	PHE	-	EXPRESSION TAG	UNP Q9WYC4
B	607	GLU	-	EXPRESSION TAG	UNP Q9WYC4
B	608	ALA	-	EXPRESSION TAG	UNP Q9WYC4
B	609	GLN	-	EXPRESSION TAG	UNP Q9WYC4
B	610	LYS	-	EXPRESSION TAG	UNP Q9WYC4
B	611	ILE	-	EXPRESSION TAG	UNP Q9WYC4
B	612	GLU	-	EXPRESSION TAG	UNP Q9WYC4
B	613	TRP	-	EXPRESSION TAG	UNP Q9WYC4
B	614	HIS	-	EXPRESSION TAG	UNP Q9WYC4
B	615	GLU	-	EXPRESSION TAG	UNP Q9WYC4
B	616	LEU	-	EXPRESSION TAG	UNP Q9WYC4
B	617	GLU	-	EXPRESSION TAG	UNP Q9WYC4
B	618	VAL	-	EXPRESSION TAG	UNP Q9WYC4
B	619	LEU	-	EXPRESSION TAG	UNP Q9WYC4
B	620	PHE	-	EXPRESSION TAG	UNP Q9WYC4
B	621	GLN	-	EXPRESSION TAG	UNP Q9WYC4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	128	Total 128	O 128	0	0

**i**

- Molecule 1: Uncharacterized ABC transporter ATP-binding protein TM 0288

Y691	Q609	K368	K372	V387	V398	R403	L413	L435	T438	F473	I474	L477	T486	L499	A501	I514	L515	D516	T519	SER	ASN	VAL	D523	T524	K525	L537	A547	E548	R549	L550	N551	D557	L558	M570	D574	G578
Y691	Q609	K368	K372	V387	V398	R403	L413	L435	T438	F473	I474	L477	T486	L499	A501	I514	L515	D516	T519	SER	ASN	VAL	D523	T524	K525	L537	A547	E548	R549	L550	N551	D557	L558	M570	D574	G578

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.30 Å 58.30 Å 208.69 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.49 – 2.30 69.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.49-2.30) 99.9 (69.56-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, $R_{free}$	0.181 , 0.236 0.181 , 0.236	Depositor DCC
$R_{free}$ test set	956 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 42.6	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19134 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2164	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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	B	0.33	0/2067	0.50	1/2784 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	LEU	CA-CB-CG	5.06	126.93	115.30

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	B	2036	0	2081	19	0
2	B	128	0	0	8	1
All	All	2164	0	2081	19	1

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 5.

All (19) 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:B:516:ASP:OD2	2:B:711:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:VAL:HG13	1:B:514:ILE:HD13	1.70	0.73
1:B:557:ASP:O	2:B:825:HOH:O	2.06	0.73
1:B:486:THR:O	2:B:821:HOH:O	2.09	0.70
1:B:474:ILE:HA	1:B:477:LEU:HD22	1.76	0.66
1:B:551:ASN:OD1	1:B:551:ASN:N	2.38	0.55
1:B:574:ASP:O	1:B:578:GLN:HG2	2.09	0.53
1:B:438:THR:HG21	1:B:501:ALA:HB2	1.90	0.52
1:B:558:LEU:HD11	1:B:570:MET:HG3	1.91	0.52
1:B:372:LYS:NZ	2:B:806:HOH:O	2.45	0.49
1:B:473:PHE:O	2:B:779:HOH:O	2.20	0.48
1:B:368:LYS:HA	1:B:369:PRO:HD3	1.81	0.44
1:B:398:VAL:CG1	1:B:514:ILE:HD13	2.45	0.44
1:B:609:GLN:CA	2:B:733:HOH:O	2.66	0.43
1:B:549:ARG:O	1:B:591:TYR:OH	2.12	0.43
1:B:519:THR:O	2:B:809:HOH:O	2.21	0.42
1:B:387:VAL:HG12	1:B:547:ALA:HB3	2.01	0.41
1:B:609:GLN:HA	2:B:733:HOH:O	2.20	0.41
1:B:502:ILE:HG23	1:B:537:LEU:HD22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:726:HOH:O	2:B:740:HOH:O[4_555]	2.15	0.05

## 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	B	253/271 (93%)	249 (98%)	4 (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	B	223 / 237 (94%)	217 (97%)	6 (3%)	52 70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	403	ARG
1	B	413	LEU
1	B	435	LEU
1	B	473	PHE
1	B	477	LEU
1	B	499	LEU

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 [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	B	255/271 (94%)	-0.25	1 (0%)	93 95	29, 42, 81, 125	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	525	LYS	2.4

### 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.