



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:18 PM UTC

PDB ID : 4K0E / pdb_00004k0e
Title : X-ray crystal structure of a heavy metal efflux pump, crystal form II
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Deposited on : 2013-04-03
Resolution : 3.71 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

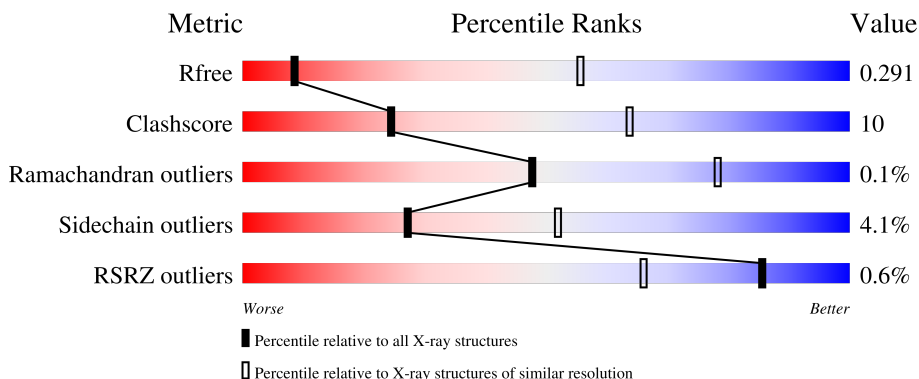
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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 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	1045	 68% 25% • 7%
1	B	1045	 67% 23% • 8%
1	C	1045	 68% 21% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22061 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 Heavy metal cation tricomponent efflux pump ZneA(CzcA-like).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	977	Total	C	N	O	S	0	0	0
			7489	4809	1303	1345	32			
1	B	957	Total	C	N	O	S	0	0	0
			7329	4710	1271	1317	31			
1	C	942	Total	C	N	O	S	0	0	0
			7239	4644	1261	1302	32			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	HIS	-	expression tag	UNP Q1LCD8
A	1041	HIS	-	expression tag	UNP Q1LCD8
A	1042	HIS	-	expression tag	UNP Q1LCD8
A	1043	HIS	-	expression tag	UNP Q1LCD8
A	1044	HIS	-	expression tag	UNP Q1LCD8
A	1045	HIS	-	expression tag	UNP Q1LCD8
B	1040	HIS	-	expression tag	UNP Q1LCD8
B	1041	HIS	-	expression tag	UNP Q1LCD8
B	1042	HIS	-	expression tag	UNP Q1LCD8
B	1043	HIS	-	expression tag	UNP Q1LCD8
B	1044	HIS	-	expression tag	UNP Q1LCD8
B	1045	HIS	-	expression tag	UNP Q1LCD8
C	1040	HIS	-	expression tag	UNP Q1LCD8
C	1041	HIS	-	expression tag	UNP Q1LCD8
C	1042	HIS	-	expression tag	UNP Q1LCD8
C	1043	HIS	-	expression tag	UNP Q1LCD8
C	1044	HIS	-	expression tag	UNP Q1LCD8
C	1045	HIS	-	expression tag	UNP Q1LCD8

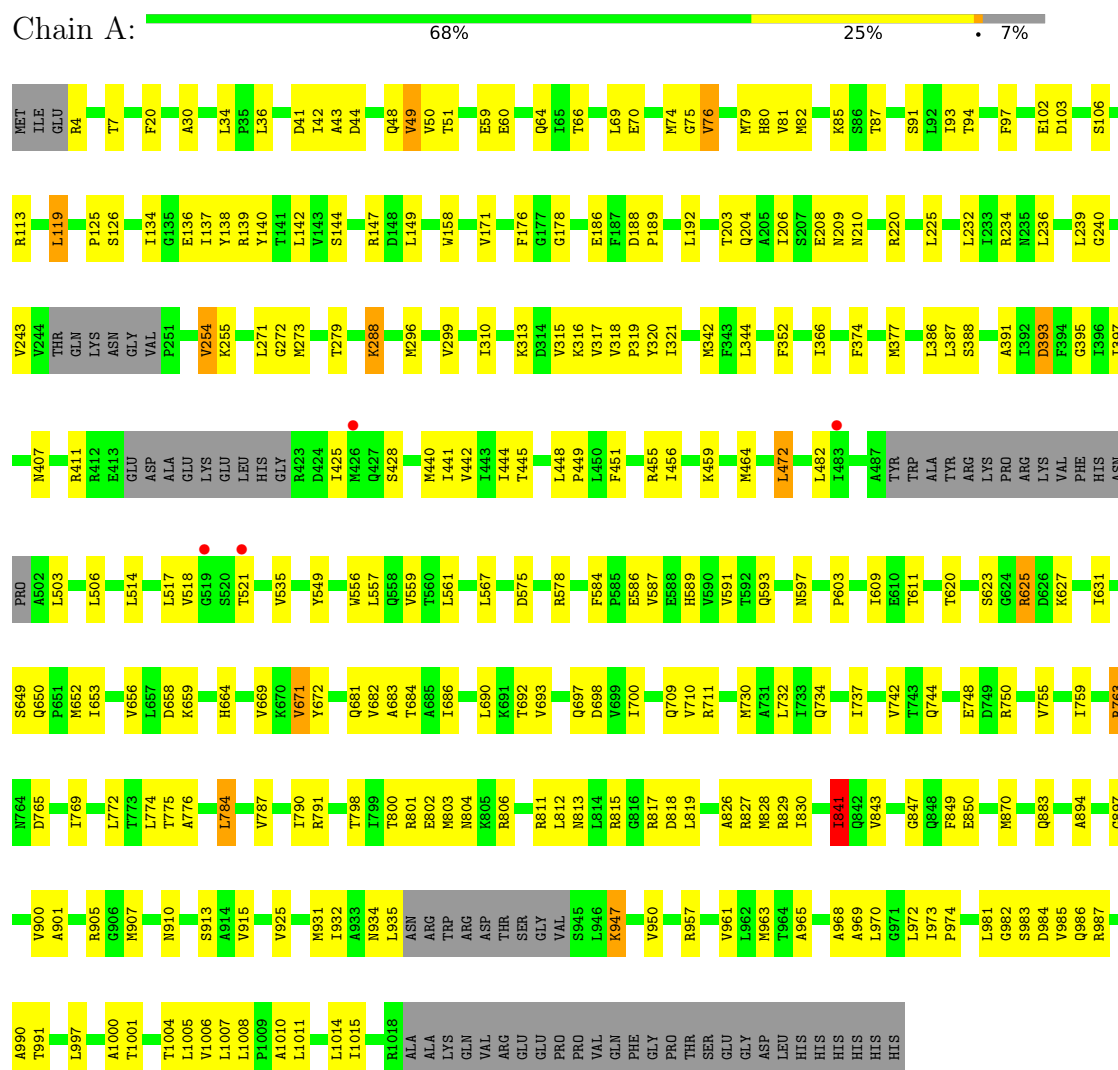
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0

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: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

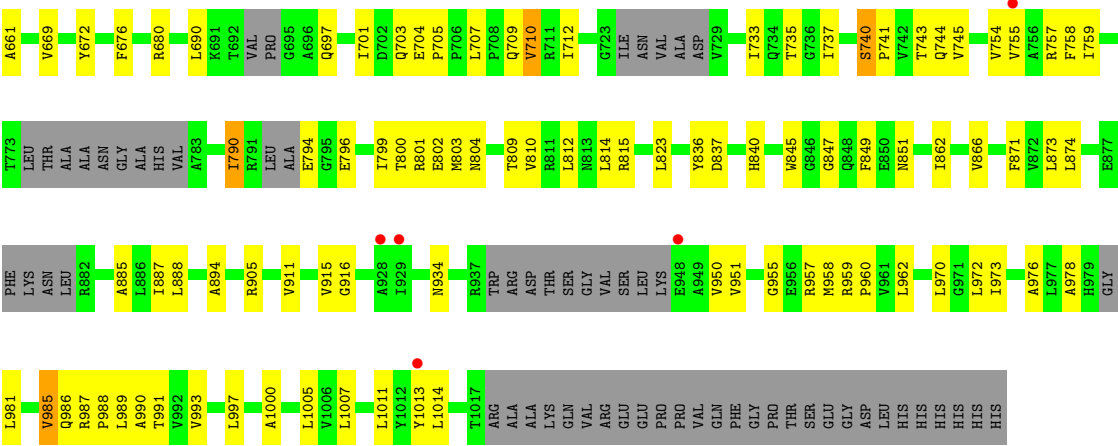


- Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)





A487	TYR	I375	VAL	I114	MET
TRP	ALA	N385	THR	P120	ILE
ALA	TYR	L386	LYS	I121	GLU
ARG	ALA	L387	ASN	S126	R4
LYS	LYS	S388	GLY	L127	C9
PRO	PRO	A391	VAL	D128	R12
ARG	ARG	I392	VAL	P129	I15
LYS	LYS	D393	LEU	L130	V16
PHE	VAL	I396	VAL	R139	F20
HIS	HIS	A401	LYS	Y140	Y26
ASN	ASN	N407	ASP	R147	L34
PRO	PRO	E413	G258	D148	P35
ALA	ALA	GLU	V260	L149	L36
L503	L503	ASP	I270	R150	A43
R509	R509	ASP	L271	E151	T46
Y510	Y510	ALA	M273	P162	S47
V513	V513	GLU	D274	Q166	Q48
L514	L514	LYS	T279	V170	V49
L517	L517	GLU	L280	V171	G55
T521	T521	LEU	Q281	G178	V61
V535	V535	GLY	G282	L179	B62
F546	F546	R423	K288	F183	T66
L547	L547	D434	N307	E186	E70
D551	D551	I425	D308	F187	V76
P563	P563	V432	N309	T202	R81
G564	G564	I436	I310	T203	R82
L567	L567	F437	D314	I206	S84
A570	A570	F438	V315	N210	S86
R578	R578	G439	K316	N212	L90
F584	F584	M440	V317	A213	I93
P585	P585	I441	I321	G214	V96
V594	V594	V442	V327	G215	F97
I609	I609	L448	D328	L218	E102
D626	D626	P449	A329	G231	D103
Q650	Q650	A452	T336	L232	R107
I653	I653	R455	V331	V226	Q111
V656	V656	K459	L349	V227	E112
G660	G660	M464	S365	R228	R13
L663	L663	L476	P366	G229	
V666	V666	L482	V362	V230	
G669	G669		T365	L241	
			L368	ILE	
				VAL	



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.34Å 127.07Å 163.33Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	19.94 – 3.71 19.94 – 3.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.94-3.71) 84.9 (19.94-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.229 , 0.283 0.240 , 0.291	Depositor DCC
R_{free} test set	2162 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.018 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22061	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: ZN

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	0.34	0/7618	0.80	5/10362 (0.0%)
1	B	0.33	0/7457	0.79	8/10146 (0.1%)
1	C	0.31	0/7358	0.78	5/9996 (0.1%)
All	All	0.33	0/22433	0.79	18/30504 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	LEU	CA-C-N	-7.16	114.42	121.65
1	C	448	LEU	C-N-CA	-7.16	114.42	121.65
1	A	119	LEU	CA-C-N	5.88	127.19	119.84
1	A	119	LEU	C-N-CA	5.88	127.19	119.84
1	B	90	LEU	N-CA-C	5.70	117.13	108.07

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	7489	0	7783	167	0
1	B	7329	0	7597	155	0
1	C	7239	0	7499	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	22061	0	22879	446	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 10.

The worst 5 of 446 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:70:GLU:HA	1:A:82:MET:HE1	1.63	0.80
1:A:984:ASP:HB3	1:A:987:ARG:HE	1.51	0.75
1:B:623:SER:OG	1:B:624:GLY:N	2.15	0.75
1:C:735:THR:HA	1:C:740:SER:HB3	1.71	0.73
1:B:978:ALA:HA	1:B:987:ARG:HE	1.55	0.71

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	967/1045 (92%)	909 (94%)	57 (6%)	1 (0%)	48	78
1	B	945/1045 (90%)	882 (93%)	61 (6%)	2 (0%)	43	71
1	C	920/1045 (88%)	855 (93%)	64 (7%)	1 (0%)	48	78
All	All	2832/3135 (90%)	2646 (93%)	182 (6%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	VAL
1	B	542	ILE
1	A	841	ILE
1	C	171	VAL

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	805/864 (93%)	776 (96%)	29 (4%)	31	54
1	B	785/864 (91%)	748 (95%)	37 (5%)	23	48
1	C	778/864 (90%)	748 (96%)	30 (4%)	28	52
All	All	2368/2592 (91%)	2272 (96%)	96 (4%)	27	52

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	784	LEU
1	C	102	GLU
1	B	808	LEU
1	B	977	LEU
1	C	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	597	ASN
1	B	842	GLN
1	C	852	GLN
1	C	650	GLN
1	B	616	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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	977/1045 (93%)	-0.21	4 (0%) 88 72	59, 104, 178, 228	0
1	B	957/1045 (91%)	-0.19	2 (0%) 91 80	61, 109, 168, 213	0
1	C	942/1045 (90%)	0.02	12 (1%) 75 50	78, 140, 198, 251	0
All	All	2876/3135 (91%)	-0.13	18 (0%) 85 66	59, 118, 187, 251	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	928	ALA	4.3
1	C	120	PRO	3.3
1	A	519	GLY	3.1
1	C	401	ALA	2.7
1	C	1013	TYR	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](#)

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($\text{\AA}^2$)	Q<0.9
2	ZN	A	1102	1/1	0.96	0.06	138,138,138,138	0
2	ZN	C	1101	1/1	0.97	0.10	151,151,151,151	0
2	ZN	B	1101	1/1	0.98	0.04	99,99,99,99	0
2	ZN	A	1101	1/1	0.98	0.07	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.