



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:10 PM GMT

PDB ID : 3T56  
Title : Crystal structure of the pre-extrusion state of the CusBA adaptor-transporter complex  
Authors : Su, C.-C.; Long, F.; Yu, E.W.  
Deposited on : 2011-07-26  
Resolution : 3.42 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

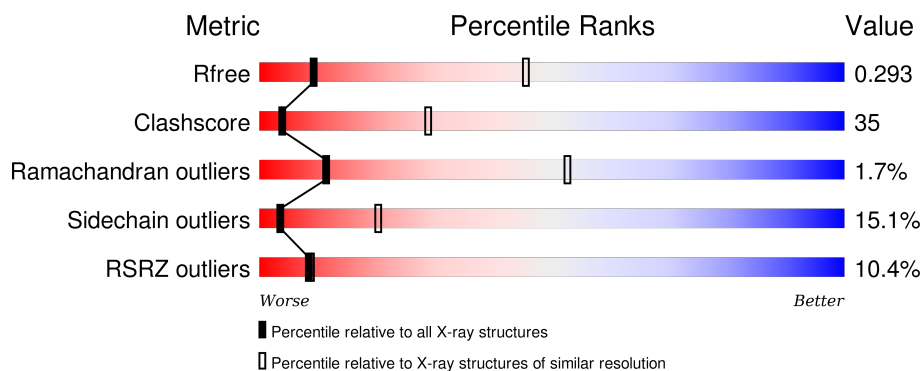
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.42 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	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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  $\geq 3$ , 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	1054	
2	B	336	
2	C	336	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CU	A	1048	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13860 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 Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1027	Total	C	N	O	S	0	225	0
			8913	5754	1502	1615	42			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	HIS	-	EXPRESSION TAG	UNP P38054

- Molecule 2 is a protein called Cation efflux system protein CusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
2	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239
C	408	HIS	-	EXPRESSION TAG	UNP P77239

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Chain	Residue	Modelled	Actual	Comment	Reference
C	409	HIS	-	EXPRESSION TAG	UNP P77239
C	410	HIS	-	EXPRESSION TAG	UNP P77239
C	411	HIS	-	EXPRESSION TAG	UNP P77239
C	412	HIS	-	EXPRESSION TAG	UNP P77239
C	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	4	Total O 4 4	0	0
4	C	8	Total O 8 8	0	0

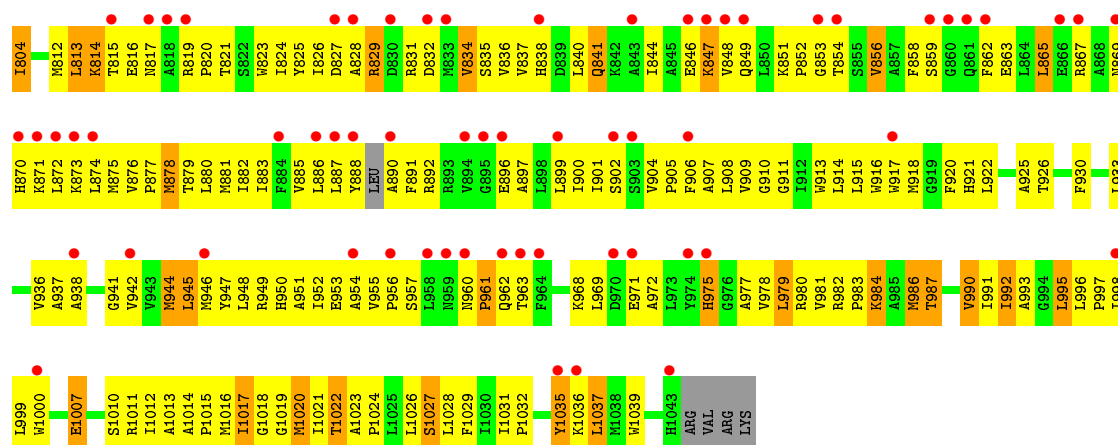
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

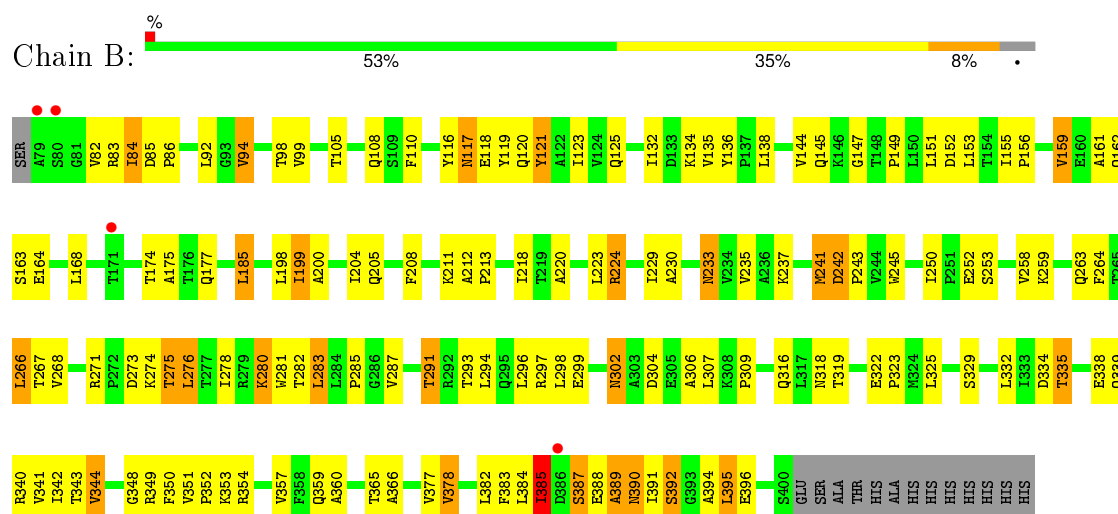
16% 38% 49% 10%

The figure displays a sequence of 100 amino acids, labeled from GLY (1) to SER (100). Each amino acid is represented by a three-letter code and a corresponding residue number. The sequence is color-coded based on a scale from 0% to 100%, with colors transitioning from red (low values) to orange, yellow, green, blue, and purple (high values). The color bar at the top indicates the distribution of values across the sequence, with markers at 16%, 38%, 49%, and 10%.

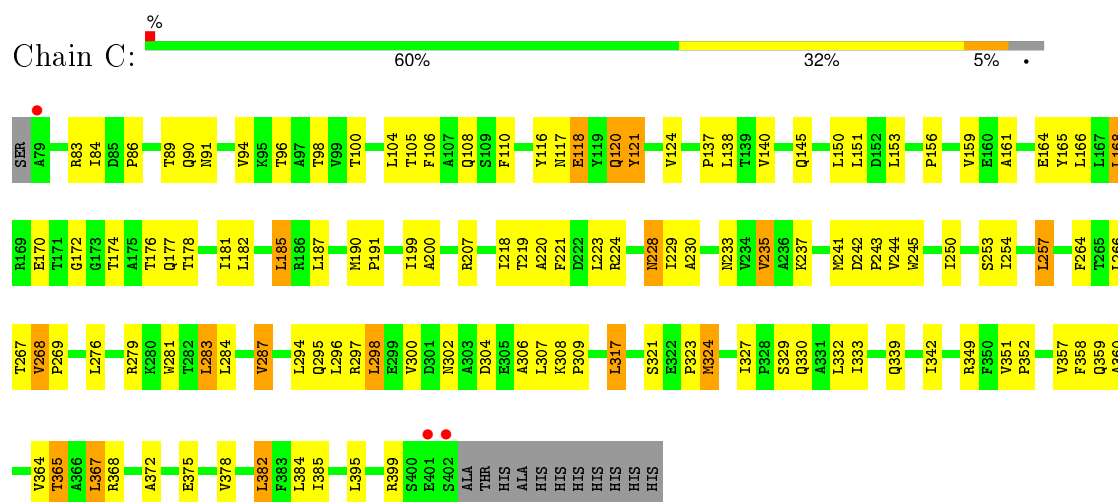
Residue	Label	Color
1	GLY	Red
2	HIS	Red
3	HIS	Red
4	HIS	Red
5	HIS	Red
6	HIS	Red
7	HIS	Red
8	HIS	Red
9	HIS	Red
10	HIS	Red
11	HIS	Red
12	HIS	Red
13	HIS	Red
14	HIS	Red
15	HIS	Red
16	HIS	Red
17	HIS	Red
18	HIS	Red
19	HIS	Red
20	HIS	Red
21	HIS	Red
22	HIS	Red
23	HIS	Red
24	HIS	Red
25	HIS	Red
26	HIS	Red
27	HIS	Red
28	HIS	Red
29	HIS	Red
30	HIS	Red
31	HIS	Red
32	HIS	Red
33	HIS	Red
34	HIS	Red
35	HIS	Red
36	HIS	Red
37	HIS	Red
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39	HIS	Red
40	HIS	Red
41	HIS	Red
42	HIS	Red
43	HIS	Red
44	HIS	Red
45	HIS	Red
46	HIS	Red
47	HIS	Red
48	HIS	Red
49	HIS	Red
50	HIS	Red
51	HIS	Red
52	HIS	Red
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56	HIS	Red
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59	HIS	Red
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62	HIS	Red
63	HIS	Red
64	HIS	Red
65	HIS	Red
66	HIS	Red
67	HIS	Red
68	HIS	Red
69	HIS	Red
70	HIS	Red
71	HIS	Red
72	HIS	Red
73	HIS	Red
74	HIS	Red
75	HIS	Red
76	HIS	Red
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78	HIS	Red
79	HIS	Red
80	HIS	Red
81	HIS	Red
82	HIS	Red
83	HIS	Red
84	HIS	Red
85	HIS	Red
86	HIS	Red
87	HIS	Red
88	HIS	Red
89	HIS	Red
90	HIS	Red
91	HIS	Red
92	HIS	Red
93	HIS	Red
94	HIS	Red
95	HIS	Red
96	HIS	Red
97	HIS	Red
98	HIS	Red
99	HIS	Red
100	SER	Red



• Molecule 2: Cation efflux system protein CusB



• Molecule 2: Cation efflux system protein CusB



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.12Å 160.12Å 684.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.25 – 3.42 49.25 – 3.42	Depositor EDS
% Data completeness (in resolution range)	88.8 (49.25-3.42) 98.7 (49.25-3.42)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.259 , 0.294 0.258 , 0.293	Depositor DCC
$R_{free}$ test set	2290 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 77.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 45646 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	13860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	0.23	0/9093	0.44	0/12371
2	B	0.22	0/2498	0.44	0/3401
2	C	0.22	0/2513	0.44	0/3421
All	All	0.23	0/14104	0.44	0/19193

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

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	8913	0	9201	752	0
2	B	2458	0	2522	135	0
2	C	2473	0	2533	104	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	8	0	0	0	0
All	All	13860	0	14256	972	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 35.

The worst 5 of 972 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:604:ARG:HG3	1:A:604:ARG:HH21	1.11	1.16
1:A:573:MET:HE2	1:A:625:GLU:HG2	1.24	1.15
1:A:828[B]:ALA:HA	1:A:829[B]:ARG:HB2	1.27	1.09
1:A:62:GLU:HB2	1:A:86:SER:HB2	1.32	1.06
1:A:62:GLU:HA	1:A:65:VAL:HG22	1.39	1.04

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	1149/1054 (109%)	1003 (87%)	119 (10%)	27 (2%)	8	46
2	B	320/336 (95%)	279 (87%)	35 (11%)	6 (2%)	10	50
2	C	322/336 (96%)	293 (91%)	28 (9%)	1 (0%)	46	83
All	All	1791/1726 (104%)	1575 (88%)	182 (10%)	34 (2%)	11	50

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	67	TYR
1	A	638	PRO
1	A	813[A]	LEU
1	A	814[A]	LYS

### 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	956/871 (110%)	811 (85%)	145 (15%)	3	20
2	B	263/275 (96%)	221 (84%)	42 (16%)	3	17
2	C	265/275 (96%)	235 (89%)	30 (11%)	7	33
All	All	1484/1421 (104%)	1267 (85%)	217 (15%)	3	22

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	722[A]	ARG
1	A	856[B]	VAL
2	C	207	ARG
1	A	731[A]	GLU
1	A	781[A]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	GLN
1	A	795[A]	GLN
2	C	228	ASN
1	A	660	ASN
1	A	744[A]	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 1 ligands modelled in this entry, 1 is 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, 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	1027/1054 (97%)	0.67	167 (16%) <b>2</b> <b>3</b>	2, 106, 283, 420	96 (9%)
2	B	322/336 (95%)	-0.20	4 (1%) <b>81</b> <b>75</b>	2, 33, 92, 166	0
2	C	324/336 (96%)	-0.18	3 (0%) <b>85</b> <b>80</b>	2, 33, 81, 209	0
All	All	1673/1726 (96%)	0.34	174 (10%) <b>8</b> <b>9</b>	2, 54, 257, 420	96 (5%)

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	THR	10.1
1	A	386	LEU	8.3
2	C	402	SER	8.0
1	A	438	VAL	7.9
1	A	890	ALA	7.7

### 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CU	A	1048	1/1	0.78	1.15	9.63	478,478,478,478	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.