



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:02 am BST

PDB ID : 3KSO  
Title : Structure and Mechanism of the Heavy Metal Transporter CusA  
Authors : Su, C.-C.  
Deposited on : 2009-11-23  
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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

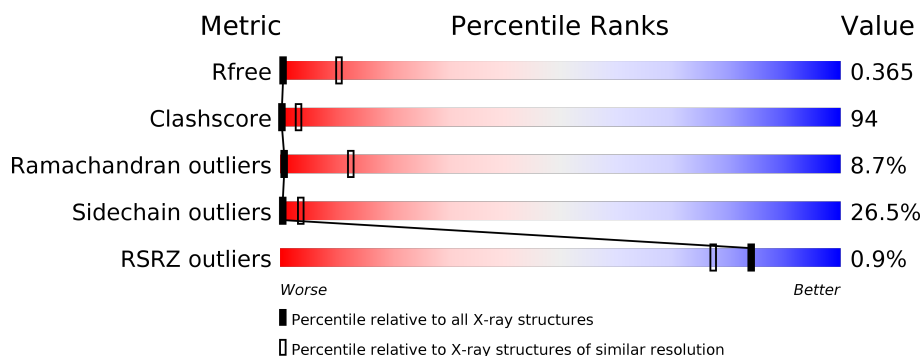
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1022 (4.92-3.80)
Clashscore	141614	1085 (4.92-3.80)
Ramachandran outliers	138981	1036 (4.92-3.80)
Sidechain outliers	138945	1019 (4.92-3.80)
RSRZ outliers	127900	1091 (5.02-3.70)

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 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	1055	<div> <div> <div></div> <div>18%</div> </div> <div> <div></div> <div>54%</div> </div> <div> <div></div> <div>23%</div> </div> <div> <div></div> <div>• •</div> </div> </div>

## 2 Entry composition

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
1	A	1014	Total	C	N	O	S	0	0	0
			7784	5031	1304	1413	36			

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

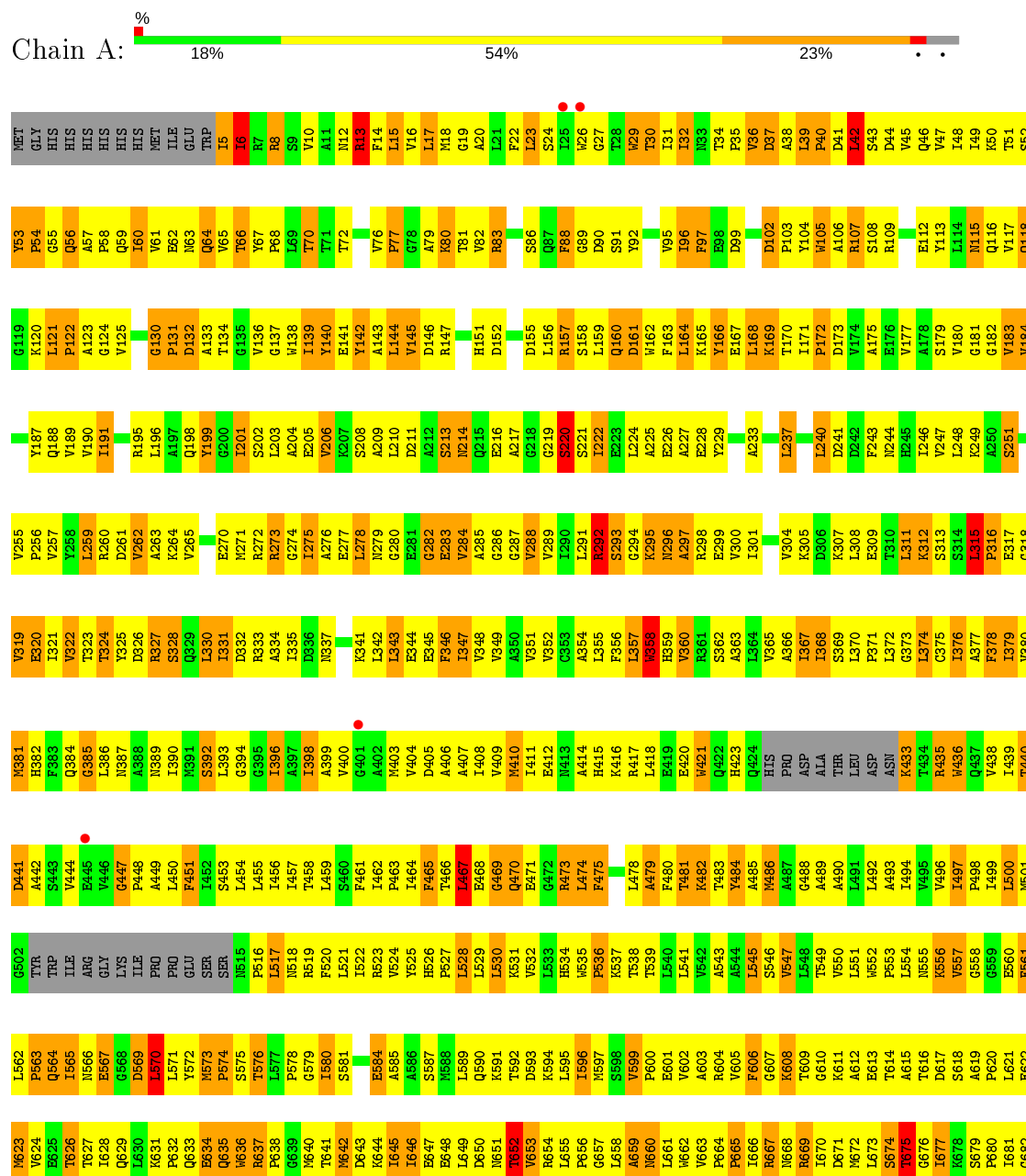
- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

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*



G994	I683	F746	S807	L874	A934	I684
L995	K684	Y747	T806	P875	G935	K685
L996	V685	T748	G809	W876	V936	V686
P997	S686	S749	F810	P877	A937	A750
I998	G687	A751	S811	W878	A938	T688
I999	A752	G752	W812	W879	E939	V689
W1000	L690	G753	L813	L880	F940	L691
G1001		A754	K814	W881	G941	
T1002	I693	A755	T815	L882	V942	I694
G1003	D694	W756	F816	L883	V943	D695
A1004	A695	V757	W817	F884	A944	A696
G1005	M696	E758	A818	W885	L945	M697
S1006	A697	T759	R819	L886	W946	A698
E1007	Q698	V760	F820	L887	Y947	Q699
W1008	E700	E761	T821	W888	L948	E701
M1009	I701	G762	W822	L889	R949	I702
S1010	A704	G763	W823	A890	H950	A705
R1011	A705	I764	I824	F891	A951	A706
T1012	A706	A764	W825	R892	I952	A707
A1013	T706	R765	L826	R893	E953	T707
A1014	F707	Y766	D827	W894	A954	F708
P1015	P707	P767	A828	G895	V955	P709
M1016	P708	I768	R829	E896	P956	P710
I1017	G709	N769	D830	A897	S957	G710
G1018	V710	L770	R831	L898	L958	V711
G1019	A711	R771	D832	L899	W959	A712
M1020	S712	Y772	R833	L900	N960	S713
T1021	A713	P773		I901	P961	A714
T1022	L714	Q774	W837	S902	Q962	L715
A1023	A715	S775	H838	T903	T963	A716
P1024	E716	W776	D839	W904	F964	E717
L1025	R716	R777	L840	P905	S965	R717
L1026	L718	D778	Q841	F906	E966	L719
S1027	E719	S779	R842	A907	Q967	E720
L1028	G720	P780	A843	L908	K968	G721
F1029	G721	Q781	I844	W909	L969	F1030
T1030	R722		A845	G910	D970	T1031
I1031	Y723	R784	E846	G911	E971	I1032
P1032	T724	Q785	R847	L912	A972	P1033
A1033	W725	L786	W848	W913	L973	A1034
A1034	N726	P787	Q849	L914	Y974	A1035
Y1035	E727	I788	L850	L915	H975	Y1036
K1036	I728	L789	K851	W916	G976	K1037
L1037	W729	T790	P852	W917	A977	L1038
TRP	M729	F791	G853	W918	V978	TRP
LEU	R730	M792	T854	G919	L979	LEU
HIS	K731	K793		F858	R980	HIS
ARG	K732	Q794	S859	W921	V981	ARG
HIS	A733	Q795	G860	L922	R982	HIS
ARG	Y736	T796	Q861	S923	P983	ARG
VAL	G737	T797	L862	W924	K984	VAL
ARG	M738	L798	E863	A925	A985	ARG
LYS	T739	D800	L864	T926	N986	LYS
	W740	W801	L865	G927	T987	
	A741	A802		T928	V988	
	D742	D803	W869	G929	A989	
	V743	I804		F930	V990	
	Q744	K805	L872	I931	I991	
	L745	V806	K873	L933	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)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.268 , 0.321 0.300 , 0.365	Depositor DCC
$R_{free}$ test set	588 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	187.4	Xtriage
Anisotropy	0.205	Xtriage
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>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	254.0	wwPDB-VP

Xtriage'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 ⓘ

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 ⓘ

### 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	1008/1055 (96%)	752 (75%)	168 (17%)	88 (9%)	<b>1</b> <b>12</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 ⓘ

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%)	0 4

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 ⓘ

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%)	-0.35	9 (0%) 84 77	127, 246, 387, 517	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1000	TRP	4.2
1	A	401	GLY	4.2
1	A	849	GLN	4.1
1	A	712	SER	2.8
1	A	26	TRP	2.7

### 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. 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	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 [i](#)

There are no such residues in this entry.