



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3KSS / pdb_00003kss
Title : Structure and Mechanism of the Heavy Metal Transporter CusA
Authors : Su, C.-C.
Deposited on : 2009-11-23
Resolution : 3.88 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

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

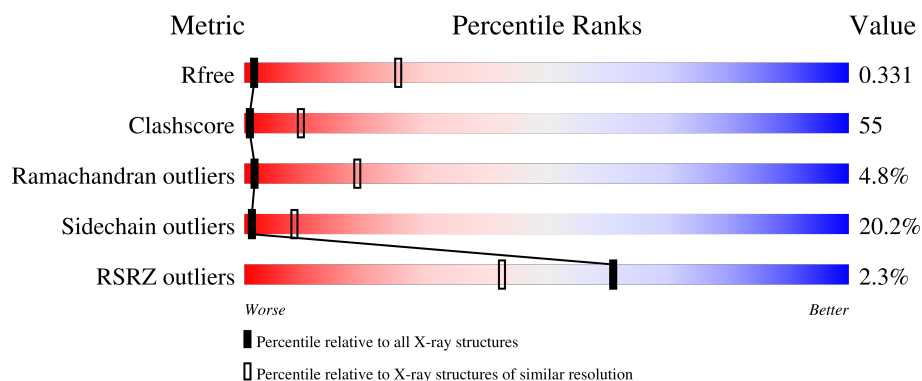
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.88 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	1186 (4.06-3.70)
Clashscore	190562	1012 (4.04-3.72)
Ramachandran outliers	187476	1167 (4.06-3.70)
Sidechain outliers	187428	1160 (4.06-3.70)
RSRZ outliers	180081	1185 (4.06-3.70)

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 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	1055	2% 32% 48% 15% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7803 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	1015	Total	C	N	O	S	0	0	0
			7802	5047	1305	1414	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 COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

W1039	A977	H917	R847	S775	L690
LEU	V978	M918	V848	S776	
HIS	R979	G919	Q849		T693
ARG	R980	F920	L850	S779	M696
HIS	V981	H921		P780	
ARG	R982	L922		Q781	Q699
VAL	P983	S923		A782	I700
ARG	K984	V924	G660	L783	E701
LYS	A985	A925	Q861	R784	E702
	M986	T926	F862	Q785	E703
	T987	T927	L864	L786	
	V988	T928	L865	P787	
	A989	G929	E866		T706
	V990	F930	R867	I788	V707
	I991	I931		L789	P708
	T992	A932	H870	T790	
		L933	K871	P791	E716
		A934	L872	M792	R717
		G935	K873	K793	L718
		V936	L874	Q794	E719
		A937	H875	Q795	
		E938	V876	I796	
		L939	P877		V726
			H878	D800	E727
			T879		I728
			L880	I804	N729
			H881	K805	E730
			L882		E731
			L883	G809	K732
			F884	P810	
			V885	S811	R735
			L886	M812	Y736
			L887	L813	Q737
			Y888	R814	
			L889	T815	V740
			F891	E816	
			I952	M817	L745
			E953	A818	F746
			A854	R819	V747
			V955	P820	T748
			P956	T821	
			S957	S822	A754
			L958	M823	M755
			N959	I824	V756
			L898	Y825	G757
			L899	I826	E758
			I900		T759
				R829	V760
				D830	E761
				P905	G762
				F906	I763
				A907	A764
				L908	R765
				V909	Y766
				G910	P767
				G911	I768
				I912	N769
				L913	L770
				L914	
				L915	P773
				Y974	Q774
				H975	
				E846	

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	180.36Å 180.36Å 287.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.28 – 3.88 35.28 – 3.88	Depositor EDS
% Data completeness (in resolution range)	92.7 (35.28-3.88) 98.2 (35.28-3.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.87Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.260 , 0.325 0.268 , 0.331	Depositor DCC
R_{free} test set	849 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	143.3	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 153.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: CU1

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	0.46	3/7960 (0.0%)	0.99	30/10834 (0.3%)

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	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	ALA	C-O	16.29	1.45	1.23
1	A	236	TYR	CA-C	-5.56	1.46	1.52
1	A	256	PRO	CA-C	-5.53	1.44	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	VAL	N-CA-CB	-26.37	82.86	111.87
1	A	254	GLY	N-CA-C	23.31	168.42	113.18
1	A	255	VAL	C-N-CD	-12.46	73.93	125.00
1	A	255	VAL	N-CA-C	12.15	122.74	109.01
1	A	254	GLY	CA-C-N	10.67	138.71	122.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	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	7802	0	8064	870	0
2	A	1	0	0	0	0
All	All	7803	0	8064	870	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 55.

The worst 5 of 870 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:530:LEU:CA	1:A:533:LEU:HD12	1.41	1.51
1:A:529:LEU:HD12	1:A:530:LEU:N	1.28	1.43
1:A:677:ILE:HG22	1:A:825:TYR:CE1	1.53	1.43
1:A:530:LEU:HA	1:A:533:LEU:CD1	1.48	1.41
1:A:572:TYR:CE1	1:A:574:PRO:HD3	1.66	1.29

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	1009/1055 (96%)	867 (86%)	94 (9%)	48 (5%)	2 19

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO
1	A	220	SER
1	A	254	GLY
1	A	256	PRO
1	A	283	GLU

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	835/872 (96%)	666 (80%)	169 (20%)	1 8

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	658	LEU
1	A	850	LEU
1	A	677	ILE
1	A	783	LEU
1	A	898	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	744	GLN
1	A	279	ASN
1	A	838	HIS
1	A	415	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 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, 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	1015/1055 (96%)	0.08	23 (2%)	61 42	75, 176, 334, 611	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	GLU	4.5
1	A	370	LEU	3.4
1	A	776	TRP	2.9
1	A	938	ALA	2.9
1	A	386	LEU	2.9

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	CU1	A	1048	1/1	0.98	0.07	124,124,124,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.