



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:55 AM GMT

PDB ID : 3F9V  
Title : Crystal Structure Of A Near Full-Length Archaeal MCM: Functional Insights For An AAA+ Hexameric Helicase  
Authors : Chen, X.J.; Brewster, A.S.; Wang, G.G.; Yu, X.; Greenleaf, W.; Tjajadi, M.; Klein, M.  
Deposited on : 2008-11-14  
Resolution : 4.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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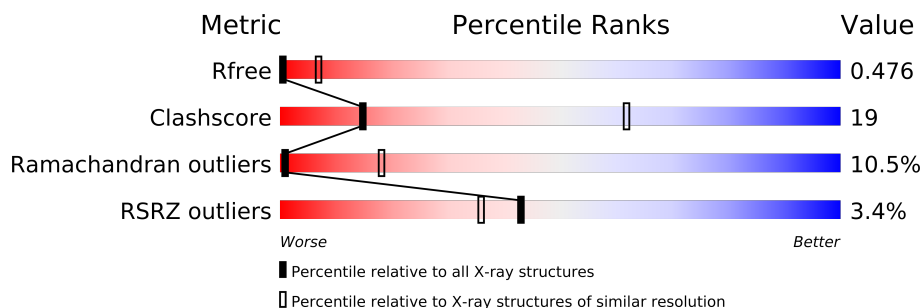
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 4.35 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))
$R_{free}$	66092	1016 (5.08-3.50)
Clashscore	79885	1280 (5.08-3.50)
Ramachandran outliers	78287	1210 (5.08-3.50)
RSRZ outliers	66119	1016 (5.08-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	595	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2944 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Minichromosome maintenance protein MCM.

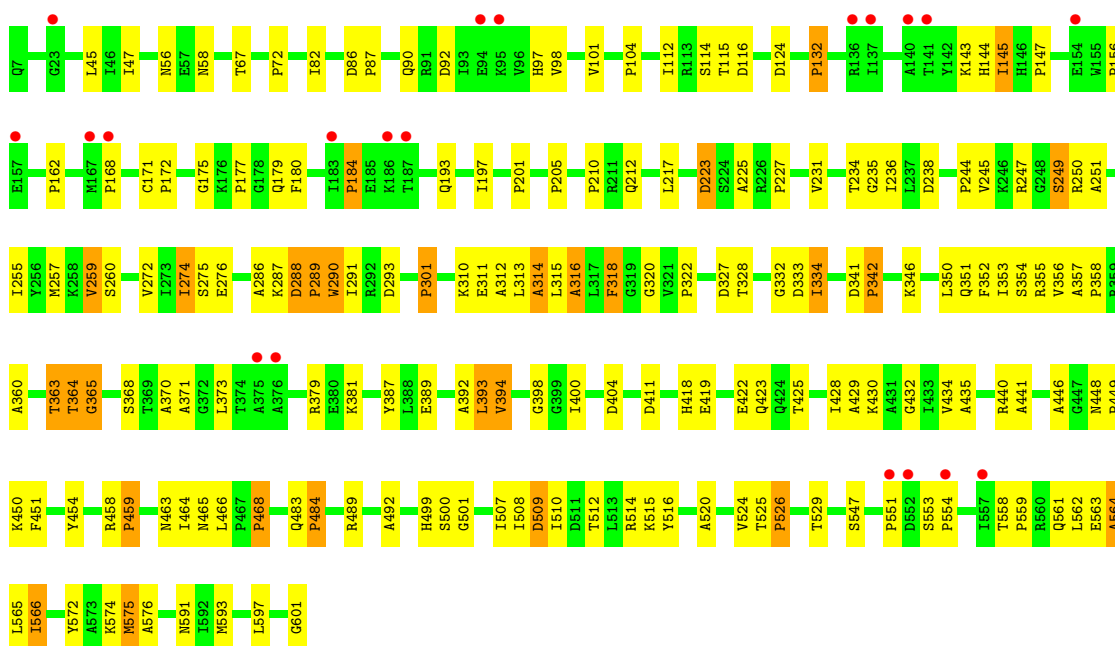
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	595	2944	1754	595	595	0	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Minichromosome maintenance protein MCM

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.53Å 202.53Å 128.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.35 29.40 – 4.35	Depositor EDS
% Data completeness (in resolution range)	82.1 (30.00-4.35) 82.0 (29.40-4.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.68 (at 4.42Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.412 , 0.481 0.412 , 0.476	Depositor DCC
$R_{free}$ test set	343 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	183.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.01 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 7388 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	2944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.45	0/2943	0.77	29/4100 (0.7%)

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	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	PRO	N-CA-CB	6.53	111.14	103.30
1	A	289	PRO	N-CA-CB	6.48	111.07	103.30
1	A	551	PRO	N-CA-CB	6.29	110.84	103.30
1	A	554	PRO	N-CA-CB	6.28	110.84	103.30
1	A	168	PRO	N-CA-CB	6.25	110.80	103.30
1	A	322	PRO	N-CA-CB	6.24	110.79	103.30
1	A	358	PRO	N-CA-CB	6.20	110.74	103.30
1	A	72	PRO	N-CA-CB	6.14	110.66	103.30
1	A	244	PRO	N-CA-CB	6.12	110.64	103.30
1	A	172	PRO	N-CA-CB	6.10	110.62	103.30
1	A	210	PRO	N-CA-CB	6.07	110.58	103.30
1	A	87	PRO	N-CA-CB	6.05	110.56	103.30
1	A	484	PRO	N-CA-CB	6.03	110.54	103.30
1	A	301	PRO	N-CA-CB	6.02	110.53	103.30
1	A	201	PRO	N-CA-CB	6.00	110.50	103.30
1	A	132	PRO	N-CA-CB	5.94	110.42	103.30
1	A	156	PRO	N-CA-CB	5.93	110.42	103.30
1	A	205	PRO	N-CA-CB	5.91	110.39	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	PRO	N-CA-CB	5.90	110.38	103.30
1	A	184	PRO	N-CA-CB	5.84	110.31	103.30
1	A	526	PRO	N-CA-CB	5.84	110.31	103.30
1	A	147	PRO	N-CA-CB	5.81	110.27	103.30
1	A	177	PRO	N-CA-CB	5.81	110.27	103.30
1	A	162	PRO	N-CA-CB	5.79	110.24	103.30
1	A	104	PRO	N-CA-CB	5.71	110.16	103.30
1	A	459	PRO	N-CA-CB	5.63	110.06	103.30
1	A	468	PRO	N-CA-CB	5.54	109.94	103.30
1	A	342	PRO	N-CA-CB	5.25	109.60	103.30
1	A	449	PRO	N-CA-CB	5.08	109.40	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	THR	Peptide
1	A	364	THR	Peptide
1	A	365	GLY	Peptide

## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2944	0	1322	82	0
All	All	2944	0	1322	82	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:370:ALA:HB1	1:A:389:GLU:CB	1.88	1.03
1:A:398:GLY:HA2	1:A:440:ARG:O	1.70	0.90
1:A:320:GLY:HA2	1:A:572:TYR:CB	2.15	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:313:LEU:C	1:A:315:LEU:H	1.90	0.73
1:A:274:ILE:O	1:A:276:GLU:N	2.26	0.69
1:A:574:LYS:C	1:A:576:ALA:H	1.97	0.67
1:A:236:ILE:O	1:A:257:MET:HA	1.94	0.66
1:A:363:THR:C	1:A:365:GLY:N	2.48	0.65
1:A:171:CYS:O	1:A:175:GLY:N	2.29	0.64
1:A:398:GLY:CA	1:A:440:ARG:O	2.42	0.64
1:A:286:ALA:O	1:A:289:PRO:N	2.31	0.64
1:A:360:ALA:HA	1:A:400:ILE:O	2.02	0.60
1:A:489:ARG:O	1:A:492:ALA:HB3	2.02	0.60
1:A:371:ALA:O	1:A:392:ALA:N	2.34	0.60
1:A:404:ASP:HA	1:A:446:ALA:HB3	1.84	0.59
1:A:572:TYR:HA	1:A:575:MET:CB	2.32	0.59
1:A:124:ASP:HA	1:A:231:VAL:O	2.02	0.59
1:A:591:ASN:C	1:A:593:MET:H	2.06	0.59
1:A:47:ILE:O	1:A:101:VAL:N	2.35	0.59
1:A:313:LEU:C	1:A:315:LEU:N	2.54	0.59
1:A:193:GLN:N	1:A:217:LEU:O	2.37	0.57
1:A:368:SER:O	1:A:371:ALA:HB3	2.04	0.56
1:A:516:TYR:O	1:A:520:ALA:N	2.38	0.56
1:A:512:THR:HA	1:A:515:LYS:CB	2.36	0.56
1:A:354:SER:C	1:A:356:VAL:H	2.10	0.55
1:A:507:ILE:C	1:A:509:ASP:H	2.10	0.55
1:A:363:THR:CB	1:A:365:GLY:HA3	2.37	0.55
1:A:310:LYS:O	1:A:314:ALA:N	2.23	0.54
1:A:574:LYS:O	1:A:576:ALA:N	2.33	0.54
1:A:313:LEU:O	1:A:315:LEU:N	2.42	0.53
1:A:574:LYS:C	1:A:576:ALA:N	2.62	0.53
1:A:311:GLU:HA	1:A:314:ALA:HB3	1.89	0.53
1:A:332:GLY:C	1:A:334:ILE:H	2.10	0.53
1:A:346:LYS:O	1:A:350:LEU:N	2.42	0.53
1:A:82:ILE:O	1:A:86:ASP:N	2.36	0.52
1:A:313:LEU:HA	1:A:316:ALA:HB3	1.92	0.52
1:A:354:SER:C	1:A:356:VAL:N	2.63	0.52
1:A:561:GLN:O	1:A:563:GLU:N	2.32	0.52
1:A:311:GLU:O	1:A:315:LEU:N	2.43	0.52
1:A:591:ASN:C	1:A:593:MET:N	2.62	0.52
1:A:354:SER:O	1:A:357:ALA:N	2.37	0.51
1:A:464:ILE:C	1:A:466:LEU:H	2.14	0.51
1:A:428:ILE:O	1:A:435:ALA:N	2.44	0.51
1:A:510:ILE:O	1:A:514:ARG:N	2.42	0.51
1:A:145:ILE:N	1:A:179:GLN:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:ASP:C	1:A:290:TRP:N	2.65	0.50
1:A:274:ILE:C	1:A:276:GLU:H	2.15	0.50
1:A:450:LYS:CB	1:A:463:ASN:HA	2.41	0.49
1:A:507:ILE:O	1:A:509:ASP:N	2.45	0.49
1:A:143:LYS:O	1:A:180:PHE:HA	2.12	0.49
1:A:381:LYS:CB	1:A:387:TYR:H	2.26	0.49
1:A:350:LEU:O	1:A:351:GLN:C	2.51	0.49
1:A:90:GLN:C	1:A:92:ASP:H	2.16	0.48
1:A:398:GLY:H	1:A:441:ALA:HB2	1.77	0.48
1:A:564:ALA:O	1:A:565:LEU:C	2.51	0.48
1:A:286:ALA:O	1:A:287:LYS:C	2.52	0.48
1:A:234:THR:O	1:A:260:SER:N	2.47	0.48
1:A:524:VAL:O	1:A:526:PRO:N	2.47	0.47
1:A:45:LEU:CB	1:A:98:VAL:HA	2.44	0.47
1:A:197:ILE:O	1:A:212:GLN:HA	2.13	0.47
1:A:429:ALA:HA	1:A:434:VAL:HA	1.96	0.47
1:A:499:HIS:O	1:A:501:GLY:N	2.47	0.47
1:A:565:LEU:O	1:A:566:ILE:C	2.53	0.46
1:A:291:ILE:C	1:A:293:ASP:H	2.19	0.46
1:A:332:GLY:C	1:A:334:ILE:N	2.69	0.46
1:A:423:GLN:O	1:A:425:THR:N	2.48	0.46
1:A:235:GLY:HA3	1:A:259:VAL:HA	1.98	0.46
1:A:249:SER:O	1:A:251:ALA:N	2.49	0.45
1:A:418:HIS:O	1:A:419:GLU:C	2.54	0.44
1:A:507:ILE:C	1:A:509:ASP:N	2.71	0.44
1:A:56:ASN:C	1:A:58:ASN:H	2.21	0.43
1:A:354:SER:O	1:A:356:VAL:N	2.52	0.42
1:A:561:GLN:C	1:A:563:GLU:H	2.18	0.42
1:A:448:ASN:O	1:A:450:LYS:N	2.45	0.42
1:A:311:GLU:O	1:A:312:ALA:C	2.58	0.42
1:A:597:LEU:O	1:A:601:GLY:N	2.53	0.41
1:A:318:PHE:C	1:A:320:GLY:H	2.24	0.41
1:A:418:HIS:O	1:A:422:GLU:N	2.50	0.41
1:A:356:VAL:O	1:A:357:ALA:C	2.59	0.40
1:A:393:LEU:O	1:A:394:VAL:C	2.59	0.40
1:A:114:SER:C	1:A:116:ASP:H	2.24	0.40
1:A:223:ASP:O	1:A:225:ALA:N	2.55	0.40

There are no symmetry-related clashes.

## 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	A	593/595 (100%)	390 (66%)	141 (24%)	62 (10%)	1 18

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	VAL
1	A	275	SER
1	A	316	ALA
1	A	334	ILE
1	A	342	PRO
1	A	373	LEU
1	A	411	ASP
1	A	454	TYR
1	A	458	ARG
1	A	468	PRO
1	A	483	GLN
1	A	484	PRO
1	A	508	ILE
1	A	525	THR
1	A	553	SER
1	A	97	HIS
1	A	145	ILE
1	A	247	ARG
1	A	249	SER
1	A	250	ARG
1	A	274	ILE
1	A	314	ALA
1	A	318	PHE
1	A	352	PHE
1	A	353	ILE
1	A	364	THR
1	A	379	ARG
1	A	394	VAL
1	A	430	LYS

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Mol	Chain	Res	Type
1	A	459	PRO
1	A	500	SER
1	A	529	THR
1	A	562	LEU
1	A	564	ALA
1	A	575	MET
1	A	115	THR
1	A	144	HIS
1	A	223	ASP
1	A	259	VAL
1	A	355	ARG
1	A	451	PHE
1	A	509	ASP
1	A	547	SER
1	A	184	PRO
1	A	290	TRP
1	A	328	THR
1	A	333	ASP
1	A	393	LEU
1	A	465	ASN
1	A	67	THR
1	A	132	PRO
1	A	238	ASP
1	A	245	VAL
1	A	255	ILE
1	A	288	ASP
1	A	327	ASP
1	A	341	ASP
1	A	112	ILE
1	A	301	PRO
1	A	432	GLY
1	A	558	THR
1	A	566	ILE

### 5.3.2 Protein sidechains ⓘ

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	595/595 (100%)	-0.02	20 (3%) 43 36	182, 185, 188, 191	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	LYS	5.0
1	A	157	GLU	4.0
1	A	167	MET	3.9
1	A	154	GLU	3.4
1	A	187	THR	3.3
1	A	137	ILE	3.0
1	A	551	PRO	2.9
1	A	23	GLY	2.8
1	A	376	ALA	2.8
1	A	554	PRO	2.8
1	A	95	LYS	2.7
1	A	557	ILE	2.6
1	A	94	GLU	2.6
1	A	552	ASP	2.5
1	A	140	ALA	2.5
1	A	375	ALA	2.3
1	A	141	THR	2.2
1	A	136	ARG	2.1
1	A	183	ILE	2.1
1	A	168	PRO	2.1

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.