Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:35 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

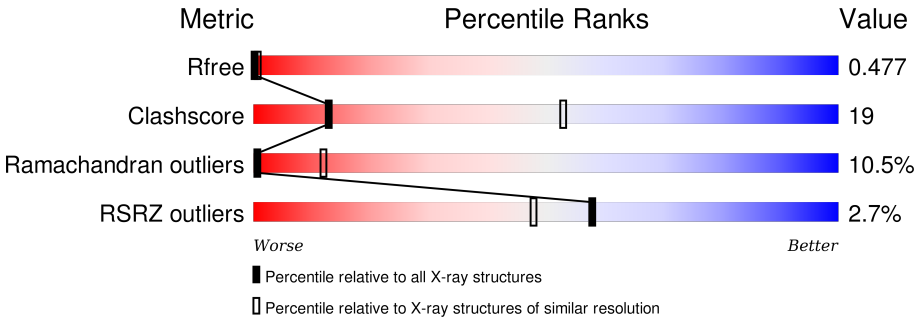
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	1063 (5.08-3.60)
Clashscore	102246	1171 (5.08-3.60)
Ramachandran outliers	100387	1110 (5.08-3.60)
RSRZ outliers	91569	1067 (5.08-3.60)

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 >=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 <=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	595	3% 69% 26% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2944 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 Minichromosome maintenance protein MCM.

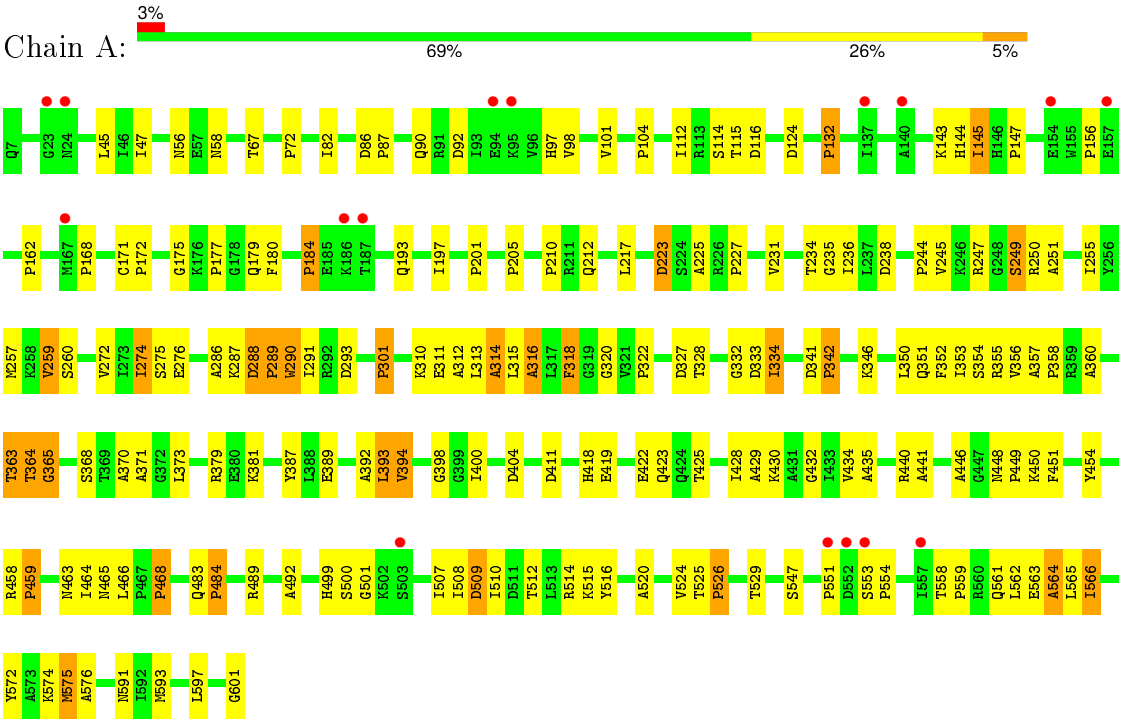
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	595	2944	1754	595	595	0	0	0

3 Residue-property plots (i)

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 (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	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) 82.1 (29.40-4.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.68 (at 4.42Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.412 , 0.481 0.410 , 0.477	Depositor DCC
R_{free} test set	343 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	183.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.02 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-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 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	2944	0	1322	82	0
All	All	2944	0	1322	82	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 19.

All (82) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLY:HA2	1:A:572:TYR:CB	2.15	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	593/595 (100%)	390 (66%)	141 (24%)	62 (10%)	1 12

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

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Mol	Chain	Res	Type
1	A	430	LYS
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 (i)

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

5.3.3 RNA (i)

There are no RNA molecules 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^{th} 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	595/595 (100%)	-0.46	16 (2%) 58 48	182, 185, 188, 191	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	LYS	4.6
1	A	187	THR	3.3
1	A	552	ASP	3.1
1	A	94	GLU	2.9
1	A	137	ILE	2.8
1	A	167	MET	2.8
1	A	157	GLU	2.7
1	A	23	GLY	2.7
1	A	503	SER	2.6
1	A	551	PRO	2.6
1	A	95	LYS	2.6
1	A	140	ALA	2.6
1	A	553	SER	2.5
1	A	154	GLU	2.4
1	A	557	ILE	2.4
1	A	24	ASN	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

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.