

# Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 - 10:25 am BST

PDB ID	:	7Z3I
Title	:	Crystal structure of the cupredoxin AcoP from Acidithiobacillus ferrooxidans,
		M171A mutant
Authors	:	Leone, P.; Sciara, G.; Ilbert, M.
Deposited on	:	2022-03-02
Resolution	:	1.82  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 (i) 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 (1)) were used in the production of this report:

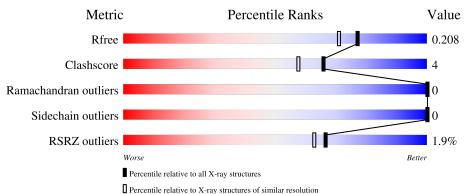
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	2.35 1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.82 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 <=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	А	171	% • 77%	•	19%		
1	В	171	<sup>2%</sup> 71%	5%	25%		



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2377 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	139	Total	С	Ν	0	S	0	1	0
	A	159	1101	709	190	199	3	0	T	0
1	В	129	Total	С	Ν	0	S	0	1	0
1	D	129	1023	662	174	184	3	0		

• Molecule 1 is a protein called AcoP.

There are $46$	discrepancies	between	the modelled	and	reference sequence	s:

Chain	Residue	Modelled	Actual	Comment	Reference
А	13	MET	-	initiating methionine	UNP A0A2W1KFF4
А	14	SER	-	expression tag	UNP A0A2W1KFF4
А	15	TYR	-	expression tag	UNP A0A2W1KFF4
А	16	TYR	-	expression tag	UNP A0A2W1KFF4
А	17	HIS	-	expression tag	UNP A0A2W1KFF4
А	18	HIS	-	expression tag	UNP A0A2W1KFF4
А	19	HIS	-	expression tag	UNP A0A2W1KFF4
А	20	HIS	-	expression tag	UNP A0A2W1KFF4
А	21	HIS	-	expression tag	UNP A0A2W1KFF4
А	22	HIS	-	expression tag	UNP A0A2W1KFF4
А	23	LEU	-	expression tag	UNP A0A2W1KFF4
А	24	GLU	-	expression tag	UNP A0A2W1KFF4
А	25	SER	-	expression tag	UNP A0A2W1KFF4
А	26	THR	-	expression tag	UNP A0A2W1KFF4
А	27	SER	-	expression tag	UNP A0A2W1KFF4
А	28	LEU	-	expression tag	UNP A0A2W1KFF4
А	29	TYR	-	expression tag	UNP A0A2W1KFF4
А	30	LYS	-	expression tag	UNP A0A2W1KFF4
А	31	LYS	-	expression tag	UNP A0A2W1KFF4
А	32	ALA	-	expression tag	UNP A0A2W1KFF4
А	33	GLY	-	expression tag	UNP A0A2W1KFF4
А	34	SER	-	expression tag	UNP A0A2W1KFF4
А	171	ALA	MET	conflict	UNP A0A2W1KFF4
В	13	MET	-	initiating methionine	UNP A0A2W1KFF4
В	14	SER	-	expression tag	UNP A0A2W1KFF4

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Chain	Residue	Modelled	Actual	Comment	Reference
В	15	TYR	-	expression tag	UNP A0A2W1KFF4
В	16	TYR	-	expression tag	UNP A0A2W1KFF4
В	17	HIS	-	expression tag	UNP A0A2W1KFF4
В	18	HIS	-	expression tag	UNP A0A2W1KFF4
В	19	HIS	-	expression tag	UNP A0A2W1KFF4
В	20	HIS	-	expression tag	UNP A0A2W1KFF4
В	21	HIS	-	expression tag	UNP A0A2W1KFF4
В	22	HIS	-	expression tag	UNP A0A2W1KFF4
В	23	LEU	-	expression tag	UNP A0A2W1KFF4
В	24	GLU	-	expression tag	UNP A0A2W1KFF4
В	25	SER	-	expression tag	UNP A0A2W1KFF4
В	26	THR	-	expression tag	UNP A0A2W1KFF4
В	27	SER	-	expression tag	UNP A0A2W1KFF4
В	28	LEU	-	expression tag	UNP A0A2W1KFF4
В	29	TYR	-	expression tag	UNP A0A2W1KFF4
В	30	LYS	-	expression tag	UNP A0A2W1KFF4
В	31	LYS	-	expression tag	UNP A0A2W1KFF4
В	32	ALA	-	expression tag	UNP A0A2W1KFF4
В	33	GLY	-	expression tag	UNP A0A2W1KFF4
В	34	SER	-	expression tag	UNP A0A2W1KFF4
В	171	ALA	MET	conflict	UNP A0A2W1KFF4

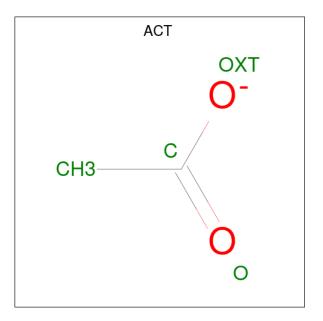
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• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

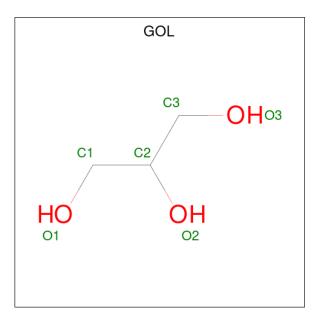
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	В	1	Total Cu 1 1	0	0

• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

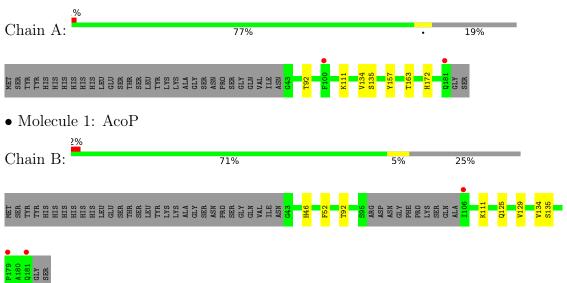
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	126	Total O 126 126	0	0
5	В	79	Total O 79 79	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: AcoP



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	73.75Å 73.75Å 113.08Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	47.40 - 1.82	Depositor
Resolution (A)	47.35 - 1.82	EDS
% Data completeness	97.6 (47.40-1.82)	Depositor
(in resolution range)	97.7 (47.35 - 1.82)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.63 (at 1.82 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.159 , $0.198$	Depositor
$R, R_{free}$	0.168 , $0.208$	DCC
$R_{free}$ test set	1396 reflections $(4.98\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	28.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, $51.5$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2377	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: ACT, CU, GOL

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 Chair		Bond	lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.76	0/1142	0.93	0/1553	
1	В	0.75	0/1061	0.87	0/1443	
All	All	0.75	0/2203	0.90	0/2996	

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	А	1101	0	1043	6	0
1	В	1023	0	969	8	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	12	0	9	0	0
3	В	4	0	3	1	0
4	А	6	0	8	3	0
4	В	24	0	32	8	0
5	А	126	0	0	1	0
5	В	79	0	0	4	0
All	All	2377	0	2064	17	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 4.

All $(17)$ close contacts	within the	same a	asymmetric	unit a	re listed	below,	sorted by	$\operatorname{their}$	$\operatorname{clash}$
magnitude.									

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:VAL:HA	4:B:204:GOL:H31	1.56	0.84
1:A:134:VAL:HA	4:A:205:GOL:H31	1.77	0.66
1:A:135:SER:H	4:A:205:GOL:C3	2.11	0.63
1:A:163:THR:HG23	5:A:413:HOH:O	2.01	0.59
1:B:135:SER:H	4:B:204:GOL:C3	2.15	0.59
1:A:135:SER:H	4:A:205:GOL:H31	1.67	0.59
1:A:92:THR:HB	1:A:111:LYS:HB2	1.88	0.56
1:B:125:GLN:HB3	4:B:203:GOL:H32	1.95	0.49
4:B:206:GOL:O3	5:B:301:HOH:O	2.13	0.47
1:B:46:HIS:HB2	5:B:374:HOH:O	2.14	0.47
4:B:206:GOL:C3	5:B:301:HOH:O	2.60	0.47
4:B:205:GOL:H12	5:B:361:HOH:O	2.15	0.46
1:B:129:VAL:HG21	4:B:203:GOL:H12	1.99	0.44
1:B:92:THR:HB	1:B:111:LYS:HB3	1.98	0.44
1:A:157:TYR:O	1:A:172:HIS:HA	2.20	0.42
1:B:129:VAL:CG2	4:B:203:GOL:H12	2.51	0.41
1:B:52:PHE:O	3:B:202:ACT:H2	2.21	0.40

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	Perce	ntiles
1	А	138/171~(81%)	135~(98%)	3~(2%)	0	100	100
1	В	126/171~(74%)	124 (98%)	2(2%)	0	100	100
All	All	264/342~(77%)	259~(98%)	5(2%)	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 side chain 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	А	117/144 (81%)	117 (100%)	0	100 100
1	В	109/144~(76%)	109 (100%)	0	100 100
All	All	226/288~(78%)	226 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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



Mol	Type	Chain	Res	Link	B	ond leng	gths	В	ond ang	gles
	Type	Ullaili	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	GOL	А	205	-	$5,\!5,\!5$	0.06	0	$5,\!5,\!5$	0.57	0
3	ACT	А	202	2	3,3,3	0.93	0	$3,\!3,\!3$	0.87	0
4	GOL	В	203	-	$5,\!5,\!5$	0.08	0	$5,\!5,\!5$	0.42	0
4	GOL	В	206	-	$5,\!5,\!5$	0.14	0	$5,\!5,\!5$	0.29	0
4	GOL	В	205	-	$5,\!5,\!5$	0.29	0	$5,\!5,\!5$	0.64	0
3	ACT	А	203	-	3,3,3	0.72	0	$3,\!3,\!3$	1.18	0
4	GOL	В	204	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.41	0
3	ACT	В	202	2	3,3,3	0.86	0	$3,\!3,\!3$	0.72	0
3	ACT	А	204	-	3,3,3	1.08	0	$3,\!3,\!3$	0.88	0

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).

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	GOL	А	205	-	-	2/4/4/4	-
4	GOL	В	203	-	-	4/4/4/4	-
4	GOL	В	206	-	-	0/4/4/4	-
4	GOL	В	205	-	-	2/4/4/4	-
4	GOL	В	204	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	205	GOL	O1-C1-C2-C3
4	В	203	GOL	O1-C1-C2-C3
4	В	203	GOL	C1-C2-C3-O3
4	В	204	GOL	C1-C2-C3-O3
4	В	205	GOL	C1-C2-C3-O3
4	А	205	GOL	O1-C1-C2-O2
4	В	203	GOL	O2-C2-C3-O3
4	В	204	GOL	O2-C2-C3-O3
4	В	205	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	В	203	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	205	GOL	3	0
4	В	203	GOL	3	0
4	В	206	GOL	2	0
4	В	205	GOL	1	0
4	В	204	GOL	2	0
3	В	202	ACT	1	0

### 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	139/171~(81%)	-0.01	2 (1%) 75 72	20, 27, 46, 80	0
1	В	129/171~(75%)	0.17	3 (2%) 60 56	22, 34, 53, 82	0
All	All	268/342 (78%)	0.08	5 (1%) 66 63	20, 30, 50, 82	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	181	GLN	4.4
1	А	100	PHE	4.2
1	А	181	GLN	3.8
1	В	179	PRO	3.0
1	В	106	ILE	2.4

### 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 monosaccharides 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,  $95^{th}$  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.

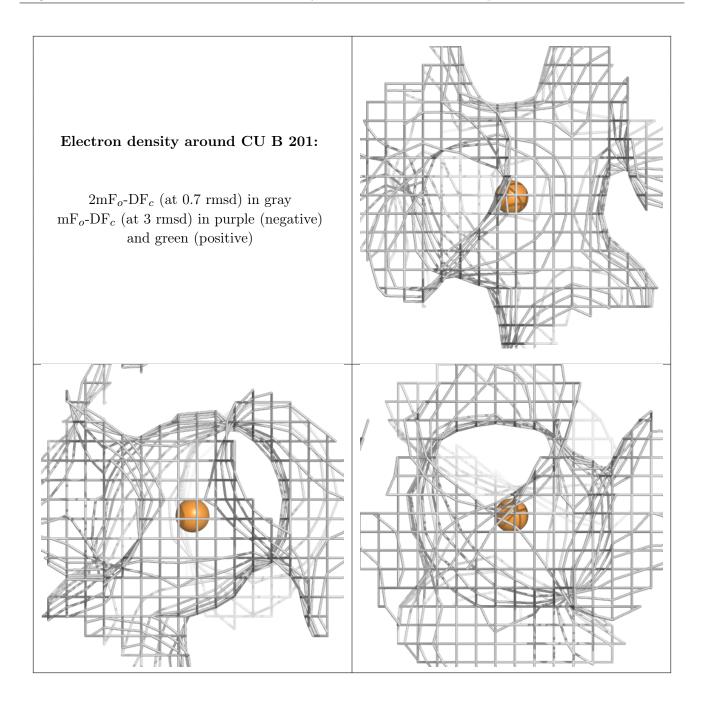


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1	4	)1

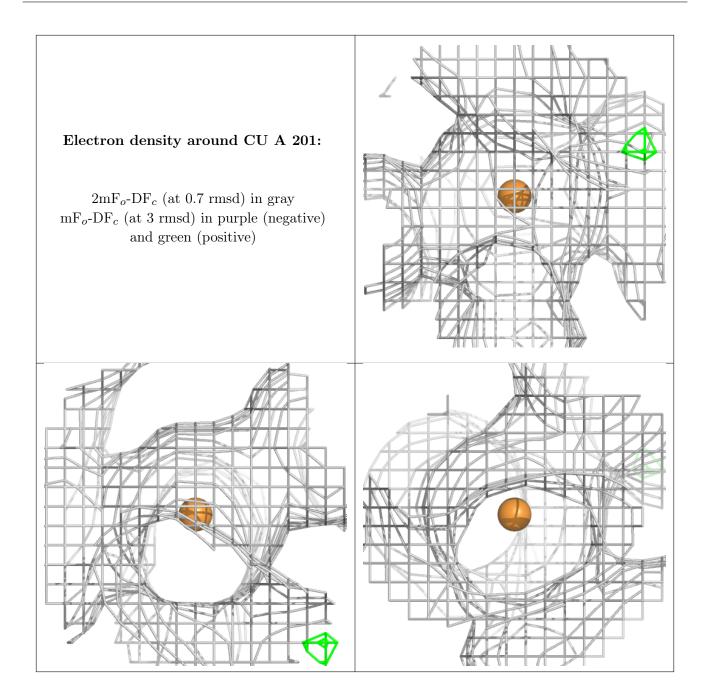
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
3	ACT	А	204	4/4	0.71	0.19	43,46,48,50	0
4	GOL	А	205	6/6	0.73	0.21	$40,\!41,\!45,\!47$	0
4	GOL	В	203	6/6	0.73	0.21	57,61,62,67	0
4	GOL	В	204	6/6	0.79	0.17	$56,\!58,\!61,\!64$	0
4	GOL	В	206	6/6	0.80	0.22	$48,\!49,\!54,\!58$	0
4	GOL	В	205	6/6	0.82	0.18	30,41,46,51	0
3	ACT	В	202	4/4	0.94	0.12	$37,\!45,\!46,\!48$	0
3	ACT	А	202	4/4	0.94	0.11	29,32,33,38	0
3	ACT	А	203	4/4	0.98	0.09	$41,\!43,\!44,\!47$	0
2	CU	В	201	1/1	1.00	0.09	28,28,28,28	0
2	CU	А	201	1/1	1.00	0.10	$24,\!24,\!24,\!24$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









### 6.5 Other polymers (i)

There are no such residues in this entry.

