



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:51 AM GMT

PDB ID : 3K0I
Title : Crystal structure of Cu(I)CusA
Authors : Su, C.-C.
Deposited on : 2009-09-24
Resolution : 4.12 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

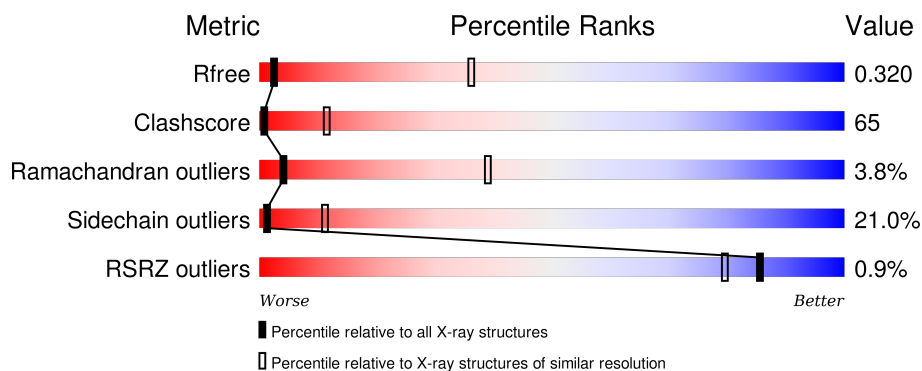
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.12 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	1020 (4.62-3.60)
Clashscore	102246	1119 (4.62-3.60)
Ramachandran outliers	100387	1065 (4.62-3.60)
Sidechain outliers	100360	1051 (4.62-3.60)
RSRZ outliers	91569	1024 (4.62-3.60)

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 ≥ 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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7804 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

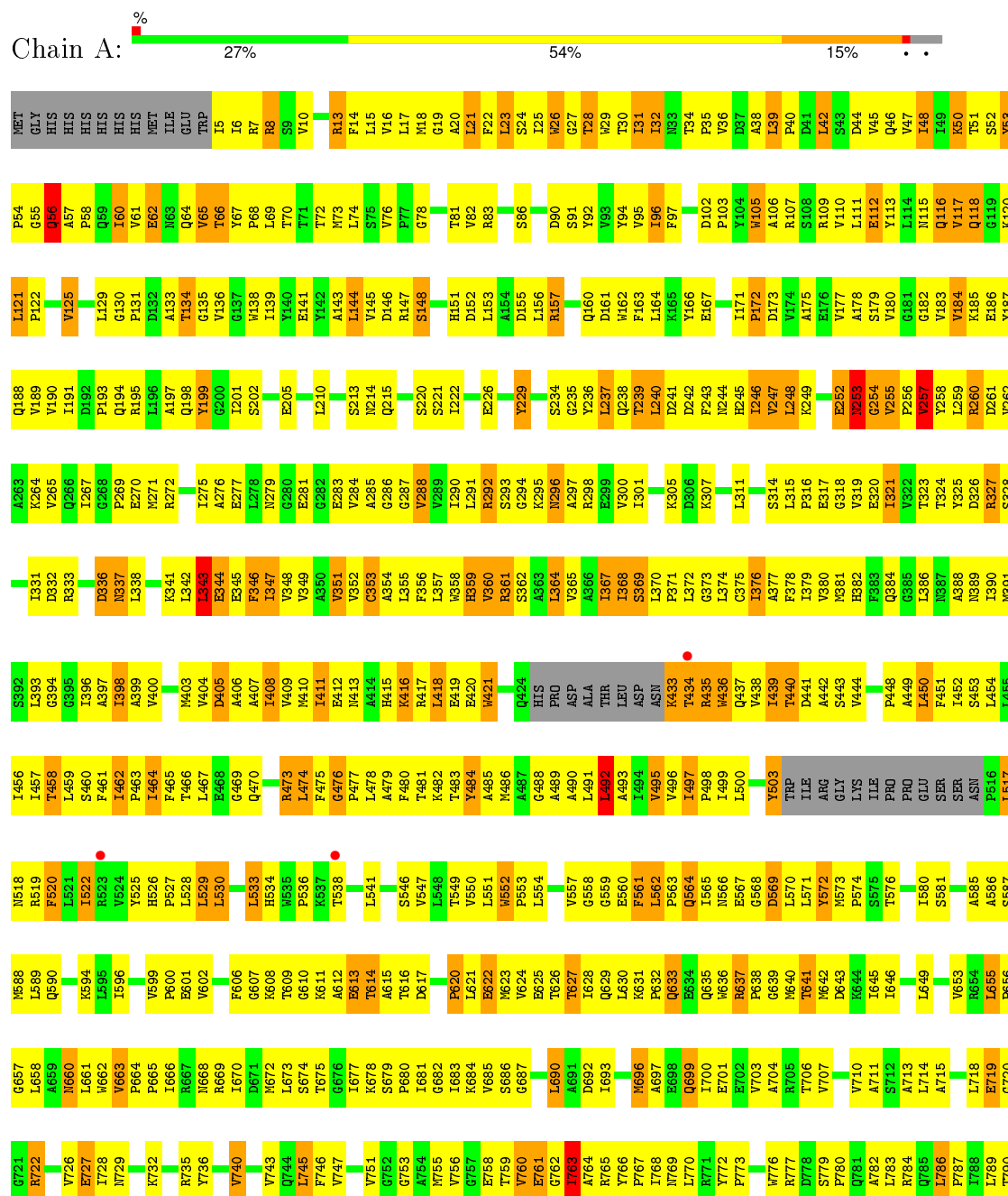
- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

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 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 ($RSRZ > 2$). 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*



K984	A985	V986	T987	V988	A989	V990	I991	I992	A993	G994	L995	L996	P997	I998	L999	G1000	G1001	T1002	S1006	S1010	R1011	I1012	A1013	A1014	P1015	M1016	I1017	G1018	G1019	M1020	I1021	T1022	A1023	P1024	L1025	L1026	S1027	L1028	F1029	I1030	I1031	P1032	A1033	A1034	F1039	I1039	HIS	ARG	HIS	ARG	VAL	ARG	LYS			
L922	S923	V924	A925	T926	G927	T928	G929	F930	I931	A932	L933	A934	G935	V936	E939	F940	G941	V942	M944	L945	M946	Y947	L948	R949	H950	A951	I952	E953	A954	V955	P956	S957	L958	M959	M960	P961	F964	S965	E966	Q967	K968	L969	D970	E971	A972	L973	Y974	H975	G976	A977	V978	L979	R980	V981	P982	P983
G860	Q861	F862	E863	L864	L865	E866	R867	H870	K871	A802	D803	I804	K805	T808	G809	P810	S811	M812	K814	T815	E816	N817	A818	R819	P820	T821	S822	M823	I824	Y825	I826	D827	A828	R829	D830	R831	D832	M833	V837	H838	D839	L840	Q841	K842	A843	I844	K847	V848	Q849	L850	K851	T854	S859			
P791	M792	K793	Q794	Q795	I796	T797	D800	V801	A802	D803	I804	K805	T808	G809	P810	S811	M812	K814	T815	E816	N817	A818	R819	P820	T821	S822	M823	I824	Y825	I826	D827	A828	R829	D830	R831	D832	M833	V837	H838	D839	L840	Q841	K842	A843	I844	K847	V848	Q849	L850	K851	T854	S859				

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	179.26 Å 179.26 Å 286.27 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.46 – 4.12 38.46 – 4.12	Depositor EDS
% Data completeness (in resolution range)	91.3 (38.46-4.12) 98.3 (38.46-4.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 4.13 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.269 , 0.308 0.268 , 0.320	Depositor DCC
R_{free} test set	679 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	132.4	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 125.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 13739 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7804	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	2/7960 (0.0%)	0.63	13/10834 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	GLY	N-CA	-8.21	1.33	1.46
1	A	254	GLY	CA-C	-7.40	1.40	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	VAL	C-N-CD	-13.31	91.33	120.60
1	A	253	ASN	O-C-N	9.21	138.86	123.20
1	A	253	ASN	CA-C-N	-8.68	98.85	116.20
1	A	257	VAL	O-C-N	8.29	135.97	122.70
1	A	257	VAL	CA-C-N	-8.14	99.28	117.20

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	A	7802	0	8064	1031	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
All	All	7804	0	8064	1031	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 65.

The worst 5 of 1031 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:669:ARG:NH2	1:A:672:MET:HB2	1.48	1.26
1:A:249:LYS:HB3	1:A:257:VAL:CG2	1.65	1.25
1:A:573:MET:CE	1:A:668:ASN:HD21	1.52	1.22
1:A:249:LYS:HB3	1:A:257:VAL:HG21	1.29	1.11
1:A:62:GLU:HA	1:A:66:THR:HG23	1.26	1.10

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%)	868 (86%)	103 (10%)	38 (4%)	4 39

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	148	SER
1	A	238	GLN
1	A	256	PRO
1	A	640	MET

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	835/872 (96%)	660 (79%)	175 (21%)	1 11

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	435	ARG
1	A	520	PHE
1	A	967	GLN
1	A	439	ILE
1	A	473	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	ASN
1	A	384	GLN
1	A	699	GLN
1	A	279	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 ⓘ

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 2 ligands modelled in this entry, 2 are 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, 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%)	-0.29	9 (0%) 85 79	58, 169, 341, 564	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	849	GLN	4.1
1	A	523	ARG	3.9
1	A	434	THR	3.6
1	A	827	ASP	3.1
1	A	866	GLU	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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CU1	A	1048	1/1	0.88	0.14	-	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CU1	A	1049	1/1	0.76	0.27	-	197,197,197,197	0

6.5 Other polymers [i](#)

There are no such residues in this entry.