



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2016 – 08:53 AM EDT

PDB ID : 5FEJ
Title : CopM in the Cu(I)-bound form
Authors : Zhao, S.; Wang, X.; Liu, L.
Deposited on : 2015-12-17
Resolution : 2.50 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

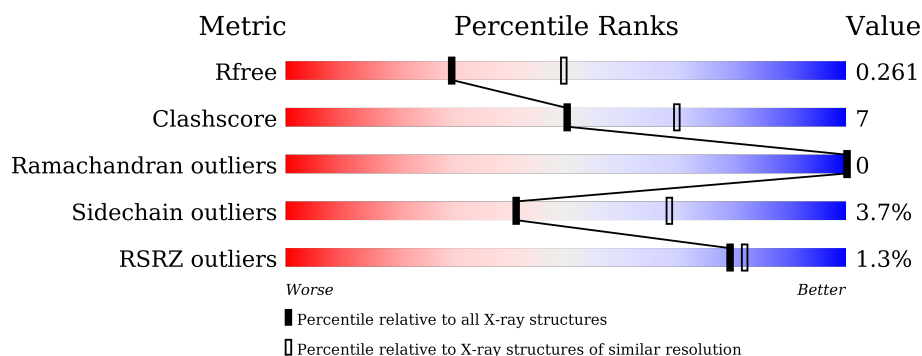
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	<div> <div></div> <div>63%16%•20%</div> </div>
1	B	172	<div> <div></div> <div>63%16%•19%</div> </div>
1	C	172	<div> <div></div> <div>68%12%20%</div> </div>
1	D	172	<div> <div></div> <div>66%15%20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4692 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
1	A	138	Total	C	N	O	S	0	0	0
			1141	720	202	207	12			
1	B	140	Total	C	N	O	S	0	0	0
			1154	728	203	212	11			
1	C	138	Total	C	N	O	S	0	0	0
			1123	707	198	207	11			
1	D	138	Total	C	N	O	S	0	0	0
			1126	711	196	208	11			

There are 8 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
C	25	GLY	-	expression tag	UNP A0A0F6QDN6
C	26	SER	-	expression tag	UNP A0A0F6QDN6
D	25	GLY	-	expression tag	UNP A0A0F6QDN6
D	26	SER	-	expression tag	UNP A0A0F6QDN6

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

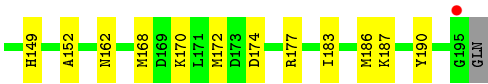
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		
2	D	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	46	Total 46	O 46	0	0
3	C	23	Total 23	O 23	0	0
3	D	30	Total 30	O 30	0	0

- Molecule 1: CopM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.82Å 86.08Å 74.97Å 90.00° 106.26° 90.00°	Depositor
Resolution (Å)	36.94 – 2.50 36.94 – 2.49	Depositor EDS
% Data completeness (in resolution range)	81.1 (36.94-2.50) 81.1 (36.94-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.259 0.212 , 0.261	Depositor DCC
R_{free} test set	914 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4692	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.60 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6565e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: CU1

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	0.23	0/1167	0.38	0/1572
1	B	0.22	0/1180	0.37	0/1590
1	C	0.25	0/1149	0.41	0/1553
1	D	0.22	0/1152	0.36	0/1556
All	All	0.23	0/4648	0.38	0/6271

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	1141	0	1088	15	0
1	B	1154	0	1100	20	0
1	C	1123	0	1036	14	0
1	D	1126	0	1050	15	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	46	0	0	6	1
3	C	23	0	0	6	1
3	D	30	0	0	4	0
All	All	4692	0	4274	62	1

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 7.

All (62) 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:62:ASP:OD1	3:B:301:HOH:O	2.02	0.78
1:D:105:PRO:O	3:D:301:HOH:O	2.01	0.77
1:C:126:MET:HG2	3:C:309:HOH:O	1.85	0.76
1:A:127:ASP:OD1	3:A:301:HOH:O	2.05	0.74
1:B:140:GLU:OE1	3:B:303:HOH:O	2.12	0.65
1:C:105:PRO:O	3:C:301:HOH:O	2.13	0.65
1:B:151:MET:SD	3:B:344:HOH:O	2.54	0.65
1:B:156:ALA:HA	1:B:172:MET:HE3	1.80	0.63
1:A:174:ASP:OD1	1:A:177:ARG:NH2	2.32	0.63
1:B:179:GLN:NE2	3:B:302:HOH:O	2.07	0.62
1:C:45:THR:N	3:C:305:HOH:O	2.32	0.62
1:B:61:ILE:HD13	1:B:88:GLU:HG3	1.82	0.62
1:B:142:ILE:HG23	1:B:186:MET:HB3	1.81	0.61
1:A:160:LYS:NZ	1:A:173:ASP:OD1	2.29	0.61
1:A:105:PRO:HG3	1:D:128:LEU:HD22	1.81	0.61
1:D:162:ASN:ND2	3:D:305:HOH:O	2.36	0.58
1:B:159:LEU:HB3	1:B:172:MET:HE2	1.84	0.58
1:A:50:ILE:HG23	1:A:94:MET:HB3	1.86	0.58
1:D:139:ARG:NH1	1:D:190:TYR:OH	2.38	0.57
1:D:83:ILE:HG23	1:D:87:GLN:HG3	1.88	0.55
1:D:142:ILE:HG23	1:D:186:MET:HB3	1.90	0.54
1:A:60:ALA:HB2	1:A:148:HIS:CE1	2.42	0.54
1:C:69:GLN:NE2	3:C:302:HOH:O	2.22	0.53
1:B:153:VAL:HG11	1:C:161:THR:HG21	1.91	0.53
1:B:193:TRP:NE1	3:B:305:HOH:O	2.29	0.49
1:B:60:ALA:HB2	1:B:148:HIS:CE1	2.47	0.49
1:B:153:VAL:HG23	1:B:176:ILE:HA	1.94	0.49
1:C:168:MET:O	1:C:172:MET:HG2	2.13	0.49
1:C:126:MET:HE1	1:C:144:GLN:HB3	1.95	0.48
1:D:56:HIS:CE1	1:D:152:ALA:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:HG23	1:B:94:MET:HB3	1.95	0.47
1:A:84:ILE:O	1:A:88:GLU:HB2	2.13	0.47
1:A:61:ILE:HD13	1:A:88:GLU:HG3	1.97	0.47
1:A:142:ILE:HG23	1:A:186:MET:HB3	1.97	0.47
1:A:60:ALA:HB2	1:A:148:HIS:HE1	1.79	0.46
1:A:168:MET:O	1:A:172:MET:HG2	2.16	0.46
1:B:84:ILE:O	1:B:88:GLU:HB2	2.14	0.46
1:B:165:ARG:NH1	3:B:311:HOH:O	2.48	0.45
1:D:183:ILE:HG22	1:D:187:LYS:HE2	1.99	0.45
1:D:174:ASP:OD1	1:D:177:ARG:NH2	2.49	0.45
1:C:84:ILE:O	1:C:88:GLU:HB2	2.16	0.45
1:C:97:TRP:CZ2	1:C:167:GLU:HB3	2.52	0.44
1:B:128:LEU:HA	1:B:128:LEU:HD13	1.85	0.44
1:B:56:HIS:CE1	1:B:152:ALA:HB2	2.51	0.44
1:C:47:GLN:HG3	1:C:98:TYR:CE2	2.53	0.43
1:D:170:LYS:NZ	3:D:303:HOH:O	2.26	0.43
1:A:149:HIS:NE2	1:A:182:GLU:OE1	2.50	0.43
1:D:168:MET:O	1:D:172:MET:HG2	2.19	0.42
1:A:102:PHE:O	1:A:104:ARG:HG2	2.20	0.42
1:A:106:VAL:HA	1:A:107:PRO:HD2	1.91	0.42
1:C:60:ALA:HB2	1:C:148:HIS:CE1	2.54	0.42
1:D:74:PRO:HD2	3:D:324:HOH:O	2.18	0.42
1:C:44:TRP:HA	3:C:305:HOH:O	2.20	0.42
1:D:84:ILE:O	1:D:88:GLU:HB2	2.20	0.41
1:A:73:HIS:HA	1:A:74:PRO:HD3	1.95	0.41
1:B:139:ARG:O	1:B:143:ARG:HB2	2.20	0.41
1:D:66:MET:HE3	1:D:128:LEU:HD23	2.03	0.41
1:B:87:GLN:HE22	1:B:179:GLN:HE22	1.70	0.40
1:C:45:THR:HG23	3:C:305:HOH:O	2.21	0.40
1:B:73:HIS:HB3	1:B:75:GLU:OE1	2.22	0.40
1:C:75:GLU:HB3	1:C:189:TRP:CZ2	2.57	0.40
1:D:63:MET:HB3	1:D:63:MET:HE2	1.88	0.40

All (1) 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)
3:B:339:HOH:O	3:C:318:HOH:O[1_655]	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	Percentiles	
1	A	134/172 (78%)	132 (98%)	2 (2%)	0	100	100
1	B	136/172 (79%)	136 (100%)	0	0	100	100
1	C	134/172 (78%)	133 (99%)	1 (1%)	0	100	100
1	D	134/172 (78%)	131 (98%)	3 (2%)	0	100	100
All	All	538/688 (78%)	532 (99%)	6 (1%)	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	116/151 (77%)	111 (96%)	5 (4%)	35	61
1	B	118/151 (78%)	110 (93%)	8 (7%)	20	36
1	C	110/151 (73%)	108 (98%)	2 (2%)	66	88
1	D	112/151 (74%)	110 (98%)	2 (2%)	66	88
All	All	456/604 (76%)	439 (96%)	17 (4%)	41	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	149	HIS

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Mol	Chain	Res	Type
1	A	151	MET
1	A	154	MET
1	A	159	LEU
1	B	57	HIS
1	B	109	LEU
1	B	128	LEU
1	B	129	ASP
1	B	139	ARG
1	B	143	ARG
1	B	149	HIS
1	B	172	MET
1	C	57	HIS
1	C	149	HIS
1	D	57	HIS
1	D	149	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	GLN
1	C	179	GLN

5.3.3 RNA ⓘ

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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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

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 [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	138/172 (80%)	0.07	1 (0%) 89 90	8, 12, 26, 40	1 (0%)
1	B	140/172 (81%)	0.22	2 (1%) 78 80	10, 15, 32, 64	1 (0%)
1	C	138/172 (80%)	0.18	2 (1%) 78 80	10, 17, 29, 39	0
1	D	138/172 (80%)	0.20	2 (1%) 78 80	9, 15, 30, 38	0
All	All	554/688 (80%)	0.17	7 (1%) 79 82	8, 15, 29, 64	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	TRP	3.9
1	D	195	GLY	2.9
1	D	125	ALA	2.5
1	A	44	TRP	2.4
1	B	44	TRP	2.3
1	B	111	SER	2.3
1	C	126	MET	2.0

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](#)

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(Å ²)	Q<0.9
2	CU1	C	202	1/1	1.00	0.13	-1.36	14,14,14,14	0
2	CU1	D	202	1/1	0.99	0.14	-1.67	10,10,10,10	0
2	CU1	A	201	1/1	1.00	0.11	-2.19	11,11,11,11	0
2	CU1	C	201	1/1	0.99	0.12	-2.23	9,9,9,9	0
2	CU1	A	202	1/1	1.00	0.12	-2.45	10,10,10,10	0
2	CU1	D	201	1/1	1.00	0.09	-2.62	13,13,13,13	0
2	CU1	B	202	1/1	1.00	0.10	-2.64	12,12,12,12	0
2	CU1	B	201	1/1	0.99	0.10	-3.48	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.