



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2025 – 04:16 pm BST

PDB ID : 9IHL / pdb_00009ihl
Title : Crystal Structure of the Human Nonmuscle Myosin 2A Motor Domain
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Deposited on : 2025-02-21
Resolution : 2.02 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

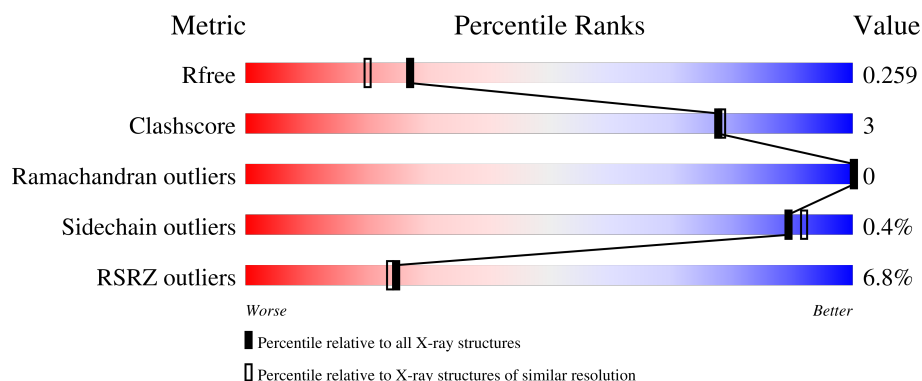
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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 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	1025	<div> <div>6%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8056 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 Myosin-9,Alpha-actinin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	953	7671	4867	1310	1460	34	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	776	ALA	-	linker	UNP P35579
A	777	SER	-	linker	UNP P35579
A	1016	ALA	-	expression tag	UNP P05095
A	1017	LEU	-	expression tag	UNP P05095
A	1018	HIS	-	expression tag	UNP P05095
A	1019	HIS	-	expression tag	UNP P05095
A	1020	HIS	-	expression tag	UNP P05095
A	1021	HIS	-	expression tag	UNP P05095
A	1022	HIS	-	expression tag	UNP P05095
A	1023	HIS	-	expression tag	UNP P05095
A	1024	HIS	-	expression tag	UNP P05095
A	1025	HIS	-	expression tag	UNP P05095

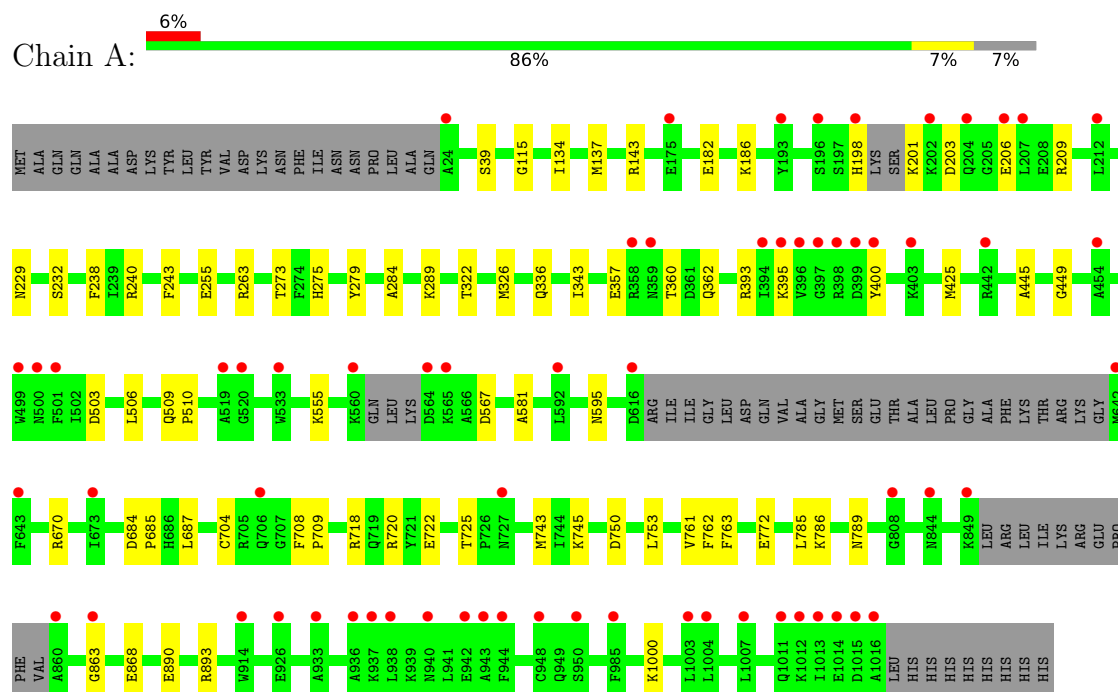
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	385	Total	O	0	0
			385	385		

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: Myosin-9,Alpha-actinin A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.99Å 120.88Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.72 – 2.02 74.72 – 2.02	Depositor EDS
% Data completeness (in resolution range)	47.0 (74.72-2.02) 47.0 (74.72-2.02)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.02Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487: ???	Depositor
R, R_{free}	0.205 , 0.259 0.205 , 0.259	Depositor DCC
R_{free} test set	1692 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8056	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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](#)

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	0.13	0/7815	0.26	0/10527

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	A	7671	0	7667	41	0
2	A	385	0	0	3	1
All	All	8056	0	7667	41	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 3.

All (41) 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:395:LYS:HE2	1:A:400:TYR:HE1	1.59	0.68
1:A:750:ASP:HB3	1:A:753:LEU:HD13	1.79	0.65
1:A:393:ARG:HB3	1:A:400:TYR:HB3	1.86	0.58
1:A:360:THR:HG22	1:A:362:GLN:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ARG:NH2	2:A:1108:HOH:O	2.36	0.57
1:A:725:THR:HG21	1:A:743:MET:HA	1.87	0.55
1:A:567:ASP:OD2	1:A:581:ALA:N	2.36	0.54
1:A:720:ARG:NH2	1:A:772:GLU:OE2	2.36	0.54
1:A:785:LEU:O	1:A:789:ASN:ND2	2.38	0.54
1:A:206:GLU:HG2	1:A:209:ARG:HH12	1.73	0.52
1:A:275:HIS:HB3	1:A:279:TYR:CZ	2.45	0.51
1:A:704:CYS:HB2	1:A:709:PRO:HB3	1.93	0.51
1:A:39:SER:HA	1:A:685:PRO:HG3	1.92	0.51
1:A:503:ASP:HB3	1:A:506:LEU:HG	1.94	0.50
1:A:890:GLU:OE2	1:A:893:ARG:NH1	2.45	0.49
1:A:863:GLY:H	1:A:868:GLU:CD	2.21	0.49
1:A:115:GLY:O	1:A:143:ARG:NH2	2.45	0.49
1:A:263:ARG:HG2	1:A:273:THR:HA	1.97	0.47
1:A:684:ASP:HB3	1:A:687:LEU:HB3	1.96	0.47
1:A:198:HIS:C	1:A:201:LYS:HD2	2.40	0.46
1:A:284:ALA:O	1:A:289:LYS:NZ	2.47	0.46
1:A:357:GLU:HG3	1:A:360:THR:HB	1.97	0.46
1:A:326:MET:HE2	1:A:336:GLN:HG2	1.98	0.46
1:A:229:ASN:HB3	1:A:232:SER:HB2	1.98	0.45
1:A:203:ASP:HA	1:A:206:GLU:HG3	1.98	0.45
1:A:240:ARG:NE	1:A:255:GLU:OE2	2.49	0.44
1:A:708:PHE:HB3	1:A:762:PHE:HB3	2.00	0.44
1:A:763:PHE:N	2:A:1101:HOH:O	2.23	0.44
1:A:718:ARG:O	1:A:722:GLU:HB2	2.17	0.44
1:A:343:ILE:HD11	1:A:425:MET:HE1	1.99	0.44
1:A:745:LYS:HE3	1:A:745:LYS:HB3	1.87	0.42
1:A:243:PHE:O	1:A:445:ALA:N	2.53	0.42
1:A:863:GLY:N	1:A:868:GLU:OE1	2.53	0.41
1:A:134:ILE:HG12	1:A:137:MET:HE2	2.02	0.41
1:A:509:GLN:N	1:A:510:PRO:HD2	2.36	0.41
1:A:182:GLU:O	1:A:186:LYS:HG2	2.21	0.41
1:A:238:PHE:CZ	1:A:449:GLY:HA3	2.55	0.41
1:A:555:LYS:HE3	2:A:1195:HOH:O	2.21	0.41
1:A:326:MET:HE2	1:A:326:MET:HB3	1.84	0.40
1:A:322:THR:O	1:A:326:MET:HG3	2.21	0.40
1:A:1000:LYS:HE3	1:A:1000:LYS:HB2	1.93	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:A:1285:HOH:O	2:A:1411:HOH:O[2_455]	2.19	0.01

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	944/1025 (92%)	915 (97%)	29 (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	835/895 (93%)	832 (100%)	3 (0%)	89	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	ASN
1	A	761	VAL
1	A	786	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	493	GLN
1	A	665	ASN
1	A	667	ASN
1	A	821	HIS
1	A	834	GLN
1	A	954	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 ⓘ

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, 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	953/1025 (92%)	0.35	65 (6%)	25 24	12, 33, 72, 101	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	TYR	5.0
1	A	1013	ILE	4.8
1	A	1016	ALA	4.7
1	A	394	ILE	4.3
1	A	565	LYS	3.9
1	A	948	CYS	3.5
1	A	944	PHE	3.4
1	A	396	VAL	3.3
1	A	212	LEU	3.3
1	A	198	HIS	3.2
1	A	616	ASP	3.1
1	A	1004	LEU	3.1
1	A	1007	LEU	3.0
1	A	936	ALA	3.0
1	A	442	ARG	3.0
1	A	643	PHE	3.0
1	A	202	LYS	3.0
1	A	207	LEU	3.0
1	A	399	ASP	2.9
1	A	499	TRP	2.9
1	A	398	ARG	2.9
1	A	560	LYS	2.8
1	A	863	GLY	2.8
1	A	844	ASN	2.7
1	A	193	TYR	2.7
1	A	1012	LYS	2.7
1	A	860	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	943	ALA	2.7
1	A	1011	GLN	2.7
1	A	501	PHE	2.7
1	A	938	LEU	2.6
1	A	1014	GLU	2.6
1	A	520	GLY	2.6
1	A	359	ASN	2.5
1	A	950	SER	2.5
1	A	24	ALA	2.5
1	A	204	GLN	2.4
1	A	500	ASN	2.4
1	A	533	TRP	2.4
1	A	397	GLY	2.4
1	A	926	GLU	2.4
1	A	933	ALA	2.3
1	A	940	ASN	2.3
1	A	673	ILE	2.3
1	A	937	LYS	2.3
1	A	642	MET	2.3
1	A	849	LYS	2.3
1	A	1015	ASP	2.2
1	A	985	PHE	2.2
1	A	808	GLY	2.2
1	A	942	GLU	2.2
1	A	914	TRP	2.2
1	A	395	LYS	2.2
1	A	403	LYS	2.2
1	A	358	ARG	2.2
1	A	175	GLU	2.1
1	A	706	GLN	2.1
1	A	592	LEU	2.1
1	A	196	SER	2.1
1	A	564	ASP	2.1
1	A	454	ALA	2.1
1	A	206	GLU	2.1
1	A	1003	LEU	2.0
1	A	727	ASN	2.0
1	A	519	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.