



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2017 – 09:55 PM EDT

PDB ID : 3KSO  
Title : Structure and Mechanism of the Heavy Metal Transporter CusA  
Authors : Su, C.-C.  
Deposited on : unknown  
Resolution : 4.37 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

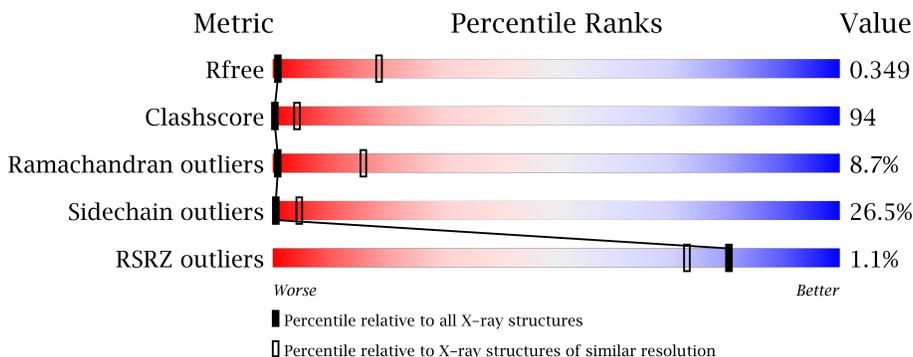
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.37 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))
$R_{free}$	100719	1024 (5.08-3.62)
Clashscore	112137	1017 (5.02-3.70)
Ramachandran outliers	110173	1017 (5.06-3.66)
Sidechain outliers	110143	1019 (5.08-3.64)
RSRZ outliers	101464	1007 (5.08-3.64)

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	1055	<p>18% 54% 23%</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7785 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
			Total	C	N	O	S			
1	A	1014	7784	5031	1304	1413	36	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP P38054
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

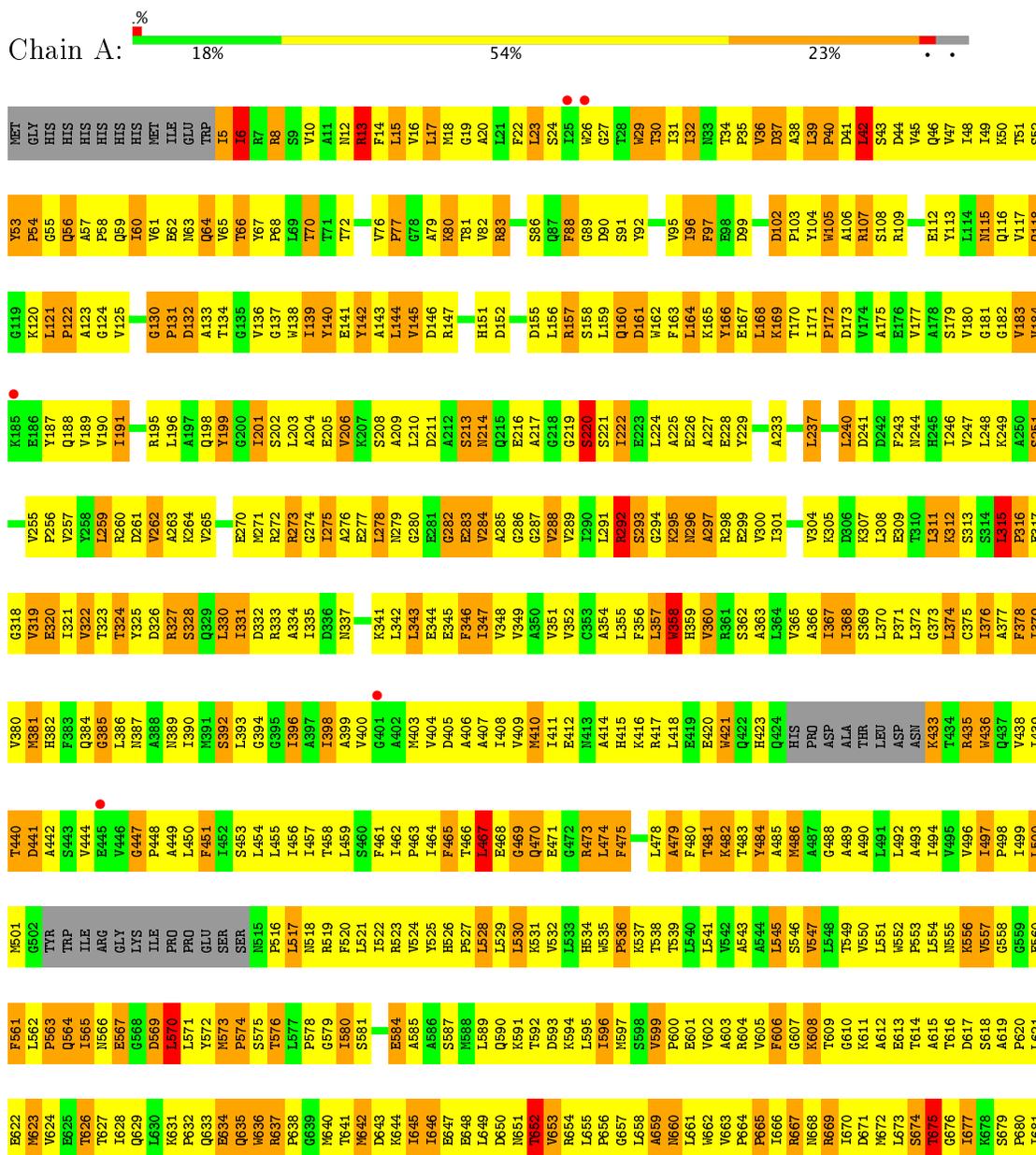
- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ag	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Cation efflux system protein cusA



4993	6882	L745	V806	K873	L893
G994	I683	F746	S807	L874	A934
L995	K684	V747	T808	M875	G935
F997	V685	T748	G809	V876	V936
I998	S686	A749	P810	M877	A937
L999	A750	S749	S811	M878	A938
M1000	T688	A751	M812	T879	E939
G1001	V689	G752	L813	L880	F940
T1002	L690	F753	K814	M881	G941
A1004	I693	A754	T815	I882	V942
G1005	D694	M755	E816	I883	V943
S1006	A695	V756	M817	F884	M944
E1007	M696	G757	A818	V885	L945
V1008	A697	E758	R819	L886	M946
M1009	E698	V759	P820	L887	Y947
S1010	Q699	F760	T821	V888	L948
R1011	I700	E761	S822	A889	R949
I1012	E701	G762	M823	A890	H950
A1013	A704	I763	I824	F891	A951
A1014	R705	A764	Y825	R892	I952
P1015	R706	R765	I826	R893	E953
M1016	T707	D827	D827	V894	A954
I1017	V708	F767	A828	G895	V955
G1018	G709	I768	R829	E896	P956
G1019	V710	M769	D830	A897	S957
M1020	A711	L770	R831	L898	L958
I1021	S712	R771	D832	L899	M959
T1022	A713	Y772	M833	I900	N960
A1023	L714	F773	V837	S902	P961
P1024	A715	M774	H838	S903	T962
L1025	E716	T775	D839	V904	F964
L1026	R717	S776	L840	F905	S965
S1027	L718	R777	K841	F906	E966
L1028	L719	D778	K842	A907	Q967
F1029	G720	S779	A843	K908	K968
I1030	G721	F780	I844	L909	L969
I1031	R722	E781	A845	G910	D970
A1033	Y723	R784	E846	G911	E971
A1034	I724	Q785	K847	I912	A972
Y1035	N725	L786	V848	M913	L973
K1036	V726	F787	Q849	L914	Y974
L1038	E727	I788	L850	L915	H975
M1038	I728	L789	K851	M916	G976
TRP	M729	T790	P852	M917	A977
LEU	M730	F791	G853	G918	V978
ARG	K731	T854	T854	G919	L979
HIS	E732	F858	F858	H921	R980
HIS	A733	Q794	S859	L922	R982
ARG	Y736	I796	G860	S923	P983
ARG	G737	T797	Q861	V924	K984
VAL	M738	L798	F862	A925	A985
ARG	T739	A799	E863	T926	M986
LYS	V740	D800	L864	T927	T987
	A741	M801	L865	T928	V988
	D742	A802	G869	G929	A989
	V743	I803	M869	F930	V990
	K805	I804	L872	I931	I991
		A932		I992	I992

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.99Å 179.99Å 286.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.47 – 4.37 35.48 – 4.37	Depositor EDS
% Data completeness (in resolution range)	92.6 (35.47-4.37) 99.6 (35.48-4.37)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 4.44Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.268 , 0.321 0.282 , 0.349	Depositor DCC
$R_{free}$ test set	588 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	187.4	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 201.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	254.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: AG

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	0.38	0/7939	0.72	7/10805 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	5	ILE	CB-CA-C	10.48	132.56	111.60
1	A	659	ALA	N-CA-C	-9.78	84.59	111.00
1	A	6	ILE	N-CA-CB	-6.77	95.23	110.80
1	A	1023	ALA	C-N-CD	-6.07	107.25	120.60
1	A	220	SER	N-CA-C	5.96	127.09	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	5	ILE	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	GLY	Peptide

## 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	7784	0	8050	1486	0
2	A	1	0	0	0	0
All	All	7785	0	8050	1486	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 94.

The worst 5 of 1486 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:370:LEU:HD21	1:A:403:MET:SD	1.40	1.59
1:A:15:LEU:HD23	1:A:16:VAL:N	1.34	1.41
1:A:409:VAL:HB	1:A:450:LEU:CD1	1.57	1.32
1:A:821:THR:HG23	1:A:823:TRP:NE1	1.46	1.31
1:A:370:LEU:CD2	1:A:403:MET:SD	2.22	1.26

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	1008/1055 (96%)	752 (75%)	168 (17%)	88 (9%)	<b>1</b> <b>16</b>

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	36	VAL
1	A	54	PRO
1	A	131	PRO
1	A	139	ILE

### 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	834/872 (96%)	613 (74%)	221 (26%)	<b>0</b> <b>5</b>

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	PHE
1	A	599	VAL
1	A	946	MET
1	A	484	TYR
1	A	560	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	437	GLN
1	A	555	ASN
1	A	253	ASN
1	A	729	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [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<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	1014/1055 (96%)	-0.34	11 (1%) 80 73	127, 246, 387, 517	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1000	TRP	4.3
1	A	401	GLY	4.2
1	A	849	GLN	4.0
1	A	712	SER	2.8
1	A	26	TRP	2.8

### 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(Å <sup>2</sup> )	Q<0.9
2	AG	A	1048	1/1	0.95	0.19	-	271,271,271,271	0

## 6.5 Other polymers

There are no such residues in this entry.