



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:17 PM GMT

PDB ID : 4RVW
Title : Structure of the bacterial Zn-transporter ZnuD from *Neisseria meningitidis*
(soaked with 20 micromolar Zinc)
Authors : Calmettes, C.; Moraes, T.F.
Deposited on : 2014-11-28
Resolution : 4.48 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

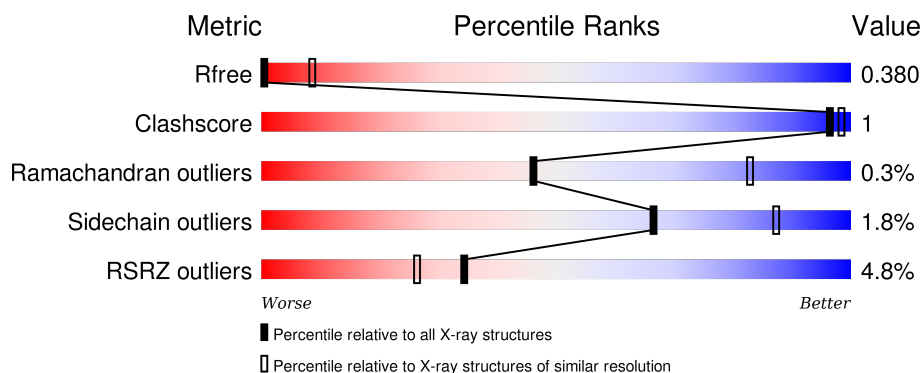
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.48 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}	91344	1070 (5.30-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1116 (5.30-3.60)
Sidechain outliers	100360	1098 (5.30-3.60)
RSRZ outliers	91569	1074 (5.30-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	748	<div> <div>4%</div> <div>78%</div> <div>18%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	804	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4839 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 ZnuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	S	0	0	0
			4831	3025	899	900	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q9JZN9
A	-12	ALA	-	EXPRESSION TAG	UNP Q9JZN9
A	-11	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-10	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-9	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-8	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-7	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-6	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-5	LEU	-	EXPRESSION TAG	UNP Q9JZN9
A	-4	VAL	-	EXPRESSION TAG	UNP Q9JZN9
A	-3	PRO	-	EXPRESSION TAG	UNP Q9JZN9
A	-2	ARG	-	EXPRESSION TAG	UNP Q9JZN9
A	-1	GLY	-	EXPRESSION TAG	UNP Q9JZN9
A	0	SER	-	EXPRESSION TAG	UNP Q9JZN9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Chain A:

4% 78% 18%

0.00 0.05 0.10 0.15 0.20 0.25

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

MET ALA HIS HIS HIS HIS HIS HIS VAL VAL ARG ARG PRO THR THR GLU GLN SER SER VAL ASP LEU LEU THR THR VAL VAL GLY LYS SER ARG ARG PRO THR ASP MET L27 H28 T29 D34 D54 H60 Q111 V112 E113 N127 R197 H206 W218 T235

THR HIS SER G300 R301 P320 F321 L327 R328 V346 G371 A387 I388 S389 V392 K393 Q394 L398 D399 N400 D416 I433 T434 T435 ASP ASN LYS PRO ALA LEU LEU ILE ASP ARG GLU ASN TYR ASN ASN PRO LEU PRO ASP LEU GLY ALA HIS R457 L465 Q474

H511 W531 L551 M552 D553 G554 P557 K558 SER ILE ASP ASP ASP S564 G583 R603 P610 SER LEU PRO GLY ARG GLU ASP ALA TYR GLY ASN ARG PRO PHE ILE GLN D628 L648 T649 D653 L667 R691 Y692 F734

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.55Å 149.59Å 157.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 4.48 47.54 – 4.48	Depositor EDS
% Data completeness (in resolution range)	94.0 (47.54-4.48) 73.6 (47.54-4.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 4.45Å)	Xtriage
Refinement program	Phenix (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.317 , 0.380 0.325 , 0.380	Depositor DCC
R_{free} test set	660 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	153.1	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 126.2	EDS
Estimated twinning fraction	0.034 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 7124 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4839	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	0.25	0/4940	0.44	0/6672

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4831	0	4698	13	0
2	A	3	0	0	0	0
3	A	5	0	0	3	0
All	All	4839	0	4698	13	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 (13) 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:551:LEU:HA	1:A:552:ASN:CB	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ARG:NH1	3:A:804:SO4:O1	2.32	0.62
1:A:551:LEU:HB3	1:A:552:ASN:O	2.10	0.51
1:A:551:LEU:HA	1:A:552:ASN:HB3	1.93	0.51
1:A:206:HIS:ND1	3:A:804:SO4:O1	2.48	0.47
1:A:551:LEU:CA	1:A:552:ASN:CB	2.94	0.46
1:A:206:HIS:CE1	3:A:804:SO4:O1	2.69	0.45
1:A:557:PRO:C	1:A:558:LYS:HG3	2.36	0.44
1:A:648:LEU:HA	1:A:649:THR:HA	1.72	0.44
1:A:553:ASP:HA	1:A:554:GLY:HA3	1.78	0.43
1:A:551:LEU:HA	1:A:552:ASN:HB2	1.98	0.42
1:A:327:LEU:HD13	1:A:328:ARG:N	2.34	0.42
1:A:27:LEU:HD22	1:A:371:GLY:HA2	2.03	0.41

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	600/748 (80%)	554 (92%)	44 (7%)	2 (0%)	46 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	PRO
1	A	416	ASP

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	502/625 (80%)	493 (98%)	9 (2%)	66 87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	TRP
1	A	321	PHE
1	A	400	ASN
1	A	465	LEU
1	A	511	HIS
1	A	531	TRP
1	A	603	ARG
1	A	653	ASP
1	A	667	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	379	GLN
1	A	394	GLN
1	A	403	GLN
1	A	707	GLN

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 [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	804	-	4,4,4	1.48	0	6,6,6	1.72	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	804	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	804	SO4	O4-S-O3	4.04	125.39	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	SO4	3	0

5.7 Other polymers [i](#)

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, 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	610/748 (81%)	0.18	29 (4%) 34 26	201, 247, 298, 434	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	GLY	5.1
1	A	241	HIS	5.1
1	A	54	ASP	4.0
1	A	29	THR	4.0
1	A	393	LYS	3.8
1	A	113	GLU	3.5
1	A	111	GLN	3.3
1	A	388	ILE	3.1
1	A	28	HIS	3.0
1	A	691	ARG	3.0
1	A	392	VAL	2.9
1	A	225	ILE	2.8
1	A	346	VAL	2.8
1	A	398	LEU	2.7
1	A	240	ALA	2.6
1	A	394	GLN	2.6
1	A	233	ARG	2.6
1	A	197	ARG	2.5
1	A	474	GLN	2.5
1	A	552	ASN	2.4
1	A	389	SER	2.4
1	A	583	GLY	2.4
1	A	433	ILE	2.3
1	A	387	ALA	2.2
1	A	127	ASN	2.2
1	A	34	ASP	2.1
1	A	399	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	692	TYR	2.0
1	A	60	HIS	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	801	1/1	0.82	0.23	-0.14	304,304,304,304	0
2	ZN	A	802	1/1	0.64	0.24	-1.03	266,266,266,266	0
3	SO4	A	804	5/5	0.88	0.13	-	268,282,302,311	0
2	ZN	A	803	1/1	0.87	0.20	-	290,290,290,290	0

6.5 Other polymers [i](#)

There are no such residues in this entry.