



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:04 AM UTC

PDB ID : 5B7M / pdb_00005b7m
Title : Structure of perdeuterated CueO - the signal peptide was truncated by HRV3C protease
Authors : Akter, M.; Higuchi, Y.; Shibata, N.
Deposited on : 2016-06-07
Resolution : 1.80 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

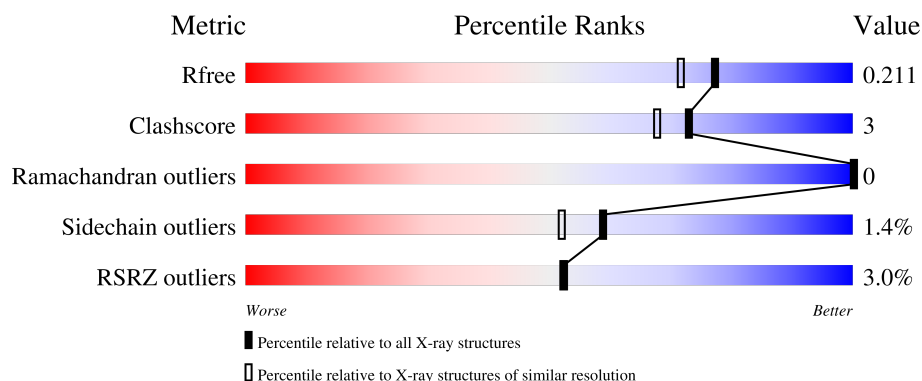
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

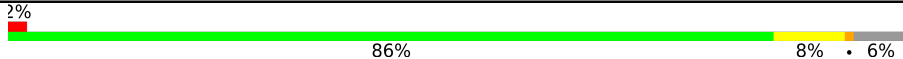
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 ≥ 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	492	
1	B	492	
1	C	492	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11511 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 Blue copper oxidase CueO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	7	0
			3593	2281	627	657	28			
1	B	464	Total	C	N	O	S	0	4	0
			3582	2274	624	658	26			
1	C	462	Total	C	N	O	S	0	3	0
			3561	2261	622	652	26			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP P36649
A	26	PRO	-	expression tag	UNP P36649
A	27	GLY	-	expression tag	UNP P36649
A	28	GLY	-	expression tag	UNP P36649
B	25	GLY	-	expression tag	UNP P36649
B	26	PRO	-	expression tag	UNP P36649
B	27	GLY	-	expression tag	UNP P36649
B	28	GLY	-	expression tag	UNP P36649
C	25	GLY	-	expression tag	UNP P36649
C	26	PRO	-	expression tag	UNP P36649
C	27	GLY	-	expression tag	UNP P36649
C	28	GLY	-	expression tag	UNP P36649

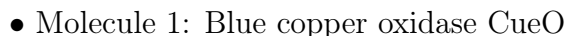
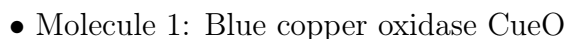
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cu	0	0
			4	4		
2	B	4	Total	Cu	0	0
			4	4		
2	C	4	Total	Cu	0	0
			4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	289	Total 289	O 289	0	0
3	B	298	Total 298	O 298	0	0
3	C	176	Total 176	O 176	0	0

- Molecule 1: Blue copper oxidase CueO



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.91Å 106.92Å 262.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.48 – 1.80 37.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.48-1.80) 99.7 (37.48-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.204 (Not available) , 0.211	Depositor DCC
R_{free} test set	2000 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.8	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	0.97	EDS
Total number of atoms	11511	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/3700	0.75	0/5022
1	B	0.48	0/3683	0.77	1/5002 (0.0%)
1	C	0.38	0/3658	0.71	1/4966 (0.0%)
All	All	0.44	0/11041	0.75	2/14990 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	PRO	O-C-N	5.35	123.77	121.31
1	B	461	PRO	O-C-N	5.13	123.67	121.31

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	3593	0	3583	26	0
1	B	3582	0	3563	22	0
1	C	3561	0	3543	20	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	289	0	0	5	0
3	B	298	0	0	1	0
3	C	176	0	0	1	0
All	All	11511	0	10689	68	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 3.

All (68) 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:C:34:LEU:HD22	1:C:317:MET:HE1	1.58	0.85
1:A:364:MET:HE3	1:A:376:MET:HE1	1.75	0.68
1:C:343:LEU:HB3	1:C:431:ARG:HD2	1.79	0.65
1:A:350:LYS:NZ	3:A:702:HOH:O	2.31	0.64
1:A:250:ASP:OD2	1:A:291:LYS:NZ	2.32	0.61
1:A:276:LEU:HD11	1:A:474:LYS:HB2	1.86	0.56
1:A:102:TRP:HB3	1:A:105:LEU:HD22	1.88	0.56
1:A:228:ARG:NH2	1:A:323:ALA:HB2	2.21	0.56
1:A:374:GLN:HG2	3:A:872:HOH:O	2.06	0.55
1:A:303:MET:HE3	1:A:379:MET:HG3	1.88	0.55
1:B:374:GLN:HG2	3:B:891:HOH:O	2.04	0.55
1:A:455:LEU:HG	1:A:483:LEU:HG	1.89	0.54
1:C:183:VAL:HB	1:C:235:LEU:HD23	1.91	0.52
1:A:124:LYS:NZ	3:A:705:HOH:O	2.42	0.52
1:A:355[A]:MET:HG3	1:A:359:LEU:HD23	1.91	0.51
1:B:227:PRO:HB2	1:B:326:ALA:HB2	1.91	0.51
1:B:265:PRO:HD3	1:B:337:LEU:HD22	1.94	0.50
1:A:93:GLN:HG2	3:A:959:HOH:O	2.11	0.50
1:B:191:SER:OG	1:B:193:ASP:OD1	2.30	0.50
1:A:368[A]:MET:SD	1:A:376:MET:HG3	2.52	0.48
1:A:228:ARG:HD3	1:A:289:ASP:HB2	1.97	0.47
1:B:358:MET:HE3	1:B:358:MET:HB2	1.78	0.47
1:C:100:LEU:O	1:C:113:GLY:HA3	2.15	0.47
1:C:355:MET:HG2	1:C:408:ASN:OD1	2.14	0.47
1:A:265:PRO:HD3	1:A:337:LEU:HD13	1.97	0.47
1:A:253:PRO:HG3	1:A:269:LYS:HE3	1.97	0.47
1:B:81:GLN:NE2	1:B:84:LYS:HE3	2.30	0.46
1:C:252:ARG:NH1	1:C:286:GLU:O	2.46	0.46
1:B:80:LEU:HB3	1:B:131:VAL:HG21	1.98	0.46
1:A:408:ASN:HB3	1:A:510:MET:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ILE:HG21	1:C:512:LEU:HD23	1.98	0.45
1:B:147:LYS:HD3	1:B:150:ARG:HH21	1.81	0.44
1:C:359:LEU:HD22	1:C:407:ALA:HB3	1.98	0.44
1:B:81:GLN:OE1	1:B:84:LYS:HG3	2.17	0.44
1:C:276:LEU:HD11	1:C:474:LYS:HB2	1.98	0.44
1:A:355[A]:MET:HE1	1:A:441:MET:HG3	1.98	0.44
1:B:492:LYS:HB2	1:B:492:LYS:HE3	1.73	0.44
1:B:276:LEU:HD11	1:B:474:LYS:HB2	2.00	0.44
1:B:482:VAL:HG23	1:B:484[B]:VAL:HG13	2.00	0.43
1:A:202:VAL:HG21	1:A:362:MET:HE2	2.00	0.43
1:A:366:MET:HB3	1:A:366:MET:HE2	1.76	0.43
1:B:41:THR:HG22	1:B:79:LYS:HB3	1.99	0.43
1:A:202:VAL:HG12	3:A:902:HOH:O	2.19	0.43
1:C:364:MET:O	1:C:368:MET:HG2	2.19	0.43
1:C:227:PRO:HB2	1:C:326:ALA:HB2	2.00	0.42
1:C:376:MET:HE3	1:C:376:MET:HB3	1.94	0.42
1:B:228:ARG:NH1	1:B:323:ALA:HB2	2.34	0.42
1:B:366:MET:HE2	1:B:366:MET:HB3	1.70	0.42
1:A:191:SER:OG	1:A:193:ASP:OD1	2.36	0.42
1:A:227:PRO:HB2	1:A:326:ALA:HB2	2.02	0.41
1:B:102:TRP:HB3	1:B:105:LEU:HD22	2.02	0.41
1:C:284:LEU:HD22	1:C:330:LEU:HD13	2.03	0.41
1:B:410:ILE:HG21	1:B:512:LEU:HD23	2.03	0.41
1:A:100:LEU:O	1:A:113:GLY:HA3	2.21	0.41
1:A:303:MET:HE1	1:A:376:MET:SD	2.61	0.41
1:C:255:TYR:OH	1:C:269:LYS:NZ	2.54	0.41
1:A:228:ARG:CZ	1:A:323:ALA:HB2	2.51	0.41
1:B:361:MET:HE3	1:B:361:MET:HB2	1.79	0.41
1:C:140:PHE:CZ	1:C:158:GLY:HA3	2.56	0.41
1:B:55:GLY:HA3	1:B:72:ASN:OD1	2.21	0.41
1:C:80:LEU:HB3	1:C:131:VAL:HG21	2.02	0.40
1:B:408:ASN:HB3	1:B:510:MET:HB2	2.04	0.40
1:C:291:LYS:HB3	1:C:291:LYS:HE3	1.77	0.40
1:C:293:PHE:CE2	1:C:319:ILE:HD12	2.56	0.40
1:C:329:ALA:O	1:C:331:PRO:HD3	2.21	0.40
1:B:147:LYS:HD3	1:B:150:ARG:NH2	2.36	0.40
1:B:81:GLN:CD	1:B:84:LYS:HG3	2.47	0.40
1:C:174:LYS:HD3	3:C:867:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	466/492 (95%)	453 (97%)	13 (3%)	0	100	100
1	B	464/492 (94%)	450 (97%)	14 (3%)	0	100	100
1	C	459/492 (93%)	443 (96%)	16 (4%)	0	100	100
All	All	1389/1476 (94%)	1346 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	376/401 (94%)	371 (99%)	5 (1%)	61	54
1	B	298/401 (74%)	294 (99%)	4 (1%)	61	54
1	C	383/401 (96%)	377 (98%)	6 (2%)	55	47
All	All	1057/1203 (88%)	1042 (99%)	15 (1%)	59	52

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	228	ARG
1	A	303	MET
1	A	350	LYS
1	A	470	LYS

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Mol	Chain	Res	Type
1	B	110	GLU
1	B	181	VAL
1	B	199	GLN
1	B	470	LYS
1	C	181	VAL
1	C	199	GLN
1	C	291	LYS
1	C	327	SER
1	C	376	MET
1	C	470	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	413	GLN
1	B	352	GLN
1	B	405	HIS
1	C	406	HIS

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 12 ligands modelled in this entry, 12 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 ⓘ

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	463/492 (94%)	-0.29	10 (2%) 62 62	7, 22, 43, 72	7 (1%)
1	B	464/492 (94%)	-0.26	10 (2%) 62 62	7, 23, 41, 62	4 (0%)
1	C	462/492 (93%)	0.26	22 (4%) 35 34	14, 36, 65, 94	3 (0%)
All	All	1389/1476 (94%)	-0.10	42 (3%) 52 52	7, 27, 53, 94	14 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	377	ALA	5.2
1	C	440	MET	4.1
1	A	290	ASN	4.0
1	C	378	GLY	3.8
1	C	288	ASN	3.8
1	C	290	ASN	3.5
1	C	323	ALA	3.5
1	B	327	SER	3.3
1	B	145	HIS	3.3
1	A	377	ALA	3.1
1	C	376	MET	3.1
1	C	379	MET	3.0
1	B	171	MET	2.9
1	C	171	MET	2.8
1	C	327	SER	2.8
1	C	145	HIS	2.7
1	B	378	GLY	2.6
1	C	84	LYS	2.6
1	B	440	MET	2.6
1	C	250	ASP	2.5
1	C	326	ALA	2.4
1	B	364	MET	2.4
1	A	483	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	368[A]	MET	2.4
1	C	403	ASP	2.3
1	C	439	ASP	2.3
1	B	326	ALA	2.3
1	A	376	MET	2.3
1	A	379	MET	2.3
1	C	355	MET	2.3
1	A	289	ASP	2.2
1	B	361	MET	2.2
1	A	327	SER	2.2
1	A	378	GLY	2.2
1	B	376	MET	2.2
1	C	130	ASN	2.1
1	C	438	GLY	2.1
1	A	171	MET	2.1
1	C	368	MET	2.1
1	C	339	ALA	2.1
1	B	379	MET	2.0
1	C	303	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 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, 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	B-factors(Å ²)	Q<0.9
2	CU	C	604	1/1	0.92	0.17	96,96,96,96	1
2	CU	B	604	1/1	0.97	0.16	41,41,41,41	1
2	CU	A	604	1/1	0.98	0.11	36,36,36,36	1
2	CU	A	602	1/1	0.99	0.02	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	B	602	1/1	0.99	0.03	24,24,24,24	1
2	CU	A	603	1/1	1.00	0.02	20,20,20,20	1
2	CU	B	603	1/1	1.00	0.01	18,18,18,18	1
2	CU	A	601	1/1	1.00	0.01	17,17,17,17	0
2	CU	C	601	1/1	1.00	0.01	30,30,30,30	0
2	CU	C	602	1/1	1.00	0.02	34,34,34,34	1
2	CU	C	603	1/1	1.00	0.02	28,28,28,28	1
2	CU	B	601	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.