

wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2023 – 09:11 PM EDT

PDB ID : 8EZW

> Title : Structure of Apo ZrgA deletion 124-184 from Vibrio cholerae

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2022-11-01 Deposited on

2.00 Å(reported) Resolution

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 (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 (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

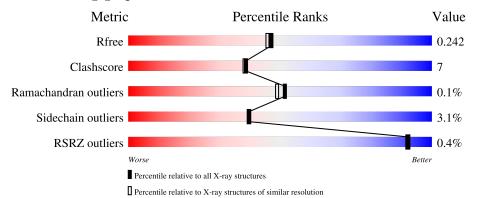
Validation Pipeline (wwPDB-VP) 2.36

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 2.00 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	160	73%	9%	18%
1	В	160	70%	11% •	18%
1	С	160	68%	15%	17%
1	D	160	74%	11%	• 14%
1	Е	160	72%	8% •	18%

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Mol	Chain	Length	Quality of cha	ain		
1	F	160	60%	20%	•	18%



2 Entry composition (i)

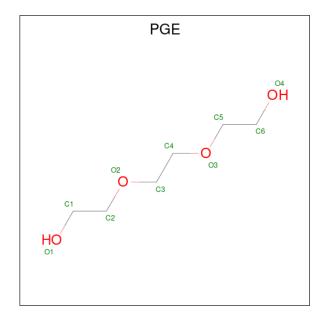
There are 3 unique types of molecules in this entry. The entry contains 6763 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Zinc-binding protein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	132	Total	С	N	О	S	0	0	0
1	Λ	152	1051	665	179	205	2	0	0	
1	В	132	Total	С	N	О	S	0	2	0
1	Ъ	152	1069	676	182	209	2	0	2	
1	С	133	Total	С	N	О	S	0	0	0
1		155	1055	667	180	206	2	0	U	
1	D	138	Total	С	N	О	S	0	0	0
1	D	130	1094	691	185	216	2	0	0	
1	Е	131	Total	С	N	О	S	0	1	0
1	l L	131	1056	669	180	205	2	U	1	
1	F	131	Total	С	N	О	S	0	1	0
1	I.	131	1056	668	180	206	2	U	1	U

• Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 10 6 4	0	0
2	F	1	Total C O 10 6 4	0	0

• Molecule 3 is water.

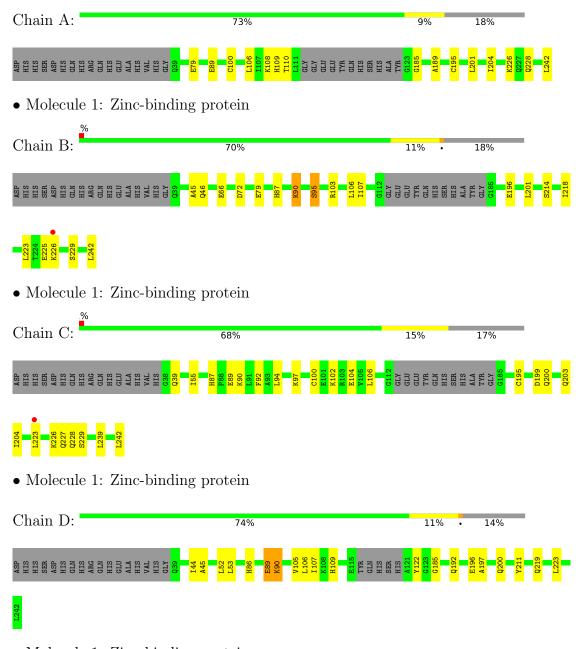
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	В	69	Total O 69 69	0	0
3	С	53	Total O 53 53	0	0
3	D	64	Total O 64 64	0	0
3	E	52	Total O 52 52	0	0
3	F	42	Total O 42 42	0	0



3 Residue-property plots (i)

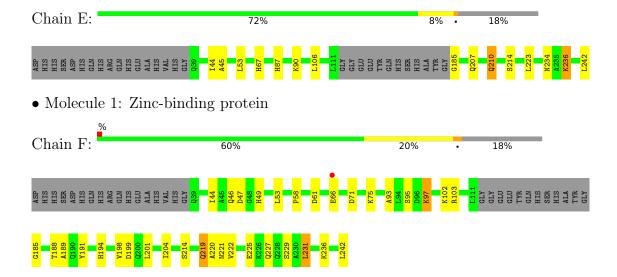
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Zinc-binding protein



• Molecule 1: Zinc-binding protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	81.06Å 65.44Å 88.73Å	Depositor
a, b, c, α , β , γ	90.00° 98.77° 90.00°	Depositor
Resolution (Å)	45.88 - 2.00	Depositor
rtesolution (A)	45.84 - 2.00	EDS
% Data completeness	99.1 (45.88-2.00)	Depositor
(in resolution range)	99.1 (45.84-2.00)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.35 (at 2.00Å)	Xtriage
Refinement program	REFMAC 7.1.018	Depositor
P. P.	0.192 , 0.236	Depositor
R, R_{free}	0.201 , 0.242	DCC
R_{free} test set	3083 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 43.5	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6763	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: PGE

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	Bo	nd lengths	Bond angles	
IVIOI	Chain	RMSZ	RMSZ $\# Z > 5$		# Z > 5
1	A	0.88	2/1069~(0.2%)	1.00	0/1443
1	В	0.94	$2/1087 \ (0.2\%)$	0.98	0/1466
1	С	0.93	1/1073 (0.1%)	0.99	0/1448
1	D	0.92	2/1113~(0.2%)	0.97	1/1502 (0.1%)
1	Е	0.89	0/1074	0.97	0/1449
1	F	0.84	0/1074	0.92	0/1450
All	All	0.90	7/6490 (0.1%)	0.97	1/8758 (0.0%)

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1
1	F	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
1	В	79	GLU	CD-OE2	7.06	1.33	1.25
1	С	89	GLU	CD-OE1	7.04	1.33	1.25
1	A	189	ALA	C-O	6.08	1.34	1.23
1	D	89	GLU	CD-OE1	5.80	1.32	1.25
1	D	89	GLU	CD-OE2	5.66	1.31	1.25

All (1) bond angle outliers are listed below:



Mo	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	D	90	LYS	N-CA-CB	-5.52	100.66	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	226	LYS	Peptide
1	F	97	LYS	Peptide

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	1051	0	1034	12	0
1	В	1069	0	1051	15	0
1	С	1055	0	1037	24	0
1	D	1094	0	1066	15	0
1	Е	1056	0	1043	10	0
1	F	1056	0	1038	25	0
2	Е	10	0	14	0	0
2	F	10	0	14	2	0
3	A	82	0	0	2	0
3	В	69	0	0	4	0
3	С	53	0	0	4	0
3	D	64	0	0	4	0
3	Е	52	0	0	3	0
3	F	42	0	0	4	0
All	All	6763	0	6297	95	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 7.

The worst 5 of 95 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	$egin{array}{c} \operatorname{Clash} \\ \operatorname{overlap}\ (\mathring{\mathbf{A}}) \end{array}$	
1:A:226:LYS:HD3	1:F:47:ASP:OD2	1.69	0.92	

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Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:C:97:LYS:HD2	1:C:200:GLN:HG2	1.61	0.81
1:D:86:HIS:CE1	1:D:107:ILE:HD12	2.17	0.79
1:A:226:LYS:CD	1:F:47:ASP:OD2	2.31	0.77
1:B:95:SER:OG	3:B:301:HOH:O	1.65	0.75

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	Perce	ntiles
1	A	128/160 (80%)	124 (97%)	4 (3%)	0	100	100
1	В	130/160 (81%)	127 (98%)	3 (2%)	0	100	100
1	С	129/160 (81%)	126 (98%)	3 (2%)	0	100	100
1	D	134/160 (84%)	127 (95%)	7 (5%)	0	100	100
1	E	128/160 (80%)	125 (98%)	3 (2%)	0	100	100
1	F	128/160 (80%)	123 (96%)	4 (3%)	1 (1%)	19	13
All	All	777/960 (81%)	752 (97%)	24 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	95	SER

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 nu	imber of residues.
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Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	A	113/136 (83%)	113 (100%)	0	100	100
1	В	115/136~(85%)	109 (95%)	6 (5%)	23	19
1	С	113/136 (83%)	109 (96%)	4 (4%)	36	35
1	D	116/136 (85%)	115 (99%)	1 (1%)	78	83
1	E	114/136 (84%)	110 (96%)	4 (4%)	36	35
1	F	114/136 (84%)	107 (94%)	7 (6%)	18	14
All	All	685/816 (84%)	663 (97%)	22 (3%)	40	38

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	242	LEU
1	F	199	ASP
1	F	97	LYS
1	F	214	SER
1	С	199	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	207	GLN
1	D	219	GLN
1	F	219	GLN
1	Е	99	GLN
1	F	70	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	True	Chain	Dag	Link	Bond lengths			В	ond ang	gles
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	PGE	F	301	-	9,9,9	0.25	0	8,8,8	0.16	0
2	PGE	Е	301	-	9,9,9	0.29	0	8,8,8	0.18	0

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
2	PGE	F	301	-	-	4/7/7/7	-
2	PGE	Е	301	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	301	PGE	O2-C3-C4-O3
2	F	301	PGE	O1-C1-C2-O2
2	F	301	PGE	O2-C3-C4-O3
2	F	301	PGE	O3-C5-C6-O4
2	F	301	PGE	C1-C2-O2-C3

There are no ring outliers.



1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	PGE	2	0

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, 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	132/160 (82%)	-0.18	0 100 100	20, 32, 52, 60	0
1	В	132/160 (82%)	-0.21	1 (0%) 86 85	21, 34, 62, 76	0
1	С	133/160 (83%)	-0.04	1 (0%) 86 85	22, 37, 65, 86	0
1	D	138/160 (86%)	-0.10	0 100 100	23, 37, 58, 71	0
1	Е	131/160 (81%)	-0.25	0 100 100	24, 33, 56, 67	0
1	F	131/160 (81%)	-0.02	1 (0%) 86 85	27, 42, 74, 92	0
All	All	797/960 (83%)	-0.13	3 (0%) 92 92	20, 36, 64, 92	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	223	LEU	3.5
1	F	66	GLU	2.4
1	В	226	LYS	2.2

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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	PGE	Е	301	10/10	0.80	0.25	69,79,87,88	0
2	PGE	F	301	10/10	0.85	0.22	69,71,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.

