



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:10 AM UTC

PDB ID : 4PD3 / pdb\_00004pd3  
Title : Crystal Structure of Rigor-Like Human Nonmuscle Myosin-2B  
Authors : Munnich, S.; Pathan-Chhatbar, S.; Manstein, D.J.  
Deposited on : 2014-04-17  
Resolution : 2.84 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](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.

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  
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

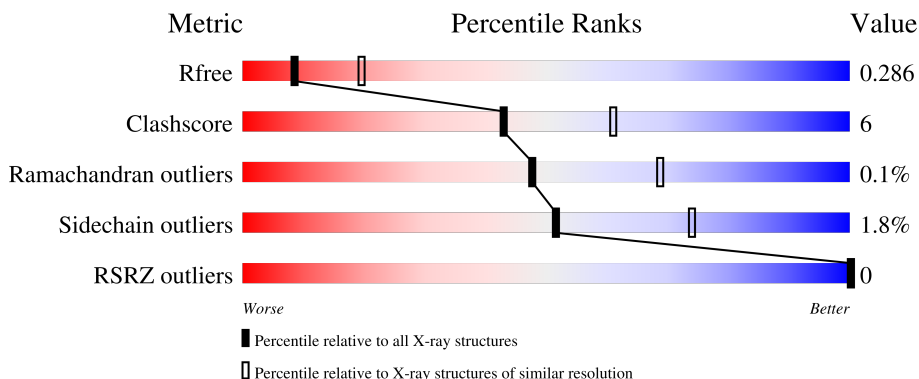
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	A	1032	 74% 15% • 11%
1	B	1032	 73% 16% • 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14828 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 Nonmuscle myosin heavy chain B, Alpha-actinin A Chimera Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	922	7379	4672	1284	1388	35	0	0	0
1	B	930	7416	4698	1288	1395	35	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	783	ALA	-	linker	UNP P35580
A	784	SER	-	linker	UNP P35580
A	1023	ALA	-	expression tag	UNP P05095
A	1024	LEU	-	expression tag	UNP P05095
A	1025	HIS	-	expression tag	UNP P05095
A	1026	HIS	-	expression tag	UNP P05095
A	1027	HIS	-	expression tag	UNP P05095
A	1028	HIS	-	expression tag	UNP P05095
A	1029	HIS	-	expression tag	UNP P05095
A	1030	HIS	-	expression tag	UNP P05095
A	1031	HIS	-	expression tag	UNP P05095
A	1032	HIS	-	expression tag	UNP P05095
B	783	ALA	-	linker	UNP P35580
B	784	SER	-	linker	UNP P35580
B	1023	ALA	-	expression tag	UNP P05095
B	1024	LEU	-	expression tag	UNP P05095
B	1025	HIS	-	expression tag	UNP P05095
B	1026	HIS	-	expression tag	UNP P05095
B	1027	HIS	-	expression tag	UNP P05095
B	1028	HIS	-	expression tag	UNP P05095
B	1029	HIS	-	expression tag	UNP P05095
B	1030	HIS	-	expression tag	UNP P05095
B	1031	HIS	-	expression tag	UNP P05095
B	1032	HIS	-	expression tag	UNP P05095

- Molecule 2 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	A	18	Total 18	O 18	0	0
2	B	15	Total 15	O 15	0	0



L386	P399	R400	I401	K402	VAL	GLY	ARG	ARG	ASP	Y407	V408	Q409	K410	A411	Q412	E415	E422	F433	R439	L444	ASP	ARG	THR	LYS	ARG	GLN	G451	I455	G456	L457	L458	D459	F463	L468	W469	S470	Y478	D510	L513	L521	I522	E523	R524	P525	A526	N527	P528			
P529	F541	P542	P566	ARG	GLN	LEU	LYS	ASP	K572	I577	E590	M593	K594	D601	N602	L607	R624	ILE	VAL	GLY	THR	LEU	ASP	GLN	VAL	THR	GLY	MET	THR	GLU	THR	ALA	PHE	GLY	SER	ALA	TYR	LYS	THR	LYS	LYS	LYS	GLY	M649	F650	R651	T652	K658	T671	I679
R686	H693	C701	I708	C711	R712	Q713	P716	R725	Q726	R727	Y728	E729	I730	P758	N759	L760	Y761	R762	F769	F770	R771	A772	G773	E779	R782	S789	L798	I818	P837	V843	R858	L859	I860	K861	R862	E863	P864	F865	V866	A867	L871									
D877	W880	L894	R895	I896	Q901	L918	E919	N920	T924	LYS	SER	VAL	TYR	LEU	GLY	SER	ASN	GLU	THR	GLY	ASP	SER	I938	T939	A940	L958	E959	N979	G980	V981	Q995	T1009	K1019	ILE	GLU	ASP	ALA	LEU	HIS	HIS	HIS	HIS	HIS	HIS						

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.85Å 157.87Å 143.48Å 90.00° 94.21° 90.00°	Depositor
Resolution (Å)	30.00 – 2.84 30.00 – 2.84	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-2.84) 83.2 (30.00-2.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.76 (at 2.85Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.253 , 0.288 0.256 , 0.286	Depositor DCC
$R_{free}$ test set	1995 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtrriage
Anisotropy	0.627	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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](#)

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	0.27	0/7515	0.73	7/10128 (0.1%)
1	B	0.28	0/7551	0.77	15/10180 (0.1%)
All	All	0.27	0/15066	0.75	22/20308 (0.1%)

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
1	B	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	TYR	N-CA-C	-10.89	97.59	112.94
1	B	859	LEU	N-CA-C	-8.51	102.91	113.38
1	A	741	MET	CB-CA-C	-8.09	107.24	116.63
1	B	524	ARG	CA-C-N	7.36	129.04	119.84
1	B	524	ARG	C-N-CA	7.36	129.04	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	GLU	Peptide
1	B	61	GLU	Peptide
1	B	858	ARG	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	7379	0	7292	80	0
1	B	7416	0	7300	103	0
2	A	18	0	0	0	0
2	B	15	0	0	0	0
All	All	14828	0	14592	182	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.

The worst 5 of 182 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:12:ARG:HD3	1:B:18:ARG:HB3	1.46	0.97
1:B:12:ARG:HB3	1:B:18:ARG:CB	2.01	0.90
1:B:12:ARG:CB	1:B:18:ARG:HB2	2.10	0.82
1:B:11:GLU:O	1:B:13:TYR:N	2.13	0.81
1:B:12:ARG:HB3	1:B:18:ARG:HB2	1.62	0.77

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	908/1032 (88%)	874 (96%)	34 (4%)	0	100 100
1	B	912/1032 (88%)	878 (96%)	33 (4%)	1 (0%)	48 69

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1820/2064 (88%)	1752 (96%)	67 (4%)	1 (0%)	48 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	ARG

### 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	792/904 (88%)	780 (98%)	12 (2%)	57 77
1	B	791/904 (88%)	774 (98%)	17 (2%)	47 70
All	All	1583/1808 (88%)	1554 (98%)	29 (2%)	51 74

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	57	GLU
1	B	939	THR
1	B	93	LEU
1	B	866	VAL
1	B	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	193	GLN
1	B	412	GLN
1	B	312	ASN
1	B	480	ASN
1	A	568	GLN

### 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](#)

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	A	922/1032 (89%)	-1.51	0 100 100	41, 77, 120, 166	0
1	B	930/1032 (90%)	-1.48	0 100 100	37, 82, 128, 161	0
All	All	1852/2064 (89%)	-1.50	0 100 100	37, 79, 124, 166	0

There are no RSRZ outliers to report.

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.