



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:06 PM UTC

PDB ID : 3K07 / pdb_00003k07
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

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

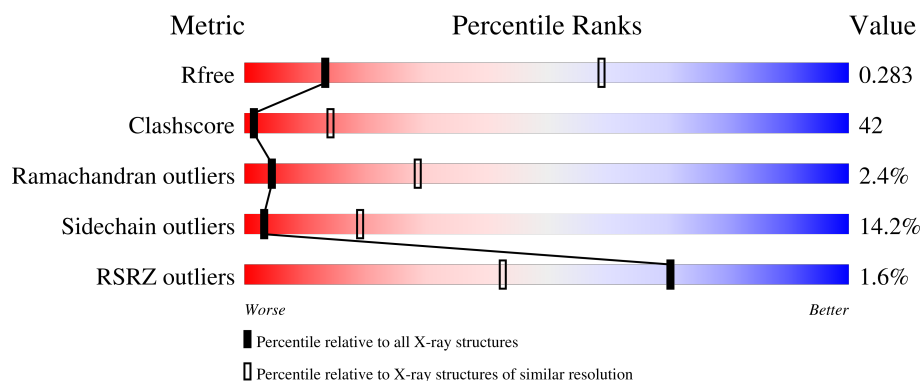
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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% 37% 49% 10% ••

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 cusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1025	Total	C	N	O	S	0	0	0
			7885	5100	1319	1430	36			

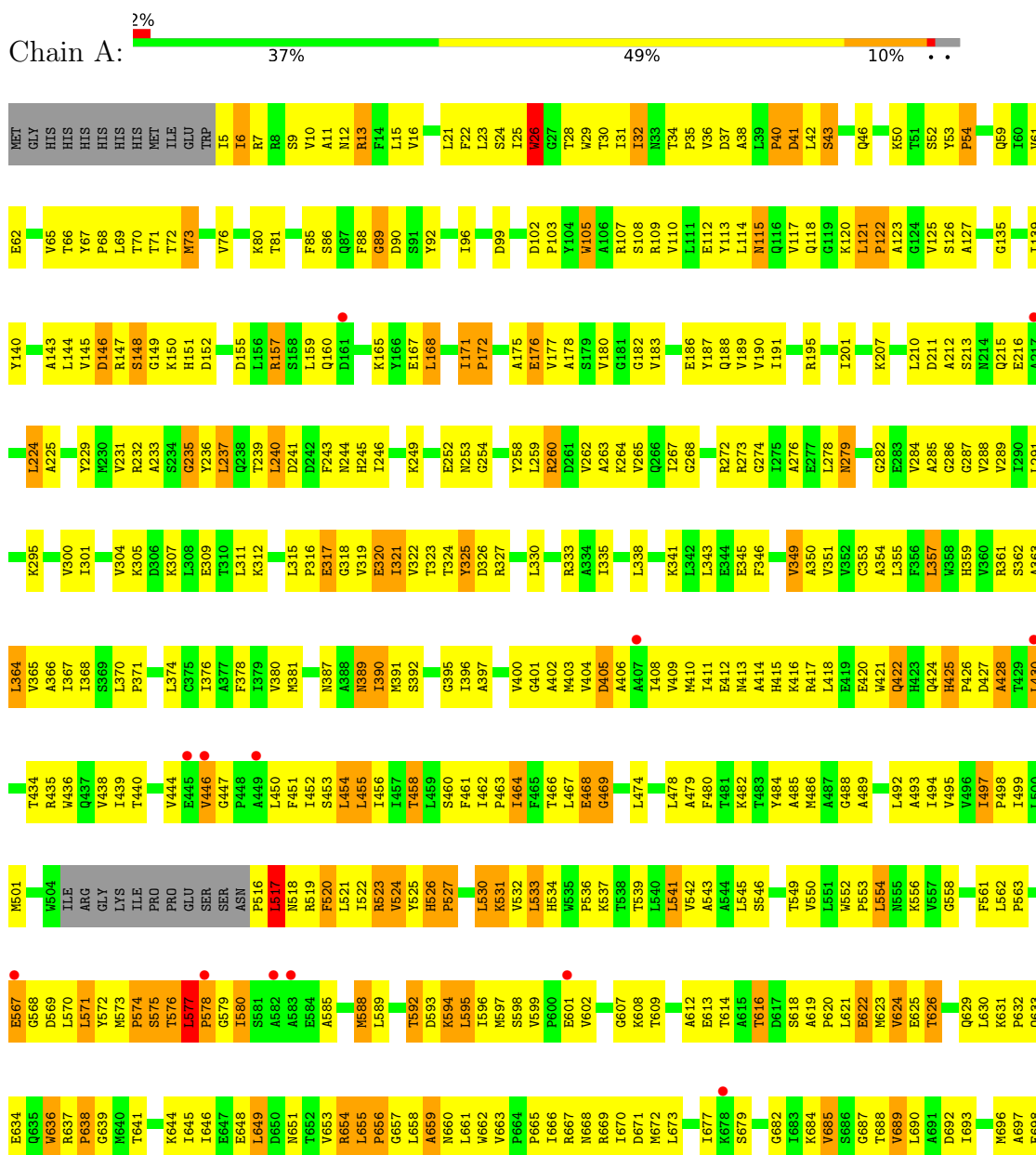
There are 8 discrepancies between the modelled and reference sequences:

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 csaA



I992	A993	G994	L995	L996	P997	I998	L999	W1000	G1001	V1008	M1009	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	Y1035	K1036	L1037	M1038	V1039	L1040	HIS	ARG	HIS	HIS	ARG	ARG	VAL	ARG	ARG	LYS								
F930	I931	A932	L933			V936	A937	A938	E939	F940	G941	V942	V943	V944	V945	V946	V947	L948	R949		I952	E953	A954	V955	P956	S957	L958	V959	N960	P961	Q962	T963	E964	S965	E966	Q967	K968	L969		A972	L973	V974	H975	G976	A977	V978	V979	R980	V981	R982	P983	K984	A985	V986	T987	V988	A989	V990	I991	
Q861		L864	L865	E866		R867	A868	R869	H870	K871	L872	K873	L874	H875	V876	P877	H878	T879	L880	R881	L882	L883		L886	L887	T888	L889		R892	R893	V894	G895	E896	A897		I900	R901	S902	S903	V904	P905	F906	A907	L908	V909		I912	V913	L914	L915	V916	V917	V918		H921	L922	S923	V924	A925	
K782	L783	K784	Q785	L786	P787	V788	L789	T790	P791	M792	K793	Q794	V795	T796	T797		D800		T804	K805	V806	S807		P810		L813	K814		T821	S822	K823	L824		A828		R831	D832	V833	V834	S835	V836	V837	H838	D839	L840	Q841	K842		I844	K845	E846	K847	V848		D849	L850	K851	P852		F858
Q699	I700	E701		V703		V707	P708	G709	V710		L714	A715	E716	R717	L718		I724	N725	V726	E727	N728	N729		K732		R735	V736	G737	M738	T739	V740	A741		L745	F746	V747	T748	S749	A750		G753	A754	M755	V756		I763		N769	L770	R771	V772	P773	Q774		R777	D778	S779	P780	Q781	

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	178.39Å 178.39Å 285.76Å 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) 97.9 (37.28-3.52)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.237 , 0.279 (Not available) , 0.283	Depositor DCC
R_{free} test set	1099 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	128.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 127.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7885	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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](#)

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	0.45	0/8048	0.92	30/10959 (0.3%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	LEU	N-CA-C	-15.47	94.41	111.28
1	A	578	PRO	N-CA-C	11.27	129.58	113.47
1	A	577	LEU	CA-C-N	10.81	130.21	118.97
1	A	577	LEU	C-N-CA	10.81	130.21	118.97
1	A	954	ALA	N-CA-C	9.67	121.59	111.14

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	679	0
All	All	7885	0	8137	679	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 42.

The worst 5 of 679 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:CD1	1:A:517:LEU:H	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%)	4 29

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%)	724 (86%)	120 (14%)	3 19

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	LEU
1	A	967	GLN
1	A	634	GLU
1	A	962	GLN
1	A	1031	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	GLN
1	A	635	GLN
1	A	921	HIS
1	A	555	ASN
1	A	668	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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	1025/1055 (97%)	-0.05	16 (1%) 70 43	63, 144, 233, 364	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	ALA	4.5
1	A	407	ALA	3.6
1	A	678	LYS	3.1
1	A	445	GLU	2.7
1	A	718	LEU	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 oligosaccharides 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.