



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 06:44 am BST

PDB ID : 3K07  
Title : Crystal structure of CusA  
Authors : Su, C.-C.  
Deposited on : 2009-09-24  
Resolution : 3.52 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

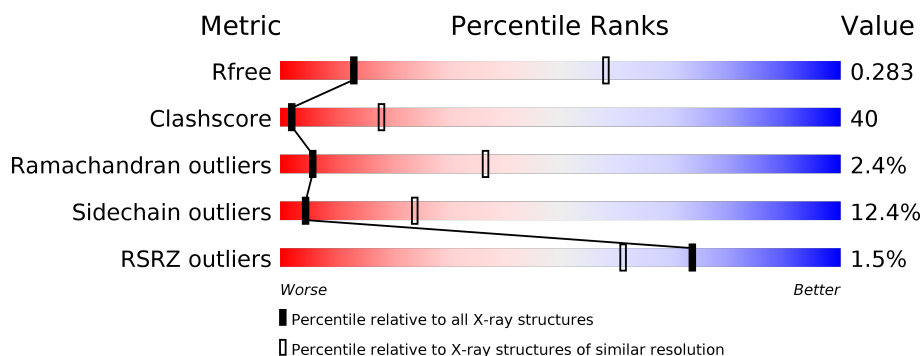
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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></div> <div>39%</div> <div>50%</div> <div>8%</div> <div></div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7885 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 csaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1025	Total	C	N	O	S	0	0	0
			7885	5100	1319	1430	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



I1012	I1013	A1014	P1015	M1016	I1017	G1018	G1019	M1020	T1022	A1023	P1024	L1025	L1026	S1027	L1028	F1029	I1030	I1031	P1032	A1033	A1034	Y1035	K1036	L1037	M1038	M1039	L1040	HIS	ARG	HIS	ARG	VAL	ARG	LYS																						
I945	M946	Y947	I948	R949	I952	E953	A954	V955	P956	S957	L958	M959	M960	P961	Q962	T963	F964	S965	E966	Q967	K968	L969	A972	L973	Y974	H975	G976	A977	V978	L979	R980	V981	R982	P983	K984	A885	M986	T987	V988	A989	V990	I991	I992	A993	G994	L995	L996	P997	I998	L999	H1000	G1001	V1008	M1009	S1010	R1011
L874	M875	P876	P877	M878	T879	L880	R881	I882	I883	L886	L887	R889	R892	R893	V894	G895	E896	A897	I900	I901	S902	S903	V904	P905	F906	H907	L908	V909	I912	M913	L914	L915	M916	M917	M918	H921	L922	S923	V924	A925	F930	I931	A932	L933	V936	A937	A938	E939	F940	G941	V942	V943	M944			
Q794	Q795	I796	T797	D800	I804	K805	V806	S807	P810	I813	K814	T821	S822	W823	I824	A828	R831	D832	M833	V834	S835	S749	V836	V837	L840	Q841	K842	A843	I844	A845	E846	K847	V848	Q849	L850	K851	P852	F858	Q861	L864	L865	E866	R867	A868	M869	H870	K871	L872	K873							
G709	V710	L714	A715	E716	R717	L718	I724	N725	V726	E727	I728	N729	K732	R735	Y736	T739	V740	A741	F746	V747	T748	S749	A750	V836	V837	G753	A754	M755	V756	N769	L770	R771	Y772	P773	Q774	R777	D778	S779	P780	Q781	A782	L783	R784	Q785	L786	P787	I788	L789	T790	P791	M792	K793				

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.39 Å   178.39 Å   285.76 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	37.28 – 3.52 37.28 – 3.52	Depositor EDS
% Data completeness (in resolution range)	92.8 (37.28-3.52) 98.1 (37.28-3.52)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 3.56 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.237   ,   0.279 0.248   ,   0.283	Depositor DCC
$R_{free}$ test set	1099 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	128.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29   ,   131.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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](#)

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	0.32	0/8048	0.52	4/10959 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	PRO	N-CA-C	6.72	129.58	112.10
1	A	517	LEU	N-CA-C	-6.14	94.41	111.00
1	A	26	TRP	CA-CB-CG	6.05	125.19	113.70
1	A	659	ALA	N-CA-C	-5.46	96.27	111.00

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	7885	0	8137	647	0
All	All	7885	0	8137	647	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 40.

The worst 5 of 647 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:516:PRO:HG2	1:A:517:LEU:CD1	1.52	1.38
1:A:523:ARG:O	1:A:527:PRO:HD3	1.27	1.25
1:A:26:TRP:CZ3	1:A:30:THR:HG21	1.80	1.16
1:A:517:LEU:H	1:A:517:LEU:CD1	1.56	1.15
1:A:26:TRP:CZ3	1:A:30:THR:CG2	2.30	1.15

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	1021/1055 (97%)	891 (87%)	105 (10%)	25 (2%)	6	36

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	PRO
1	A	148	SER
1	A	172	PRO
1	A	425	HIS
1	A	469	GLY

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	844/872 (97%)	739 (88%)	105 (12%)	4 24

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	530	LEU
1	A	595	LEU
1	A	962	GLN
1	A	531	LYS
1	A	576	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	ASN
1	A	470	GLN
1	A	959	ASN
1	A	415	HIS
1	A	526	HIS

### 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 ⓘ

There are no ligands in this entry.

## 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	1025/1055 (97%)	-0.24	15 (1%)	73 61	63, 144, 233, 364	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	THR	5.6
1	A	428	ALA	5.3
1	A	427	ASP	5.0
1	A	526	HIS	3.9
1	A	405	ASP	3.7

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.