



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2017 – 11:11 PM EST

PDB ID : 5MU3
Title : Crystal structure of Ctf19-Mcm21 kinetochore assembly bound with Ctf19-Mcm21 binding motif of central kinetochore subunit Okp1
Authors : Schmitzberger, F.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

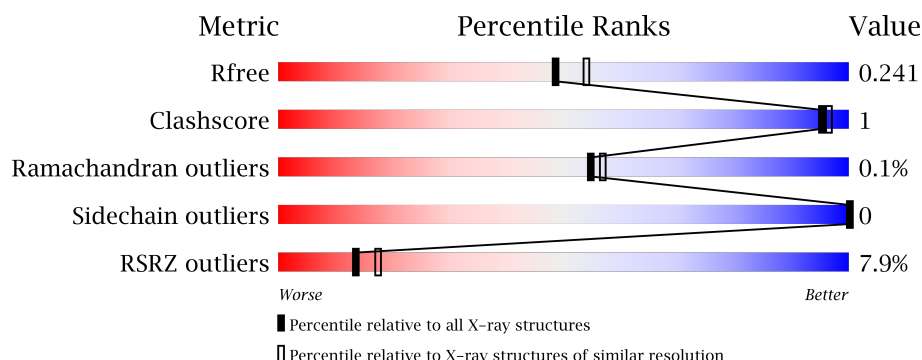
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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. 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	189	<div> <div>5%</div> <div>93%</div> <div>• •</div> </div>
1	D	189	<div> <div>7%</div> <div>95%</div> <div>• •</div> </div>
2	B	165	<div> <div>8%</div> <div>93%</div> <div>5% •</div> </div>
3	C	67	<div> <div>6%</div> <div>33%</div> <div>•</div> <div>64%</div> </div>
3	F	67	<div> <div>4%</div> <div>37%</div> <div>63%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	165	<div><div></div><div>10%</div><div></div><div>95%</div><div></div><div></div></div>

2 Entry composition

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	A	184	Total	C	H	N	O	S	0	1	0
			3046	987	1521	255	278	5			
1	D	185	Total	C	H	N	O	S	0	1	0
			3064	993	1531	256	279	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP Q6CVQ9
A	-2	ASN	-	expression tag	UNP Q6CVQ9
A	-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	B	163	Total	C	H	N	O	S	0	1	0
			2678	851	1354	217	249	7			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	24	Total	C	H	N	O	0	0	0
			414	134	209	32	39			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	25	Total	C	H	N	O	0	0	0
			426	137	215	33	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	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	C	H	N	O	S	0	0
			2684	853	1356	217	250	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	67	Total	O	0	0
			67	67		
5	C	20	Total	O	0	0
			20	20		
5	D	67	Total	O	0	0
			67	67		
5	E	60	Total	O	0	0
			60	60		
5	F	14	Total	O	0	0
			14	14		

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



- Molecule 1: Central kinetochore subunit MCM21



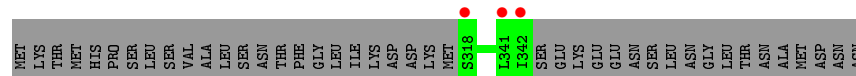
- Molecule 2: Central kinetochore subunit CTF19



- Molecule 3: Central kinetochore subunit Okp1

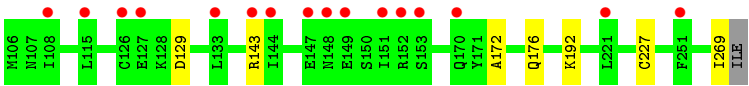


- Molecule 3: Central kinetochore subunit Okp1



- Molecule 4: Central kinetochore subunit CTF19





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	93.34Å 105.48Å 122.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.06 – 2.10 80.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (80.06-2.10) 94.7 (80.06-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.222 , 0.248 0.213 , 0.241	Depositor DCC
R_{free} test set	1729 reflections (2.43%)	DCC
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

5.1 Standard geometry

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/1564	0.39	0/2113
1	D	0.25	0/1572	0.40	0/2124
2	B	0.25	0/1349	0.46	0/1827
3	C	0.25	0/208	0.35	0/278
3	F	0.25	0/214	0.36	0/286
4	E	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

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	1525	1521	1520	5	1
1	D	1533	1531	1531	2	1
2	B	1324	1354	1352	6	1
3	C	205	209	209	1	0
3	F	211	215	214	0	0
4	E	1328	1356	1356	5	1
5	A	110	0	0	0	0

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

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-2	Interatomic distance (Å)	Clash 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

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	183/189 (97%)	180 (98%)	3 (2%)	0	100	100
1	D	184/189 (97%)	179 (97%)	5 (3%)	0	100	100
2	B	162/165 (98%)	153 (94%)	8 (5%)	1 (1%)	28	24
3	C	22/67 (33%)	22 (100%)	0	0	100	100
3	F	23/67 (34%)	23 (100%)	0	0	100	100
4	E	161/165 (98%)	152 (94%)	9 (6%)	0	100	100
All	All	735/842 (87%)	709 (96%)	25 (3%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	108	ILE

5.3.2 Protein sidechains

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	172/176 (98%)	172 (100%)	0	100	100
1	D	173/176 (98%)	173 (100%)	0	100	100
2	B	151/152 (99%)	151 (100%)	0	100	100
3	C	24/63 (38%)	24 (100%)	0	100	100
3	F	25/63 (40%)	25 (100%)	0	100	100
4	E	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 ⓘ

There are no RNA molecules in this entry.

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

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CSX	E	227	4	3,6,7	1.23	0	1,6,8	0.15	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	E	227	4	-	0/1/5/7	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	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 ⓘ

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	184/189 (97%)	0.88	9 (4%)	30 37	36, 51, 87, 105	0
1	D	185/189 (97%)	0.82	13 (7%)	17 22	42, 58, 95, 115	0
2	B	163/165 (98%)	1.02	14 (8%)	11 14	37, 55, 98, 120	0
3	C	24/67 (35%)	1.02	4 (16%)	2 2	38, 53, 81, 104	0
3	F	25/67 (37%)	0.99	3 (12%)	5 6	42, 55, 86, 104	0
4	E	163/165 (98%)	1.03	16 (9%)	8 11	37, 54, 106, 120	0
All	All	744/842 (88%)	0.94	59 (7%)	13 17	36, 55, 98, 120	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	GLY	9.2
1	D	164	LEU	6.4
3	F	342	ILE	5.2
1	A	224	GLY	4.8
4	E	108	ILE	4.8
3	C	342	ILE	4.2
2	B	127	GLU	4.1
1	D	163	ARG	4.0
2	B	108	ILE	3.8
2	B	107	ASN	3.7
1	A	227	VAL	3.5
4	E	152	ARG	3.2
2	B	191	ILE	3.2
2	B	149	GLU	3.2
1	D	291	ILE	3.1
4	E	148	ASN	3.1
2	B	151	ILE	3.1
4	E	127	GLU	3.1
4	E	147	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	143	ARG	3.0
4	E	143	ARG	2.9
3	C	340	PRO	2.9
2	B	133	LEU	2.9
4	E	149	GLU	2.9
4	E	251	PHE	2.9
1	A	182	GLN	2.9
1	D	289	GLN	2.8
4	E	133	LEU	2.8
2	B	251	PHE	2.8
4	E	115	LEU	2.7
1	A	228	ASN	2.7
4	E	151	ILE	2.7
2	B	228	TYR	2.6
3	C	339	LYS	2.6
1	A	281	ILE	2.5
2	B	144	ILE	2.4
1	D	-1	ALA	2.4
1	D	112	GLN	2.4
1	D	162	LYS	2.4
4	E	144	ILE	2.4
1	A	169	LEU	2.4
1	D	242	LEU	2.3
1	D	275	ILE	2.3
2	B	152	ARG	2.3
4	E	170	GLN	2.3
1	A	275	ILE	2.2
2	B	146	VAL	2.2
1	A	209	LEU	2.2
3	C	341	LEU	2.2
4	E	221	LEU	2.2
4	E	153	SER	2.2
1	D	186	LEU	2.2
4	E	126	CYS	2.2
2	B	229	TRP	2.1
1	A	289	GLN	2.1
3	F	341	LEU	2.1
3	F	318	SER	2.0
1	D	191	THR	2.0
1	D	176	LYS	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
4	CSX	E	227	7/8	0.93	0.20	-	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.