



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:40 AM UTC

PDB ID : 5FFC / pdb\_00005ffc  
Title : CopM in the Cu(II)-bound form  
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Deposited on : 2015-12-18  
Resolution : 2.01 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

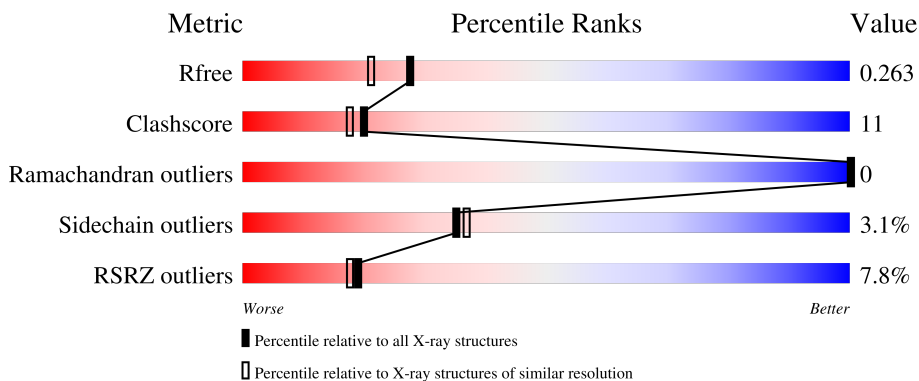
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	172	 3% 67% 18% 14%
1	B	172	 10% 63% 13% 23%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2470 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 CopM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	148	1207	760	212	220	15	0	1	0
1	B	133	1099	697	188	203	11	0	3	0

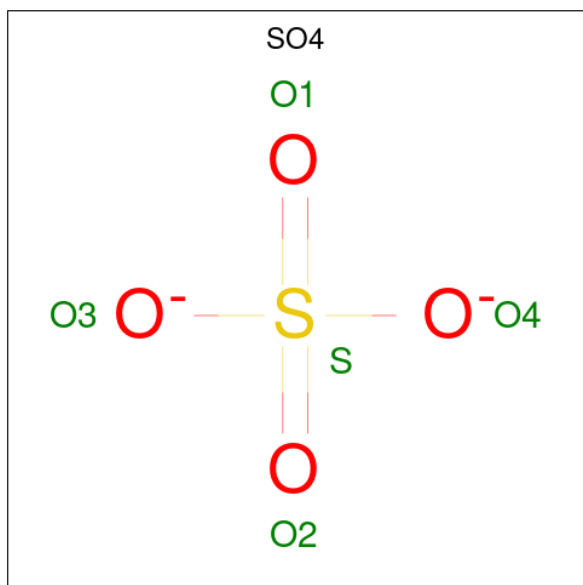
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP A0A0F6QDN6
A	26	SER	-	expression tag	UNP A0A0F6QDN6
B	25	GLY	-	expression tag	UNP A0A0F6QDN6
B	26	SER	-	expression tag	UNP A0A0F6QDN6

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	48	Total	O	0	0
			48	48		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	32.24Å 86.67Å 53.43Å 90.00° 92.33° 90.00°	Depositor
Resolution (Å)	27.10 – 2.01 27.10 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.3 (27.10-2.01) 97.4 (27.10-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.226 , 0.269 0.227 , 0.263	Depositor DCC
$R_{free}$ test set	975 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtrriage
Anisotropy	0.338	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2470	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<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.

## 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: SO4, CU

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	0.39	0/1233	0.69	0/1661
1	B	0.34	0/1131	0.70	0/1529
All	All	0.36	0/2364	0.69	0/3190

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	A	1207	0	1125	31	0
1	B	1099	0	1023	21	0
2	A	2	0	0	0	0
3	A	5	0	0	0	0
4	A	109	0	0	16	2
4	B	48	0	0	7	1
All	All	2470	0	2148	51	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 11.

All (51) 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:108:ALA:N	4:A:301:HOH:O	1.80	1.10
1:A:43:GLN:CA	4:A:303:HOH:O	2.02	1.07
1:A:43:GLN:HA	4:A:303:HOH:O	1.56	1.01
1:A:191[A]:GLN:OE1	4:A:302:HOH:O	1.83	0.97
1:A:43:GLN:HB3	4:A:303:HOH:O	1.67	0.95
1:B:148:HIS:ND1	4:B:202:HOH:O	2.01	0.92
1:A:43:GLN:CB	4:A:303:HOH:O	2.14	0.91
1:B:61:ILE:O	4:B:201:HOH:O	1.91	0.88
1:A:107:PRO:HA	4:A:301:HOH:O	1.76	0.86
1:A:136:ASN:HB3	4:A:306:HOH:O	1.78	0.81
1:A:107:PRO:CA	4:A:301:HOH:O	2.30	0.79
1:A:42:MET:O	4:A:303:HOH:O	2.00	0.79
1:A:72:GLU:OE1	4:A:304:HOH:O	2.03	0.74
1:A:72:GLU:OE1	1:A:72:GLU:CG	2.38	0.72
1:A:72:GLU:CG	1:A:72:GLU:OE2	2.38	0.71
1:B:58:GLN:OE1	4:B:204:HOH:O	2.07	0.71
1:B:182:GLU:OE1	4:B:205:HOH:O	2.10	0.69
1:A:72:GLU:OE1	1:A:72:GLU:OE2	2.19	0.61
1:A:187:LYS:NZ	4:A:305:HOH:O	2.21	0.61
1:A:107:PRO:C	4:A:301:HOH:O	2.22	0.60
1:A:42:MET:N	4:A:311:HOH:O	2.36	0.58
1:B:82:ASN:OD1	1:B:85:ARG:NH1	2.36	0.56
1:A:49:PHE:CZ	1:A:53:MET:HG3	2.42	0.55
1:B:61:ILE:HD11	1:B:88:GLU:HG3	1.89	0.54
1:B:57[B]:HIS:HB3	1:B:91:ILE:HD11	1.90	0.54
1:A:42:MET:C	4:A:303:HOH:O	2.47	0.51
1:B:126:MET:HB2	1:B:144:GLN:OE1	2.11	0.49
1:B:69:GLN:HG3	4:B:241:HOH:O	2.12	0.48
1:B:66:MET:HE3	1:B:131:LEU:HD23	1.95	0.48
1:A:59:ASP:OD1	1:A:60:ALA:N	2.48	0.47
1:A:139:ARG:HB2	1:A:194:TYR:CZ	2.50	0.46
1:B:168:MET:O	1:B:172:MET:HG2	2.16	0.46
1:B:62:ASP:HB3	1:B:128:LEU:HD21	1.99	0.45
1:A:54:THR:HB	1:A:55:PRO:HD3	1.99	0.45
1:B:126:MET:N	4:B:211:HOH:O	2.50	0.45
1:A:63:MET:SD	1:A:131:LEU:HD22	2.57	0.44
1:A:75:GLU:HB3	1:A:189:TRP:CZ2	2.53	0.44
1:A:168:MET:O	1:A:172:MET:HG2	2.17	0.43
1:B:66:MET:HG2	1:B:137:PHE:CE1	2.53	0.43
1:B:49:PHE:CE2	1:B:53:MET:HG3	2.53	0.43
1:B:57[A]:HIS:HD1	1:B:148:HIS:HE1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HB2	1:B:194:TYR:CZ	2.55	0.42
1:A:63:MET:HE3	1:A:126:MET:HB3	2.01	0.42
1:A:90:GLU:HG2	1:A:171:LEU:HD11	2.00	0.42
1:B:53:MET:O	1:B:57[B]:HIS:HB2	2.20	0.42
1:B:91:ILE:HD13	4:B:204:HOH:O	2.19	0.41
1:A:51:GLU:HG2	1:A:107:PRO:HD2	2.01	0.41
1:A:140:GLU:OE2	1:A:143:ARG:NH2	2.47	0.41
1:A:99:GLN:O	1:B:69:GLN:NE2	2.54	0.41
1:A:88:GLU:OE1	4:A:307:HOH:O	2.22	0.40
1:B:159:LEU:HD12	1:B:172:MET:SD	2.62	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)
4:A:308:HOH:O	4:B:226:HOH:O[1_554]	1.86	0.34
4:A:403:HOH:O	4:A:405:HOH:O[2_645]	2.19	0.01

## 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	145/172 (84%)	145 (100%)	0	0	100	100
1	B	132/172 (77%)	131 (99%)	1 (1%)	0	100	100
All	All	277/344 (80%)	276 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Percentiles	
1	A	119/151 (79%)	116 (98%)	3 (2%)	42	45
1	B	111/151 (74%)	107 (96%)	4 (4%)	31	31
All	All	230/302 (76%)	223 (97%)	7 (3%)	35	38

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	63	MET
1	A	149	HIS
1	B	59	ASP
1	B	61	ILE
1	B	69	GLN
1	B	159	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	69	GLN
1	A	179	GLN
1	B	148	HIS
1	B	179	GLN
1	B	188	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
3	SO4	A	203	-	4,4,4	0.24	0	6,6,6	0.11	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.

No monomer is involved in short contacts.

## 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, 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	148/172 (86%)	0.36	5 (3%) 48 47	21, 36, 51, 70	3 (2%)
1	B	133/172 (77%)	0.89	17 (12%) 7 6	22, 45, 73, 85	5 (3%)
All	All	281/344 (81%)	0.61	22 (7%) 19 18	21, 41, 64, 85	8 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57[A]	HIS	4.5
1	B	60	ALA	4.5
1	B	56	HIS	3.4
1	B	131	LEU	3.0
1	B	66	MET	2.9
1	A	114	MET	2.8
1	A	57	HIS	2.8
1	B	61	ILE	2.7
1	A	108	ALA	2.6
1	B	129	ASP	2.6
1	B	190	TYR	2.6
1	B	132	ALA	2.5
1	A	117	MET	2.4
1	B	133	THR	2.3
1	B	128	LEU	2.3
1	A	115	MET	2.3
1	B	54	THR	2.2
1	B	192	ASN	2.2
1	B	59	ASP	2.2
1	B	126	MET	2.2
1	B	134	ALA	2.2
1	B	85	ARG	2.1

## 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 oligosaccharides in this entry.

## 6.4 Ligands [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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	A	202	1/1	0.96	0.05	56,56,56,56	0
3	SO4	A	203	5/5	0.97	0.07	42,45,49,51	0
2	CU	A	201	1/1	0.98	0.06	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.