Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 06:06 pm GMT

PDB ID	:	9T44 / pdb_00009t44
Title	:	Inward-open structure of a Zn2+-transporting P-type ATPase
Authors	:	Lyu, P.; Longhin, E.; Wang, K.; Croll, T.; Bagenholm, V.; Gourdon, P.
Deposited on	:	2025-10-30
Resolution	:	3.58 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

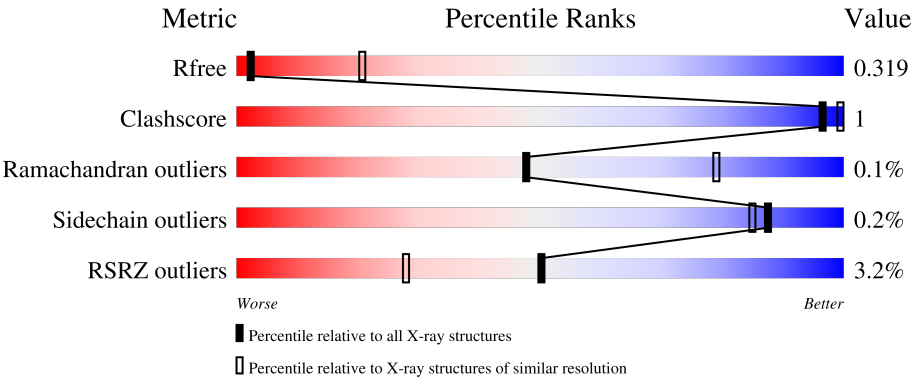
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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 <=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	910	2% 66% · 32%
1	B	910	2% 65% · 32%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9010 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 P-type Zn(2+) transporter.

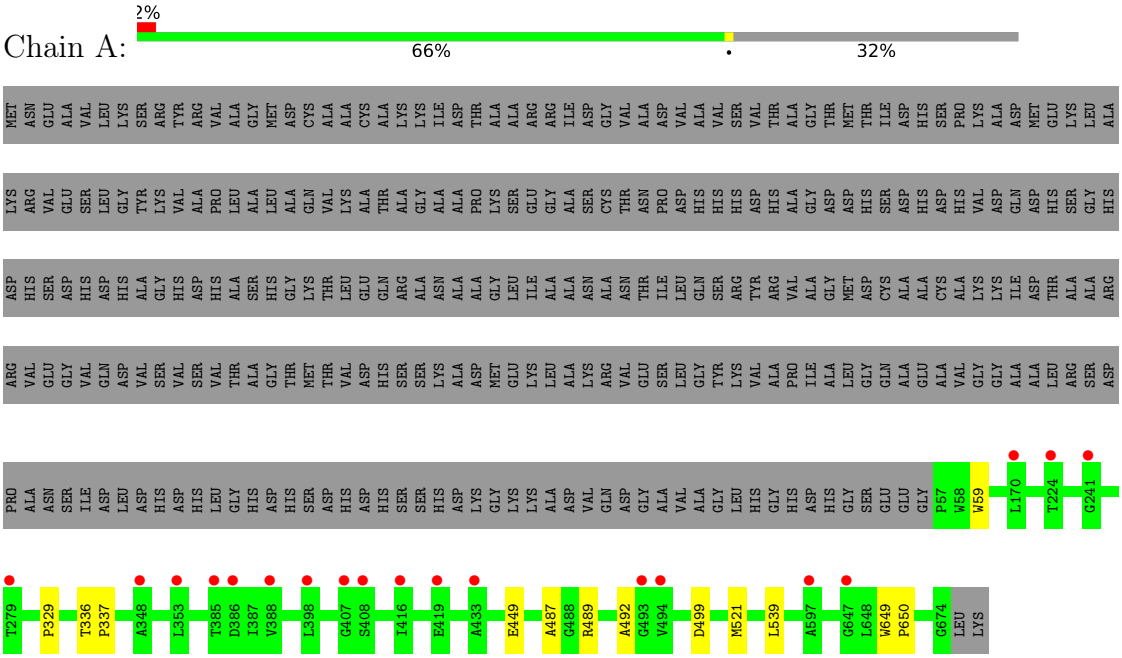
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	0	0
			4505	2860	781	844	20			
1	B	618	Total	C	N	O	S	0	0	0
			4505	2860	781	844	20			

3 Residue-property plots (i)

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.

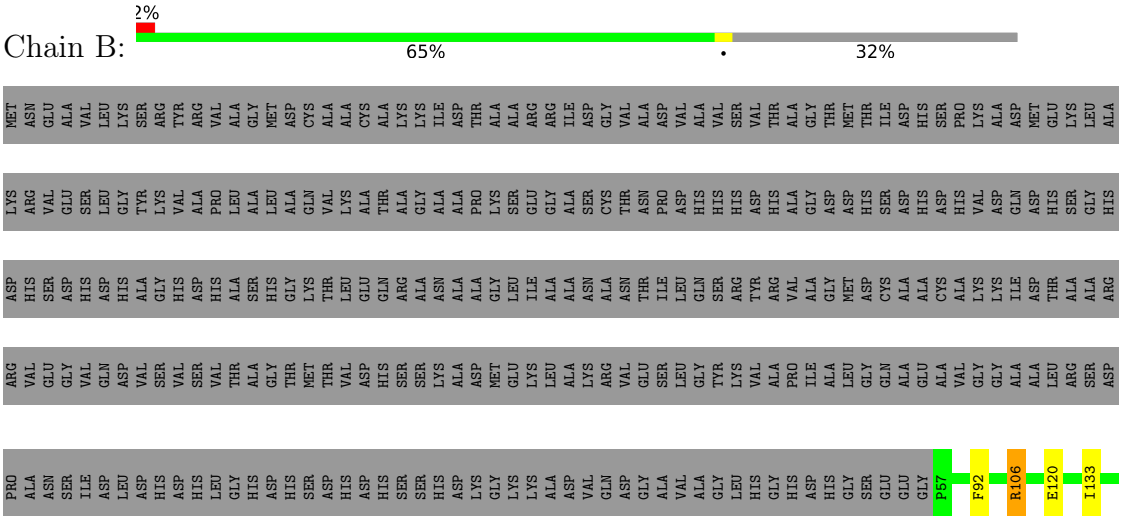
• Molecule 1: P-type Zn(2+) transporter

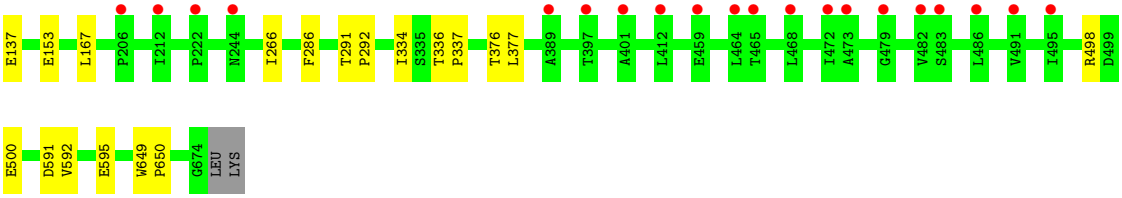
Chain A:



• Molecule 1: P-type Zn(2+) transporter

Chain B:




E137
E153
L167
P206
I212
P222
N244
I266
F286
T291
P292
I334
S335
T336
P337
T376
L377
A389
T397
A401
L412
E459
L464
T465
L468
I472
A473
G479
V482
S483
L486
V491
I495
R498
D499

E500
D591
V592
E595
W649
P650
G674
LEU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.19Å 337.99Å 56.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.58 49.56 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.56-3.58) 99.8 (49.56-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 3.57Å)	Xtriage
Refinement program	PHENIX (dev_4386: ???)	Depositor
R, R_{free}	0.277 , 0.315 0.277 , 0.319	Depositor DCC
R_{free} test set	1176 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	103.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 102.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.18	0/4565	0.48	0/6203
1	B	0.18	0/4565	0.48	0/6203
All	All	0.18	0/9130	0.48	0/12406

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	ARG	Sidechain

5.2 Too-close contacts

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	4505	0	4743	6	0
1	B	4505	0	4743	13	0
All	All	9010	0	9486	19	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 1.

All (19) 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:449:GLU:OE1	1:A:489:ARG:NH1	2.17	0.72
1:A:521:MET:HB2	1:A:539:LEU:HD13	1.92	0.52
1:B:92:PHE:CE2	1:B:137:GLU:HG3	2.48	0.48
1:B:498:ARG:NH1	1:B:500:GLU:OE2	2.45	0.47
1:A:649:TRP:CD1	1:A:650:PRO:HD3	2.51	0.46
1:B:106:ARG:NH1	1:B:120:GLU:OE2	2.47	0.46
1:A:487:ALA:HB3	1:A:492:ALA:HB2	1.98	0.46
1:B:591:ASP:CG	1:B:592:VAL:H	2.23	0.46
1:A:499:ASP:OD1	1:A:499:ASP:N	2.45	0.45
1:B:336:THR:HB	1:B:337:PRO:HD3	1.99	0.44
1:B:133:ILE:HG22	1:B:133:ILE:O	2.18	0.43
1:B:167:LEU:HD23	1:B:266:ILE:HD11	2.00	0.43
1:B:291:THR:OG1	1:B:292:PRO:HD3	2.19	0.43
1:B:153:GLU:HB2	1:B:334:ILE:HG21	2.02	0.42
1:B:649:TRP:CD1	1:B:650:PRO:HD3	2.54	0.42
1:A:336:THR:HB	1:A:337:PRO:HD3	2.02	0.41
1:B:595:GLU:OE1	1:B:595:GLU:N	2.51	0.41
1:B:376:THR:OG1	1:B:377:LEU:N	2.53	0.40
1:B:649:TRP:CG	1:B:650:PRO:HD3	2.56	0.40

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	616/910 (68%)	602 (98%)	13 (2%)	1 (0%)	43 72
1	B	616/910 (68%)	600 (97%)	16 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1232/1820 (68%)	1202 (98%)	29 (2%)	1 (0%)	48 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO

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	464/683 (68%)	463 (100%)	1 (0%)	87 85
1	B	464/683 (68%)	463 (100%)	1 (0%)	87 85
All	All	928/1366 (68%)	926 (100%)	2 (0%)	87 85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TRP
1	B	286	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	572	ASN
1	B	622	ASN
1	B	626	ASN
1	B	665	ASN

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

There are no ligands in this entry.

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

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^{th} 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	618/910 (67%)	0.24	19 (3%)	51	28	45, 150, 220, 264	0
1	B	618/910 (67%)	0.31	20 (3%)	50	28	33, 162, 230, 255	0
All	All	1236/1820 (67%)	0.28	39 (3%)	50	28	33, 158, 226, 264	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	GLY	5.7
1	A	386	ASP	4.6
1	B	459	GLU	4.2
1	B	472	ILE	4.1
1	B	468	LEU	3.7
1	A	416	ILE	2.9
1	A	385	THR	2.9
1	B	491	VAL	2.8
1	A	279	THR	2.8
1	A	353	LEU	2.7
1	B	244	ASN	2.6
1	B	222	PRO	2.6
1	A	388	VAL	2.6
1	A	348	ALA	2.5
1	B	401	ALA	2.5
1	A	419	GLU	2.4
1	A	398	LEU	2.4
1	B	412	LEU	2.4
1	A	647	GLY	2.3
1	B	473	ALA	2.3
1	A	224	THR	2.3
1	B	397	THR	2.3
1	A	597	ALA	2.3
1	B	479	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	483	SER	2.2
1	A	170	LEU	2.2
1	B	495	ILE	2.2
1	B	464	LEU	2.2
1	A	494	VAL	2.2
1	B	465	THR	2.2
1	A	408	SER	2.2
1	B	486	LEU	2.2
1	A	241	GLY	2.1
1	B	206	PRO	2.1
1	A	407	GLY	2.1
1	B	212	ILE	2.0
1	A	433	ALA	2.0
1	B	389	ALA	2.0
1	B	482	VAL	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 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.