

# Full wwPDB X-ray Structure Validation Report (i)

#### May 25, 2020 - 05:19 am BST

PDB ID	:	5MU3
$\operatorname{Title}$	:	Crystal structure of Ctf19-Mcm21 kinetochore assembly bound with Ctf19-
		Mcm21 binding motif of central kinetochore subunit Okp1
Authors	:	Schmitzberger, F.
Deposited on	:	2017-01-12
Resolution	:	2.10  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 (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	:	1.8.5 (274361), CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	5197(2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647(2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 <=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		Qu	ality of chain	1	
1		100	5%				
	A	189			93%		• •
			6%				
1	D	189			95%		• •
			8%				
2	В	165			93%		5% •
			6%				
3	C	67	33%	•		64%	
	_		3%				
3	F	67	37%			63%	
			10%				
4	E	165			95%		• •



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12650 atoms, of which 6186 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 Central kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Δ	184	Total	С	Η	Ν	Ο	S	0	1	0
	104	3046	987	1521	255	278	5	0	I	0	
1	1 D 195	185	Total	С	Η	Ν	Ο	S	0	1	0
	100	3064	993	1531	256	279	5	0			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
А	-3	SER	-	expression tag	UNP Q6CVQ9
А	-2	ASN	-	expression tag	UNP Q6CVQ9
А	-1	ALA	-	expression tag	UNP Q6CVQ9
D	-3	SER	-	expression tag	UNP Q6CVQ9
D	-2	ASN	-	expression tag	UNP Q6CVQ9
D	-1	ALA	-	expression tag	UNP Q6CVQ9

• Molecule 2 is a protein called Central kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	В	163	Total 2678	C 851	H 1354	N 217	O 249	${f S}$ 7	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference		
В	106	MET	-	initiating methionine	UNP Q6CRN7		

• Molecule 3 is a protein called Central kinetochore subunit Okp1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	24	Total 414	C 134	Н 209	N 32	O 39	0	0	0



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	F	25	Total 426	$\begin{array}{c} \mathrm{C} \\ 137 \end{array}$	Н 215	N 33	O 41	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference		
С	294	MET	-	initiating methionine	UNP Q6CJY0		
F	294	MET	-	initiating methionine	UNP Q6CJY0		

• Molecule 4 is a protein called Central kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	164	Total 2684	m C  m 853	H 1356	N 217	O 250	S 8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	106	MET	-	initiating methionine	UNP Q6CRN7

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	110	Total O 110 110	0	0
5	В	67	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 67 & 67 \end{array}$	0	0
5	С	20	TotalO2020	0	0
5	D	67	Total O 67 67	0	0
5	Е	60	Total O 60 60	0	0
5	F	14	Total O 14 14	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 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: Central kinetochore subunit MCM21







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	93.34Å $105.48$ Å $122.98$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}\left(\mathring{A}\right)$	80.06 - 2.10	Depositor
Resolution (A)	80.06 - 2.00	EDS
% Data completeness	98.0 (80.06-2.10)	Depositor
(in resolution range)	94.7 (80.06 - 2.00)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.02 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D D.	0.222 , $0.248$	Depositor
II, II, <i>free</i>	0.222 , $0.248$	DCC
$R_{free}$ test set	1896 reflections $(2.42\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.42 , 57.4	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12650	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 17.81% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: CSX

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).

Mal	Chain	Bond	Bond lengths		angles
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/1564	0.39	0/2113
1	D	0.25	0/1572	0.40	0/2124
2	В	0.25	0/1349	0.46	0/1827
3	С	0.25	0/208	0.35	0/278
3	F	0.25	0/214	0.36	0/286
4	Е	0.25	0/1341	0.44	0/1813
All	All	0.25	0/6248	0.42	0/8441

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	А	1525	1521	1520	5	1
1	D	1533	1531	1531	2	1
2	В	1324	1354	1352	6	1
3	С	205	209	209	1	0
3	F	211	215	214	0	0
4	Е	1328	1356	1356	5	1
5	А	110	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes			
5	В	67	0	0	2	0			
5	С	20	0	0	0	0			
5	D	67	0	0	0	0			
5	Е	60	0	0	1	0			
5	F	14	0	0	0	0			
All	All	6464	6186	6182	17	2			

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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 1.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 9	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
4:E:129:ASP:OD1	4:E:143:ARG:NH1	2.18	0.76
4:E:192:LYS:NZ	4:E:227:CSX:SG	2.60	0.74
2:B:204:GLU:OE1	5:B:301:HOH:O	2.08	0.72
1:D:247[A]:ARG:NH1	1:D:249:GLY:O	2.26	0.68
2:B:213:ASN:ND2	5:B:302:HOH:O	2.26	0.67
1:D:211:LYS:NZ	1:D:260:GLY:O	2.27	0.67
2:B:136:GLY:O	2:B:137:SER:OG	2.10	0.64
1:A:247[B]:ARG:NH1	1:A:249:GLY:O	2.38	0.54
4:E:192:LYS:NZ	4:E:227:CSX:HG	2.05	0.53
1:A:114:GLU:OE1	2:B:111:ARG:NH2	2.49	0.46
1:A:211:LYS:NZ	1:A:260:GLY:O	2.50	0.45
4:E:172:ALA:O	4:E:176:GLN:N	2.50	0.44
1:A:114:GLU:OE2	2:B:111:ARG:NH2	2.51	0.43
3:C:336:ASP:OD2	3:C:339:LYS:NZ	2.43	0.42
4:E:269:ILE:O	5:E:301:HOH:O	2.22	0.41
2:B:148:ASN:OD1	2:B:149:GLU:N	2.54	0.40
1:A:151:PRO:HA	1:A:152:PRO:HD3	1.97	0.40

All (2) 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:B:143:ARG:NH1	4:E:129:ASP:OD1[1_565]	2.04	0.16
1:A:280:SER:OG	1:D:130:ASP:OD2[3_755]	2.15	0.05



## 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	Perce	ntiles
1	А	183/189~(97%)	180~(98%)	3~(2%)	0	100	100
1	D	184/189~(97%)	$179 \ (97\%)$	5(3%)	0	100	100
2	В	162/165~(98%)	153~(94%)	8 (5%)	1 (1%)	25	21
3	С	22/67~(33%)	22~(100%)	0	0	100	100
3	F	23/67~(34%)	23~(100%)	0	0	100	100
4	Е	161/165~(98%)	152 (94%)	9 (6%)	0	100	100
All	All	735/842 (87%)	709 (96%)	25 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	108	ILE

#### 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	Perce	ntiles
1	А	172/176~(98%)	172~(100%)	0	100	100
1	D	173/176~(98%)	173~(100%)	0	100	100
2	В	151/152~(99%)	151 (100%)	0	100	100
3	С	24/63~(38%)	24~(100%)	0	100	100
3	F	25/63~(40%)	25~(100%)	0	100	100
4	Ε	150/151~(99%)	150~(100%)	0	100	100



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	695/781~(89%)	695~(100%)	0	100	100

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

Some 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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Type	Type Chain		Res Link	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CSX	Е	227	4	$3,\!6,\!7$	0.99	0	$1,\!6,\!8$	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CSX	Ε	227	4	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:



Mol	Chain	$\mathbf{Res}$	Type	Atoms
4	Ε	227	CSX	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Е	227	CSX	2	0

### 5.5 Carbohydrates (i)

There are no carbohydrates 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 $>$	# <b>RSRZ</b> >	>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	184/189~(97%)	0.88	9 (4%) 29	35	36,51,87,105	0
1	D	185/189~(97%)	0.82	12 (6%) 18	23	42, 58, 95, 115	0
2	В	163/165~(98%)	1.02	14 (8%) 10	13	37, 55, 98, 120	0
3	С	24/67~(35%)	1.02	4 (16%) 1	2	38,53,81,104	0
3	F	25/67~(37%)	0.99	2 (8%) 12	16	42, 55, 86, 104	0
4	Ε	163/165~(98%)	1.03	16 (9%) 7	10	37, 54, 106, 120	0
All	All	744/842~(88%)	0.94	57 (7%) 13	17	36, 55, 98, 120	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	GLY	9.1
1	D	164	LEU	6.4
3	F	342	ILE	5.2
1	А	224	GLY	4.8
4	Ε	108	ILE	4.8
3	С	342	ILE	4.2
2	В	127	GLU	4.1
1	D	163	ARG	4.0
2	В	108	ILE	3.8
2	В	107	ASN	3.7
1	А	227	VAL	3.5
4	Е	152	ARG	3.2
2	В	149	GLU	3.2
2	В	191	ILE	3.2
4	Е	148	ASN	3.1
1	D	291	ILE	3.1
2	В	151	ILE	3.1
4	Е	127	GLU	3.1
2	В	143	ARG	3.0



Mol	Chain	Res	Type	RSRZ
4	Е	147	GLU	3.0
4	Е	143	ARG	2.9
3	С	340	PRO	2.9
4	Е	149	GLU	2.9
2	В	133	LEU	2.9
4	Е	251	PHE	2.9
1	А	182	GLN	2.9
4	Е	133	LEU	2.8
1	D	289	GLN	2.8
2	В	251	PHE	2.8
1	А	228	ASN	2.7
4	Е	115	LEU	2.7
4	Е	151	ILE	2.7
2	В	228	TYR	2.6
3	С	339	LYS	2.5
1	D	112	GLN	2.5
1	А	281	ILE	2.5
1	D	-1	ALA	2.4
2	В	144	ILE	2.4
4	Е	144	ILE	2.4
1	А	169	LEU	2.4
1	D	162	LYS	2.4
1	D	275	ILE	2.4
1	D	242	LEU	2.3
2	В	152	ARG	2.3
4	Е	170	GLN	2.3
2	В	146	VAL	2.2
1	А	275	ILE	2.2
4	E	221	LEU	2.2
4	Е	153	SER	2.2
1	A	209	LEU	2.2
3	С	341	LEU	2.2
1	D	186	LEU	2.1
4	Ε	126	CYS	2.1
3	F	341	LEU	2.1
2	В	229	TRP	2.1
1	А	289	GLN	2.1
1	D	176	LYS	2.0

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### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
4	CSX	Е	227	7/8	0.94	0.21	$40,\!54,\!85,\!102$	0

### 6.3 Carbohydrates (i)

There are no carbohydrates 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.

