



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:36 pm BST

PDB ID : 3IWP
Title : Crystal structure of human copper homeostasis protein CutC
Authors : Li, Y.; Du, J.; Zhang, P.; Ding, J.
Deposited on : 2009-09-03
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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	:	2.11
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)	:	2.11

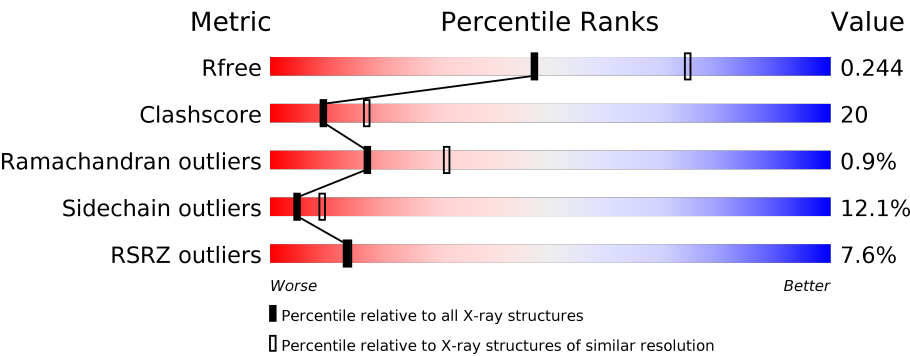
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	287	<div><div>3%</div><div><div></div><div>47%</div><div>32%</div><div>8%</div><div>13%</div></div></div>
1	B	287	<div><div>%</div><div><div></div><div>57%</div><div>23%</div><div>6%</div><div>15%</div></div></div>
1	C	287	<div><div>%</div><div><div></div><div>58%</div><div>23%</div><div>•</div><div>14%</div></div></div>
1	D	287	<div><div>%</div><div><div></div><div>48%</div><div>28%</div><div>9%</div><div>15%</div></div></div>
1	E	287	<div><div>6%</div><div><div></div><div>55%</div><div>25%</div><div>5%</div><div>16%</div></div></div>
1	F	287	<div><div>4%</div><div><div></div><div>47%</div><div>31%</div><div>5%</div><div>•</div><div>16%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	287	
1	H	287	
1	I	287	
1	J	287	
1	K	287	
1	L	287	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22740 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 Copper homeostasis protein cutC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1870	1166	329	357	18			
1	B	244	Total	C	N	O	S	0	0	0
			1837	1145	324	350	18			
1	C	247	Total	C	N	O	S	0	0	0
			1856	1157	327	354	18			
1	D	245	Total	C	N	O	S	0	0	0
			1843	1150	324	351	18			
1	E	242	Total	C	N	O	S	0	0	0
			1825	1138	322	348	17			
1	F	241	Total	C	N	O	S	0	0	0
			1817	1135	320	345	17			
1	G	237	Total	C	N	O	S	0	0	0
			1792	1119	317	340	16			
1	H	236	Total	C	N	O	S	0	0	0
			1779	1111	315	337	16			
1	I	241	Total	C	N	O	S	0	0	0
			1822	1138	321	347	16			
1	J	239	Total	C	N	O	S	0	0	0
			1807	1129	318	344	16			
1	K	238	Total	C	N	O	S	0	0	0
			1800	1127	317	340	16			
1	L	239	Total	C	N	O	S	0	0	0
			1804	1129	318	341	16			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
A	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
A	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
A	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
A	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
A	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
A	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
A	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
A	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
A	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
A	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
A	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
A	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
B	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
B	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
B	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
B	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
B	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9
B	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
B	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
B	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
B	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
B	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
B	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
B	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
B	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
B	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
C	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
C	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
C	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
C	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
C	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9
C	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
C	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
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C	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
C	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
C	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
C	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
D	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
D	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
D	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
D	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
D	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
D	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
D	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
D	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
D	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
D	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
D	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
D	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
D	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
E	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
E	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
E	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
E	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
E	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9
E	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
E	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
E	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
E	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
E	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
E	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
E	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
E	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
E	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
F	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
F	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
F	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
F	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
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F	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
F	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
F	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
F	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
F	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
G	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
G	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
G	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
G	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
G	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
G	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
G	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
G	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
G	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
G	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
G	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
G	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
G	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
H	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
H	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
H	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
H	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
H	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9
H	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
H	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
H	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
H	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
H	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
H	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
H	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
H	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
H	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
I	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
I	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
I	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
I	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
I	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9
I	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
I	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
I	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
I	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
I	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
I	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
I	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
I	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
I	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
J	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
J	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
J	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
J	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
J	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
J	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
J	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
J	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
J	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
J	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
J	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
J	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
J	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
K	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
K	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
K	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
K	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
K	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9
K	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
K	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
K	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
K	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
K	-4	HIS	-	EXPRESSION TAG	UNP Q9NTM9
K	-3	GLY	-	EXPRESSION TAG	UNP Q9NTM9
K	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
K	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
K	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9
L	-13	MET	-	EXPRESSION TAG	UNP Q9NTM9
L	-12	ARG	-	EXPRESSION TAG	UNP Q9NTM9
L	-11	GLY	-	EXPRESSION TAG	UNP Q9NTM9
L	-10	SER	-	EXPRESSION TAG	UNP Q9NTM9
L	-9	HIS	-	EXPRESSION TAG	UNP Q9NTM9
L	-8	HIS	-	EXPRESSION TAG	UNP Q9NTM9
L	-7	HIS	-	EXPRESSION TAG	UNP Q9NTM9
L	-6	HIS	-	EXPRESSION TAG	UNP Q9NTM9
L	-5	HIS	-	EXPRESSION TAG	UNP Q9NTM9
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L	-2	SER	-	EXPRESSION TAG	UNP Q9NTM9
L	-1	ALA	-	EXPRESSION TAG	UNP Q9NTM9
L	0	CYS	-	EXPRESSION TAG	UNP Q9NTM9

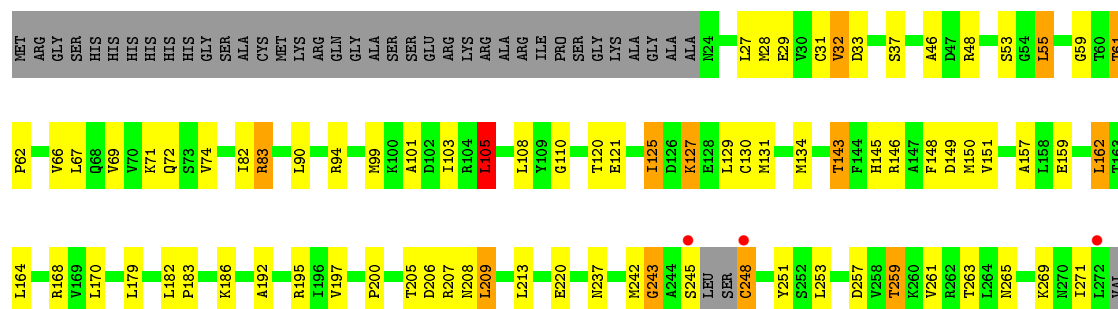
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	145	Total O 145 145	0	0

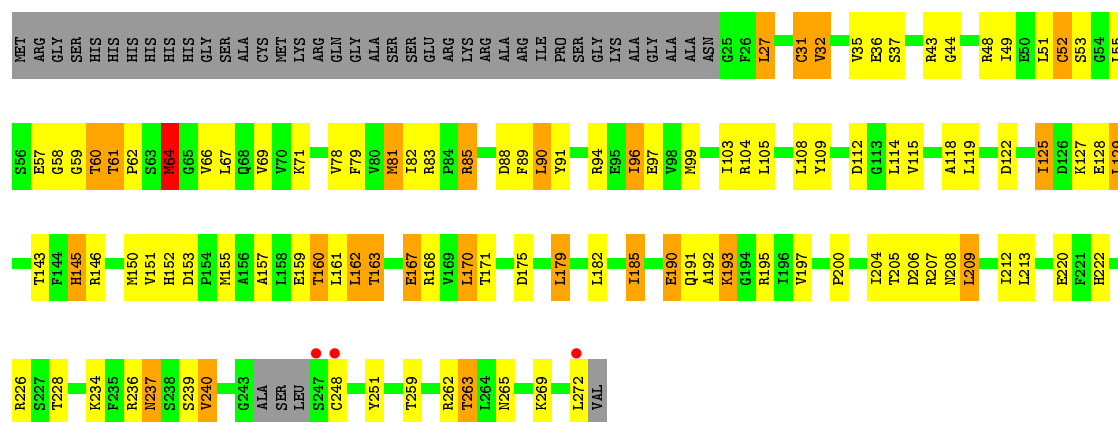
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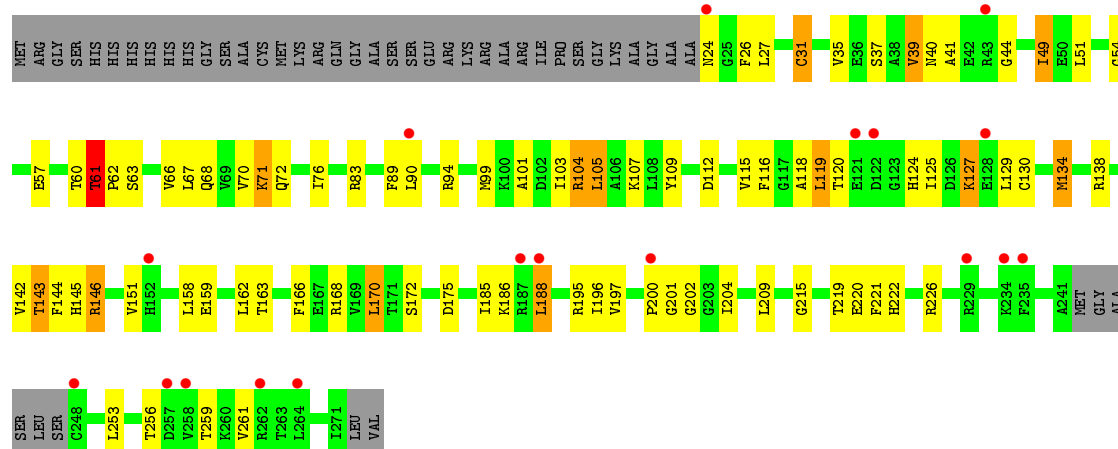
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	134	Total 134	O 134	0	0
2	C	137	Total 137	O 137	0	0
2	D	157	Total 157	O 157	0	0
2	E	58	Total 58	O 58	0	0
2	F	47	Total 47	O 47	0	0
2	G	25	Total 25	O 25	0	0
2	H	33	Total 33	O 33	0	0
2	I	56	Total 56	O 56	0	0
2	J	43	Total 43	O 43	0	0
2	K	26	Total 26	O 26	0	0
2	L	27	Total 27	O 27	0	0



- Molecule 1: Copper homeostasis protein cutC homolog



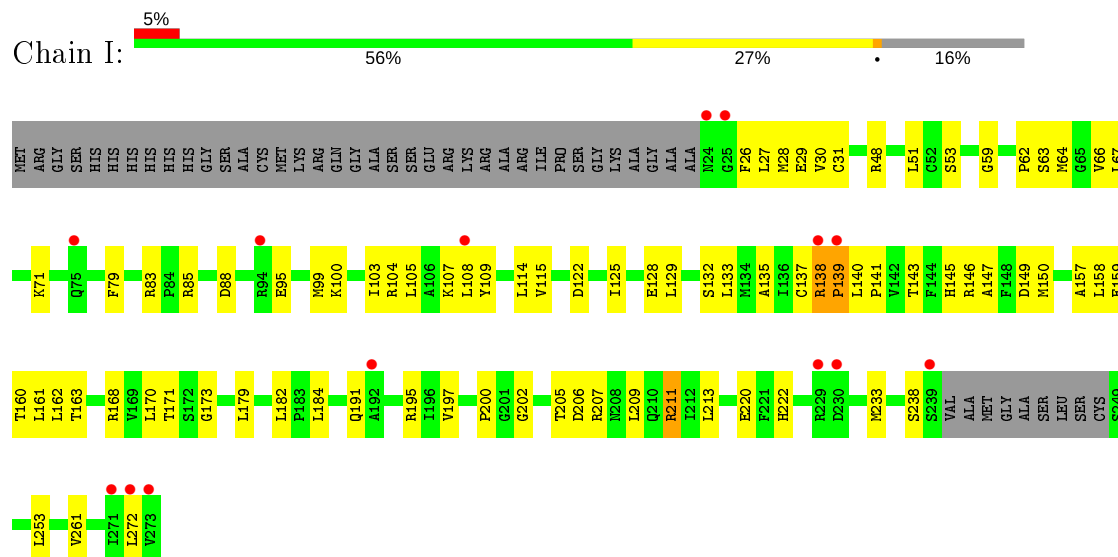
- Molecule 1: Copper homeostasis protein cutC homolog



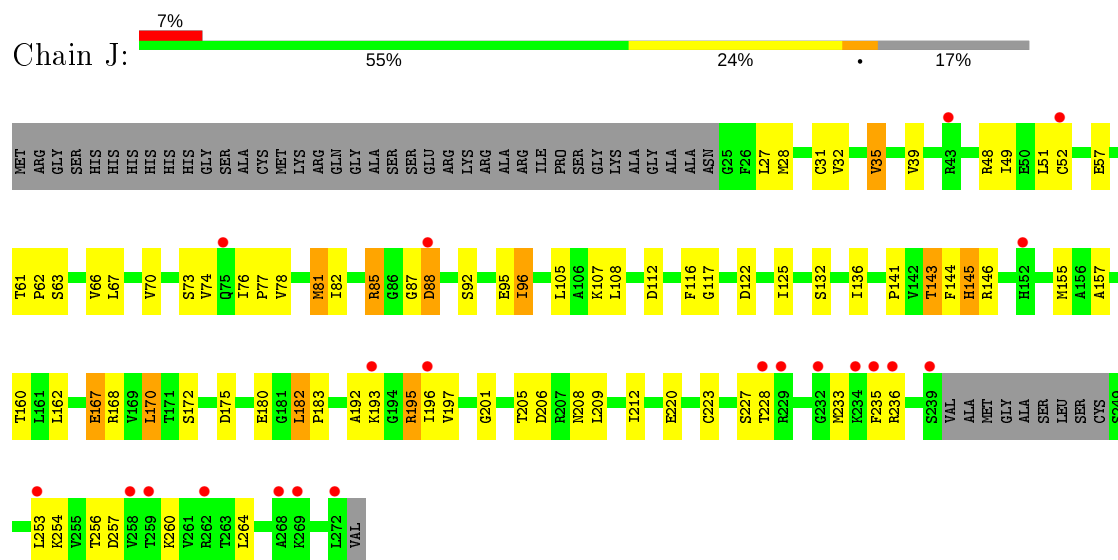
- Molecule 1: Copper homeostasis protein cutC homolog



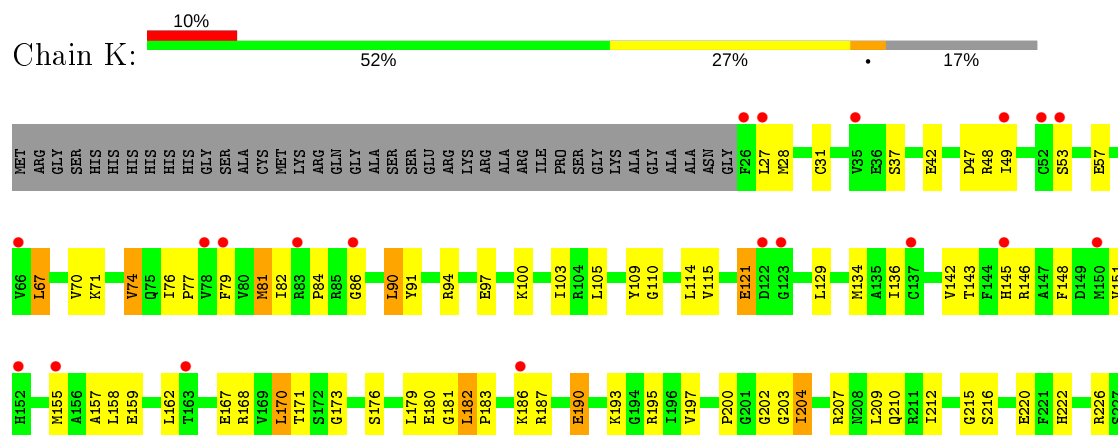
- Molecule 1: Copper homeostasis protein cutC homolog

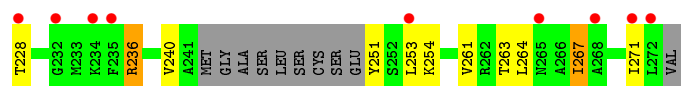


- Molecule 1: Copper homeostasis protein cutC homolog

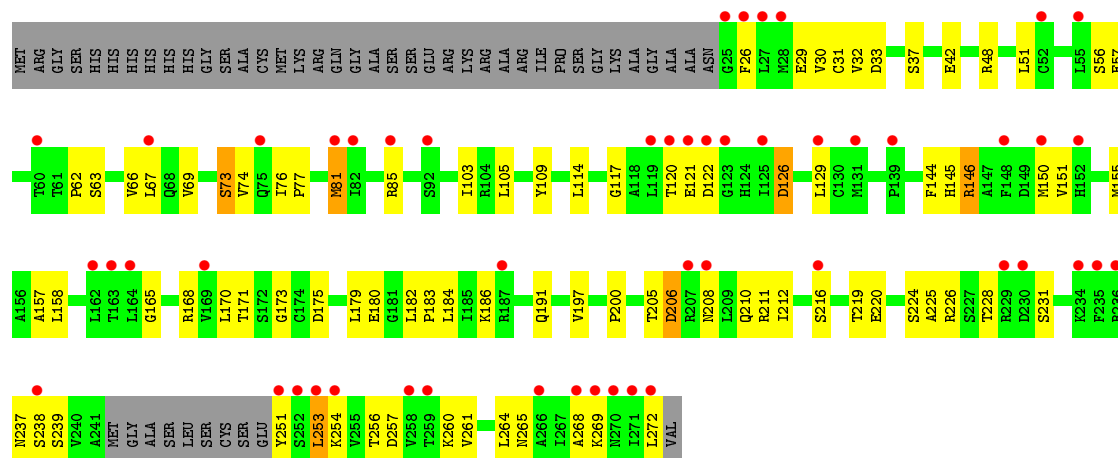


- Molecule 1: Copper homeostasis protein cutC homolog





- Molecule 1: Copper homeostasis protein cutC homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.16Å 78.41Å 170.35Å 76.84° 87.88° 71.86°	Depositor
Resolution (Å)	50.00 – 2.50 40.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.50) 98.5 (40.13-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.51Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.283 0.241 , 0.244	Depositor DCC
R_{free} test set	6413 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22740	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

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	0.64	0/1893	0.82	2/2549 (0.1%)
1	B	0.67	0/1859	0.78	0/2501
1	C	0.69	0/1878	0.84	1/2527 (0.0%)
1	D	0.69	1/1865 (0.1%)	0.83	3/2509 (0.1%)
1	E	0.46	0/1847	0.63	0/2486
1	F	0.49	0/1839	0.67	2/2474 (0.1%)
1	G	0.39	0/1814	0.58	0/2441
1	H	0.36	0/1800	0.58	0/2422
1	I	0.44	0/1844	0.61	0/2482
1	J	0.44	0/1829	0.61	0/2461
1	K	0.36	0/1822	0.57	0/2453
1	L	0.37	0/1826	0.55	0/2458
All	All	0.52	1/22116 (0.0%)	0.68	8/29763 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	CYS	CB-SG	6.06	1.92	1.82

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	LEU	CA-CB-CG	6.59	130.46	115.30
1	F	264	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	85	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	C	105	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	64	MET	CG-SD-CE	5.46	108.94	100.20

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	1870	0	1905	125	0
1	B	1837	0	1867	70	0
1	C	1856	0	1888	70	0
1	D	1843	0	1877	107	0
1	E	1825	0	1855	67	0
1	F	1817	0	1851	73	0
1	G	1792	0	1825	74	0
1	H	1779	0	1819	69	0
1	I	1822	0	1856	63	0
1	J	1807	0	1841	61	0
1	K	1800	0	1841	75	0
1	L	1804	0	1844	50	0
2	A	145	0	0	14	0
2	B	134	0	0	9	0
2	C	137	0	0	12	0
2	D	157	0	0	17	0
2	E	58	0	0	8	0
2	F	47	0	0	4	0
2	G	25	0	0	4	0
2	H	33	0	0	3	0
2	I	56	0	0	9	0
2	J	43	0	0	4	0
2	K	26	0	0	6	0
2	L	27	0	0	5	0
All	All	22740	0	22269	863	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 20.

The worst 5 of 863 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:61:THR:HG21	2:B:280:HOH:O	1.38	1.23
1:A:249:SER:CB	1:A:250:GLU:HA	1.68	1.18
1:J:88:ASP:HB2	2:J:294:HOH:O	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:ARG:HB3	1:I:139:PRO:HD2	1.38	1.04
1:C:61:THR:HG21	2:C:276:HOH:O	1.57	1.02

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	247/287 (86%)	231 (94%)	13 (5%)	3 (1%)	13	24
1	B	240/287 (84%)	228 (95%)	10 (4%)	2 (1%)	19	35
1	C	243/287 (85%)	237 (98%)	5 (2%)	1 (0%)	34	54
1	D	241/287 (84%)	235 (98%)	6 (2%)	0	100	100
1	E	238/287 (83%)	217 (91%)	18 (8%)	3 (1%)	12	21
1	F	237/287 (83%)	214 (90%)	20 (8%)	3 (1%)	12	21
1	G	233/287 (81%)	208 (89%)	21 (9%)	4 (2%)	9	16
1	H	232/287 (81%)	211 (91%)	20 (9%)	1 (0%)	34	54
1	I	237/287 (83%)	225 (95%)	10 (4%)	2 (1%)	19	35
1	J	235/287 (82%)	216 (92%)	18 (8%)	1 (0%)	34	54
1	K	234/287 (82%)	213 (91%)	17 (7%)	4 (2%)	9	16
1	L	235/287 (82%)	210 (89%)	22 (9%)	3 (1%)	12	21
All	All	2852/3444 (83%)	2645 (93%)	180 (6%)	27 (1%)	17	31

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	CYS
1	F	267	ILE
1	I	138	ARG

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Mol	Chain	Res	Type
1	I	139	PRO
1	L	121	GLU

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	206/233 (88%)	172 (84%)	34 (16%)	2	4
1	B	202/233 (87%)	176 (87%)	26 (13%)	4	8
1	C	204/233 (88%)	179 (88%)	25 (12%)	4	9
1	D	203/233 (87%)	165 (81%)	38 (19%)	1	2
1	E	201/233 (86%)	179 (89%)	22 (11%)	6	12
1	F	199/233 (85%)	169 (85%)	30 (15%)	3	5
1	G	197/233 (84%)	182 (92%)	15 (8%)	13	25
1	H	196/233 (84%)	171 (87%)	25 (13%)	4	8
1	I	201/233 (86%)	185 (92%)	16 (8%)	12	23
1	J	199/233 (85%)	175 (88%)	24 (12%)	5	9
1	K	198/233 (85%)	180 (91%)	18 (9%)	9	18
1	L	198/233 (85%)	180 (91%)	18 (9%)	9	18
All	All	2404/2796 (86%)	2113 (88%)	291 (12%)	5	9

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	119	LEU
1	F	179	LEU
1	K	193	LYS
1	E	143	THR
1	F	64	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	124	HIS
1	E	24	ASN
1	K	124	HIS
1	D	152	HIS
1	E	68	GLN

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 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, 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	249/287 (86%)	0.09	10 (4%) 38 41	9, 25, 57, 151	0
1	B	244/287 (85%)	-0.23	2 (0%) 86 87	9, 24, 48, 100	0
1	C	247/287 (86%)	-0.22	3 (1%) 79 80	12, 22, 50, 91	0
1	D	245/287 (85%)	-0.13	3 (1%) 79 80	9, 23, 48, 89	0
1	E	242/287 (84%)	0.58	18 (7%) 14 15	36, 60, 94, 119	0
1	F	241/287 (83%)	0.32	12 (4%) 28 30	26, 55, 89, 113	0
1	G	237/287 (82%)	0.91	30 (12%) 3 3	52, 77, 99, 134	0
1	H	236/287 (82%)	0.86	28 (11%) 4 4	52, 79, 103, 120	0
1	I	241/287 (83%)	0.54	14 (5%) 23 24	37, 57, 91, 136	0
1	J	239/287 (83%)	0.42	21 (8%) 10 10	35, 57, 92, 113	0
1	K	238/287 (82%)	0.96	29 (12%) 4 3	54, 80, 108, 125	0
1	L	239/287 (83%)	1.23	51 (21%) 0 0	61, 87, 121, 143	0
All	All	2898/3444 (84%)	0.44	221 (7%) 13 14	9, 58, 100, 151	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	273	VAL	11.7
1	A	245	SER	9.8
1	A	246	LEU	7.5
1	K	145	HIS	7.2
1	L	271	ILE	7.0

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 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.