



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:59 pm BST

PDB ID : 2PS3  
Title : Structure and metal binding properties of ZnuA, a periplasmic zinc transporter from *Escherichia coli*  
Authors : Yatsunyk, L.A.; Kim, L.R.; Vorontsov, I.I.; Rosenzweig, A.C.  
Deposited on : 2007-05-04  
Resolution : 2.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

---

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

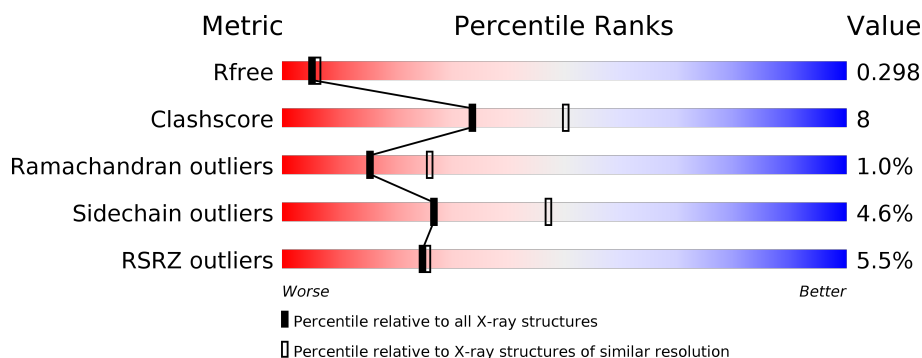
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	284	
1	B	284	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4115 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 High-affinity zinc uptake system protein znuA.

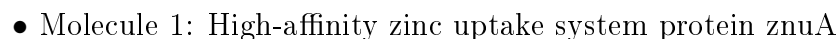
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	3	0	0
			2038	1299	347	384	8			
1	B	264	Total	C	N	O	S	0	0	0
			2028	1293	344	383	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total	O	0	0
			28	28		
2	B	21	Total	O	0	0
			21	21		



- Molecule 1: High-affinity zinc uptake system protein *znuA*



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.88Å 89.84Å 91.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.10 – 2.47 35.10 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.10-2.47) 98.0 (35.10-2.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.240 , 0.303 0.236 , 0.298	Depositor DCC
$R_{free}$ test set	1068 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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	0.55	1/2081 (0.0%)	0.64	2/2820 (0.1%)
1	B	0.50	0/2070	0.61	0/2805
All	All	0.53	1/4151 (0.0%)	0.63	2/5625 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	GLU	CG-CD	-6.18	1.42	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASN	C-N-CD	-5.66	108.15	120.60
1	A	228	ASN	N-CA-C	5.08	124.73	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	2038	0	2043	29	0
1	B	2028	0	2036	42	0
2	A	28	0	0	4	0
2	B	21	0	0	1	0
All	All	4115	0	4079	69	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 8.

All (69) 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:229:PRO:HB2	1:A:259:PHE:HA	1.42	1.02
1:B:229:PRO:O	1:B:259:PHE:HB2	1.62	0.99
1:B:64:LEU:H	1:B:64:LEU:HD12	1.24	0.99
1:A:61:ASP:O	1:B:66:PRO:HD2	1.64	0.94
1:B:64:LEU:CD1	1:B:64:LEU:H	1.87	0.87
1:B:258:GLN:HG2	1:B:259:PHE:N	2.01	0.74
1:B:159:HIS:HE1	1:B:174:ASP:OD1	1.72	0.72
1:B:238:LEU:HD21	1:B:266:SER:HB3	1.73	0.71
1:B:64:LEU:N	1:B:64:LEU:HD12	2.03	0.70
1:B:241:ILE:CG2	1:B:267:VAL:HG11	2.27	0.65
1:A:34:PRO:HA	1:A:37:PHE:CD2	2.34	0.63
1:A:229:PRO:HB3	1:A:259:PHE:CD1	2.33	0.63
1:A:171:ALA:O	2:A:318:HOH:O	2.15	0.62
1:A:285:ILE:HD13	1:A:295:PHE:HA	1.82	0.60
1:A:229:PRO:CB	1:A:259:PHE:HA	2.24	0.60
1:A:59:GLU:HG3	1:A:85:MET:SD	2.42	0.59
1:B:159:HIS:CE1	1:B:174:ASP:OD1	2.53	0.58
1:A:165:LEU:O	1:A:167:PRO:HD3	2.04	0.58
1:A:229:PRO:HB3	1:A:259:PHE:CG	2.40	0.57
1:B:34:PRO:HA	1:B:37:PHE:CD2	2.41	0.55
1:B:225:PHE:CD1	1:B:241:ILE:HD12	2.42	0.55
1:B:230:GLU:O	1:B:260:ARG:HB2	2.08	0.53
1:B:233:PRO:HD3	1:B:263:VAL:HG13	1.91	0.52
1:B:241:ILE:HG22	1:B:267:VAL:HG11	1.91	0.52
1:A:236:GLN:NE2	2:A:330:HOH:O	2.43	0.51
1:B:228:ASN:HD22	1:B:230:GLU:H	1.59	0.51
1:B:147:SER:HB2	1:B:212:TYR:HB3	1.93	0.51
1:A:196:ALA:N	1:A:197:PRO:HD2	2.26	0.50
1:B:237:ARG:O	1:B:241:ILE:HG12	2.12	0.50
1:B:29:VAL:HG11	1:B:72:LEU:HD12	1.94	0.50
1:A:116:LYS:O	1:A:117:SER:HB3	2.10	0.49
1:B:228:ASN:H	1:B:229:PRO:HA	1.78	0.49
1:A:200:GLY:H	1:A:220:THR:HG21	1.77	0.48
1:B:144:LEU:HB3	1:B:150:ILE:HG21	1.97	0.47
1:A:115:MET:HB2	1:A:212:TYR:CE2	2.50	0.47
1:A:61:ASP:O	1:B:65:ARG:HB2	2.14	0.47
1:B:80:TRP:CE2	1:B:93:VAL:HG11	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG12	1:A:228:ASN:H	1.80	0.47
1:B:169:SER:O	1:B:170:ARG:C	2.52	0.47
1:A:37:PHE:CD1	1:A:291:SER:HB2	2.50	0.46
1:B:227:VAL:HB	1:B:228:ASN:H	1.53	0.46
1:B:104:ILE:HG12	1:B:154:THR:HG23	1.98	0.46
1:B:241:ILE:HG21	1:B:267:VAL:HG11	1.97	0.46
1:A:101:GLN:O	1:A:161:LYS:NZ	2.49	0.46
1:A:225:PHE:HE1	1:A:244:GLN:OE1	1.99	0.46
1:B:233:PRO:CD	1:B:263:VAL:HG13	2.46	0.45
1:A:31:SER:OG	1:A:32:LEU:HG	2.17	0.45
1:B:263:VAL:O	1:B:266:SER:HB2	2.17	0.44
1:B:101:GLN:NE2	1:B:103:THR:OG1	2.51	0.44
1:B:91:LYS:HB2	1:B:92:PRO:CD	2.47	0.43
1:A:195:LEU:HD13	1:A:219:LEU:HD22	2.01	0.43
1:A:265:GLU:HA	1:A:275:MET:SD	2.59	0.43
1:B:81:VAL:HG13	1:B:144:LEU:HD12	2.00	0.43
1:B:198:LEU:HD11	1:B:304:ALA:HA	2.00	0.43
1:B:33:LYS:HE3	1:B:285:ILE:O	2.19	0.43
1:A:200:GLY:H	1:A:220:THR:CG2	2.32	0.42
1:B:284:ASN:HD22	1:B:298:GLN:NE2	2.17	0.42
1:A:147:SER:HB2	1:A:212:TYR:HB3	2.01	0.42
1:A:207:HIS:CE1	1:A:209:ALA:HB2	2.55	0.42
1:B:141:ASN:HD22	1:B:212:TYR:HE1	1.68	0.42
1:B:64:LEU:HG	1:B:88:PHE:O	2.19	0.42
1:A:171:ALA:HB3	2:A:334:HOH:O	2.21	0.41
1:A:108:GLU:HB2	2:A:337:HOH:O	2.19	0.41
1:B:228:ASN:HD22	1:B:230:GLU:N	2.18	0.41
1:B:221:PRO:HD2	2:B:330:HOH:O	2.20	0.41
1:B:65:ARG:O	1:B:68:ASP:HB2	2.20	0.41
1:B:166:MET:HB3	1:B:169:SER:OG	2.21	0.40
1:A:28:VAL:HG11	1:A:39:ALA:HB1	2.02	0.40
1:B:263:VAL:O	1:B:267:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	261/284 (92%)	247 (95%)	13 (5%)	1 (0%)	34	52
1	B	260/284 (92%)	236 (91%)	20 (8%)	4 (2%)	10	16
All	All	521/568 (92%)	483 (93%)	33 (6%)	5 (1%)	15	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ARG
1	B	230	GLU
1	B	88	PHE
1	B	227	VAL
1	A	228	ASN

### 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	219/236 (93%)	210 (96%)	9 (4%)	30	53
1	B	218/236 (92%)	207 (95%)	11 (5%)	24	43
All	All	437/472 (93%)	417 (95%)	20 (5%)	27	47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	80	TRP
1	A	101	GLN
1	A	117	SER
1	A	139	ASP
1	A	163	VAL
1	A	219	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	220	THR
1	A	297	SER
1	B	32	LEU
1	B	53	LEU
1	B	64	LEU
1	B	80	TRP
1	B	113	LEU
1	B	116	LYS
1	B	169	SER
1	B	227	VAL
1	B	236	GLN
1	B	258	GLN
1	B	267	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	90	GLN
1	A	101	GLN
1	A	159	HIS
1	A	236	GLN
1	B	60	HIS
1	B	73	GLN
1	B	90	GLN
1	B	101	GLN
1	B	141	ASN
1	B	159	HIS
1	B	228	ASN
1	B	284	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 [i](#)

There are no carbohydrates 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

### 6.1 Protein, DNA and RNA chains

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	265/284 (93%)	0.32	6 (2%) 60 62	36, 54, 71, 78	2 (0%)
1	B	264/284 (92%)	0.64	23 (8%) 10 9	40, 59, 82, 93	1 (0%)
All	All	529/568 (93%)	0.48	29 (5%) 25 26	36, 56, 79, 93	3 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	GLY	6.1
1	A	310	ASP	5.5
1	B	233	PRO	4.9
1	B	232	GLN	4.4
1	B	261	PRO	4.2
1	B	263	VAL	4.1
1	B	231	ILE	3.9
1	B	310	ASP	3.7
1	B	309	GLY	3.5
1	A	227	VAL	3.2
1	B	268	ALA	3.1
1	B	220	THR	3.0
1	B	227	VAL	2.9
1	B	260	ARG	2.6
1	A	138	GLY	2.6
1	A	168	GLN	2.6
1	A	137	HIS	2.5
1	B	287	LEU	2.4
1	B	116	LYS	2.3
1	B	266	SER	2.3
1	B	270	GLY	2.3
1	B	81	VAL	2.2
1	B	165	LEU	2.2
1	B	234	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	168	GLN	2.1
1	B	264	VAL	2.1
1	A	231	ILE	2.1
1	B	56	GLY	2.0
1	B	206	PHE	2.0

## 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.