



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2021 – 10:08 PM JST

PDB ID : 7DPD  
Title : Human MCM9 N-terminal domain  
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Deposited on : 2020-12-18  
Resolution : 2.55 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  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

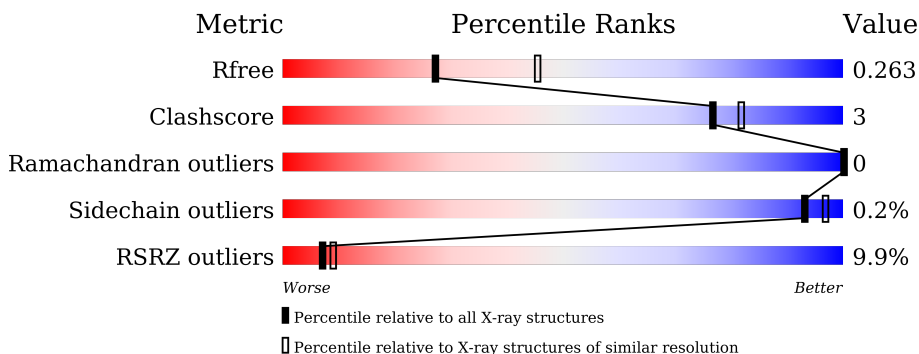
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	291	
1	B	291	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4574 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 DNA helicase MCM9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2169	1372	362	418	17	0	0	0
1	B	273	2185	1381	365	421	18	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q9NXL9
A	-12	GLY	-	expression tag	UNP Q9NXL9
A	-11	SER	-	expression tag	UNP Q9NXL9
A	-10	SER	-	expression tag	UNP Q9NXL9
A	-9	HIS	-	expression tag	UNP Q9NXL9
A	-8	HIS	-	expression tag	UNP Q9NXL9
A	-7	HIS	-	expression tag	UNP Q9NXL9
A	-6	HIS	-	expression tag	UNP Q9NXL9
A	-5	HIS	-	expression tag	UNP Q9NXL9
A	-4	HIS	-	expression tag	UNP Q9NXL9
A	-3	SER	-	expression tag	UNP Q9NXL9
A	-2	ASN	-	expression tag	UNP Q9NXL9
A	-1	GLY	-	expression tag	UNP Q9NXL9
A	0	SER	-	expression tag	UNP Q9NXL9
A	168	PRO	ARG	engineered mutation	UNP Q9NXL9
A	257	ALA	CYS	engineered mutation	UNP Q9NXL9
B	-13	MET	-	initiating methionine	UNP Q9NXL9
B	-12	GLY	-	expression tag	UNP Q9NXL9
B	-11	SER	-	expression tag	UNP Q9NXL9
B	-10	SER	-	expression tag	UNP Q9NXL9
B	-9	HIS	-	expression tag	UNP Q9NXL9
B	-8	HIS	-	expression tag	UNP Q9NXL9
B	-7	HIS	-	expression tag	UNP Q9NXL9
B	-6	HIS	-	expression tag	UNP Q9NXL9
B	-5	HIS	-	expression tag	UNP Q9NXL9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q9NXL9
B	-3	SER	-	expression tag	UNP Q9NXL9
B	-2	ASN	-	expression tag	UNP Q9NXL9
B	-1	GLY	-	expression tag	UNP Q9NXL9
B	0	SER	-	expression tag	UNP Q9NXL9
B	168	PRO	ARG	engineered mutation	UNP Q9NXL9
B	257	ALA	CYS	engineered mutation	UNP Q9NXL9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

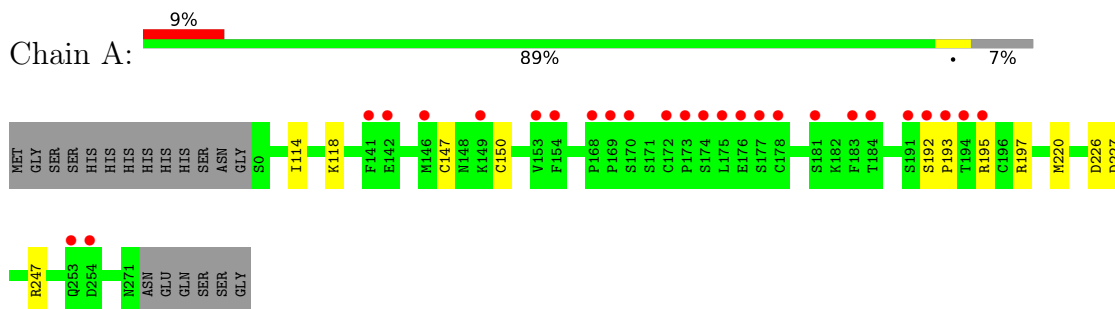
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	97	Total O 97 97	0	0
4	B	120	Total O 120 120	0	0

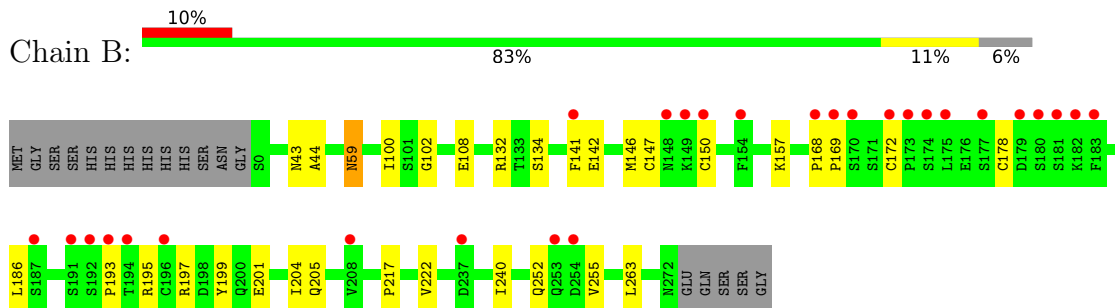
### 3 Residue-property plots [i](#)

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: DNA helicase MCM9



- Molecule 1: DNA helicase MCM9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.29Å 85.90Å 111.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.11 – 2.55 46.77 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.11-2.55) 93.0 (46.77-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.54Å)	Xtrriage
Refinement program	PHENIX dev_3139	Depositor
R, $R_{free}$	0.208 , 0.264 0.209 , 0.263	Depositor DCC
$R_{free}$ test set	1997 reflections (8.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7991e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN, 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	0.26	0/2210	0.42	0/2991
1	B	0.26	0/2226	0.44	0/3012
All	All	0.26	0/4436	0.43	0/6003

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	2169	0	2160	8	0
1	B	2185	0	2174	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	97	0	0	2	0
4	B	120	0	0	2	0
All	All	4574	0	4334	26	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 3.

All (26) 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:146:MET:HB2	1:B:186:LEU:HD11	1.85	0.59
1:A:114:ILE:HD12	1:A:220:MET:HB2	1.84	0.57
1:B:147:CYS:HB3	1:B:150:CYS:SG	2.45	0.57
1:A:193:PRO:HB2	1:A:195:ARG:HG3	1.88	0.56
1:A:147:CYS:HB3	1:A:150:CYS:SG	2.48	0.54
1:B:172:CYS:HB2	1:B:178:CYS:HB3	1.93	0.51
1:B:222:VAL:HG22	1:B:263:LEU:HB3	1.92	0.51
1:B:252:GLN:HB2	1:B:255:VAL:HB	1.93	0.51
1:B:59:ASN:ND2	4:B:404:HOH:O	2.44	0.50
1:B:132:ARG:HH12	1:B:134:SER:HB3	1.80	0.46
1:A:192:SER:HB2	1:A:193:PRO:HD3	1.97	0.46
1:A:247:ARG:NH2	4:A:405:HOH:O	2.49	0.46
1:B:199:TYR:OH	1:B:201:GLU:OE1	2.30	0.45
1:B:43:ASN:HD22	1:B:102:GLY:HA3	1.81	0.44
1:A:118:LYS:HB3	1:A:118:LYS:HE2	1.86	0.44
1:B:205:GLN:HG3	1:B:217:PRO:HB2	2.00	0.43
1:A:227:ASP:OD2	4:A:401:HOH:O	2.21	0.43
1:A:197:ARG:HD2	1:A:226:ASP:OD1	2.18	0.43
1:B:141:PHE:CD2	1:B:197:ARG:HG3	2.54	0.42
1:B:44:ALA:HB2	1:B:100:ILE:HG23	2.01	0.42
1:B:204:ILE:HD13	1:B:240:ILE:HD12	2.01	0.42
1:B:142:GLU:HG2	1:B:157:LYS:HD3	2.02	0.42
1:B:222:VAL:HG11	1:B:240:ILE:HD13	2.01	0.41
1:B:193:PRO:O	1:B:195:ARG:HA	2.21	0.41
1:B:108:GLU:HB2	4:B:474:HOH:O	2.21	0.40
1:B:168:PRO:HA	1:B:169:PRO:HD3	1.94	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	270/291 (93%)	261 (97%)	9 (3%)	0	100	100
1	B	272/291 (94%)	260 (96%)	12 (4%)	0	100	100
All	All	542/582 (93%)	521 (96%)	21 (4%)	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	254/270 (94%)	254 (100%)	0	100	100
1	B	256/270 (95%)	255 (100%)	1 (0%)	91	95
All	All	510/540 (94%)	509 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	ASN

Sometimes 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are 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 [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, 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	272/291 (93%)	0.46	26 (9%) <b>8</b>   <b>10</b>	21, 43, 105, 142	0
1	B	273/291 (93%)	0.53	28 (10%) <b>6</b>   <b>8</b>	19, 40, 111, 130	0
All	All	545/582 (93%)	0.50	54 (9%) <b>7</b>   <b>9</b>	19, 41, 110, 142	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	LYS	9.0
1	B	191	SER	7.8
1	A	192	SER	6.7
1	B	148	ASN	6.2
1	B	194	THR	6.2
1	A	176	GLU	5.8
1	B	181	SER	5.4
1	A	174	SER	5.4
1	B	183	PHE	5.2
1	A	175	LEU	4.6
1	A	178	CYS	4.4
1	B	180	SER	4.3
1	B	170	SER	4.3
1	B	175	LEU	4.2
1	A	169	PRO	4.1
1	A	153	VAL	3.9
1	A	183	PHE	3.9
1	A	177	SER	3.9
1	A	195	ARG	3.8
1	A	146	MET	3.7
1	B	193	PRO	3.6
1	B	182	LYS	3.4
1	A	170	SER	3.4
1	B	208	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	THR	3.3
1	B	187	SER	3.3
1	A	154	PHE	3.3
1	B	196	CYS	3.2
1	B	254	ASP	3.1
1	B	253	GLN	3.0
1	A	142	GLU	2.9
1	A	168	PRO	2.9
1	A	191	SER	2.9
1	A	149	LYS	2.9
1	B	172	CYS	2.9
1	A	184	THR	2.8
1	B	174	SER	2.8
1	B	179	ASP	2.8
1	A	181	SER	2.7
1	B	192	SER	2.6
1	A	193	PRO	2.6
1	A	172	CYS	2.5
1	A	173	PRO	2.5
1	B	150	CYS	2.5
1	B	169	PRO	2.5
1	A	253	GLN	2.5
1	B	173	PRO	2.4
1	B	237	ASP	2.4
1	B	154	PHE	2.3
1	B	168	PRO	2.3
1	B	177	SER	2.2
1	A	254	ASP	2.1
1	B	141	PHE	2.1
1	A	141	PHE	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 monosaccharides 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, 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(Å <sup>2</sup> )	Q<0.9
2	ZN	B	300	1/1	0.85	0.06	151,151,151,151	0
2	ZN	A	300	1/1	0.87	0.08	142,142,142,142	0
3	NA	A	301	1/1	0.92	0.20	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.