



# wwPDB X-ray Structure Validation Summary Report

Nov 20, 2014 – 11:39 AM EST

PDB ID : 3WZM  
Title : ZEN lactonase mutant complex  
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Deposited on : 2014-10-01  
Resolution : 2.48 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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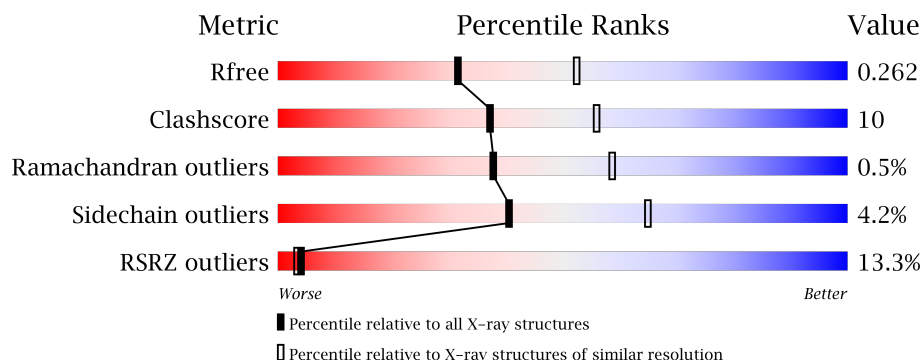
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24195  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24195

# 1 Overall quality at a glance

The reported resolution of this entry is 2.48 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))
$R_{free}$	66092	3277 (2.50-2.46)
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	278	
1	B	278	
1	C	278	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZER	A	300	-	X
2	ZER	B	300	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6558 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total 2021	C 1282	N 341	O 387	S 11	0	0	0
1	B	264	Total 2021	C 1282	N 341	O 387	S 11	0	0	0
1	C	264	Total 2021	C 1282	N 341	O 387	S 11	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

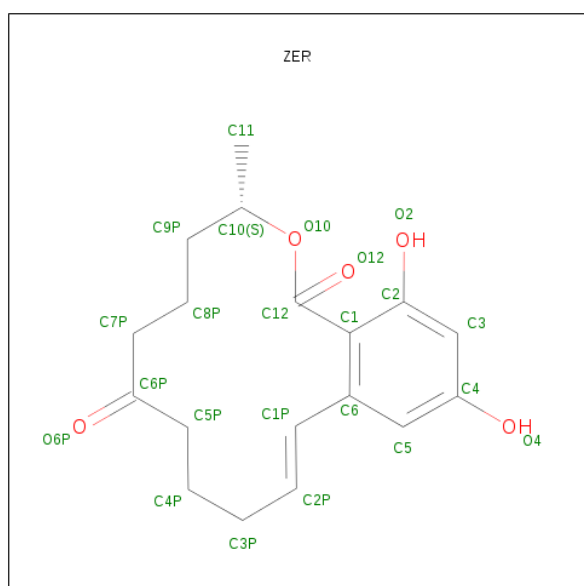
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8NKB0
A	-12	ALA	-	EXPRESSION TAG	UNP Q8NKB0
A	-11	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-10	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-9	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-8	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-7	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-6	HIS	-	EXPRESSION TAG	UNP Q8NKB0
A	-5	VAL	-	EXPRESSION TAG	UNP Q8NKB0
A	-4	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	-3	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	-2	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	-1	ASP	-	EXPRESSION TAG	UNP Q8NKB0
A	0	LYS	-	EXPRESSION TAG	UNP Q8NKB0
A	102	ALA	SER	ENGINEERED MUTATION	UNP Q8NKB0
B	-13	MET	-	EXPRESSION TAG	UNP Q8NKB0
B	-12	ALA	-	EXPRESSION TAG	UNP Q8NKB0
B	-11	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-10	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-9	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-8	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-7	HIS	-	EXPRESSION TAG	UNP Q8NKB0
B	-6	HIS	-	EXPRESSION TAG	UNP Q8NKB0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	VAL	-	EXPRESSION TAG	UNP Q8NKB0
B	-4	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	-3	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	-2	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	-1	ASP	-	EXPRESSION TAG	UNP Q8NKB0
B	0	LYS	-	EXPRESSION TAG	UNP Q8NKB0
B	102	ALA	SER	ENGINEERED MUTATION	UNP Q8NKB0
C	-13	MET	-	EXPRESSION TAG	UNP Q8NKB0
C	-12	ALA	-	EXPRESSION TAG	UNP Q8NKB0
C	-11	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-10	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-9	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-8	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-7	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-6	HIS	-	EXPRESSION TAG	UNP Q8NKB0
C	-5	VAL	-	EXPRESSION TAG	UNP Q8NKB0
C	-4	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	-3	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	-2	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	-1	ASP	-	EXPRESSION TAG	UNP Q8NKB0
C	0	LYS	-	EXPRESSION TAG	UNP Q8NKB0
C	102	ALA	SER	ENGINEERED MUTATION	UNP Q8NKB0

- Molecule 2 is (3S,11E)-14,16-DIHYDROXY-3-METHYL-3,4,5,6,9,10-HEXAHYDRO-1H-2-BENZOXACYCLOTETRADECINE-1,7(8H)-DIONE (three-letter code: ZER) (formula:  $C_{18}H_{22}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	18	5		
2	B	1	Total	C	O	0	0
			23	18	5		
2	C	1	Total	C	O	0	0
			23	18	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	0
			185	185		
3	B	162	Total	O	0	0
			162	162		
3	C	79	Total	O	0	0
			79	79		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.84Å 86.84Å 471.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.48 19.95 – 2.48	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.95-2.48) 95.5 (19.95-2.48)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.30 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.204 , 0.268 0.200 , 0.262	Depositor DCC
$R_{free}$ test set	1848 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36961 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.99	2/2072 (0.1%)	0.87	3/2829 (0.1%)
1	B	0.96	2/2072 (0.1%)	0.86	1/2829 (0.0%)
1	C	0.73	0/2072	0.72	0/2829
All	All	0.90	4/6216 (0.1%)	0.82	4/8487 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	GLU	CG-CD	5.79	1.60	1.51
1	B	258	GLU	CG-CD	5.74	1.60	1.51
1	A	82	SER	CB-OG	-5.70	1.34	1.42
1	B	258	GLU	CD-OE2	5.07	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	185	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	2	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	B	2	ARG	NE-CZ-NH1	-6.23	117.19	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,



and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2021	0	1991	30	0
1	B	2021	0	1991	14	0
1	C	2021	0	1991	78	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
3	A	185	0	0	3	1
3	B	162	0	0	2	0
3	C	79	0	0	9	1
All	All	6558	0	5973	122	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 122 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:123:MET:HE1	1:B:256:VAL:HA	1.23	1.07
1:A:38:MET:HG2	1:A:168:MET:HE1	1.45	0.98
1:C:40:ASP:HB3	3:C:436:HOH:O	1.67	0.95
1:C:125:HIS:CD2	1:C:126:GLU:HG3	2.02	0.93
1:A:158:VAL:HA	1:A:241:MET:HE2	1.53	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:668:HOH:O	3:C:430:HOH:O[8_555]	1.94	0.26

## 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	262/278 (94%)	251 (96%)	10 (4%)	1 (0%)	43	64
1	B	262/278 (94%)	250 (95%)	10 (4%)	2 (1%)	27	44
1	C	262/278 (94%)	229 (87%)	32 (12%)	1 (0%)	43	64
All	All	786/834 (94%)	730 (93%)	52 (7%)	4 (0%)	38	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	ASP
1	A	187	TYR
1	B	161	GLY
1	B	187	TYR

### 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	220/233 (94%)	217 (99%)	3 (1%)	78	93
1	B	220/233 (94%)	208 (94%)	12 (6%)	30	51
1	C	220/233 (94%)	207 (94%)	13 (6%)	28	46
All	All	660/699 (94%)	632 (96%)	28 (4%)	40	65

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	219	GLU
1	C	8	SER
1	C	223	ASP
1	B	245	TYR
1	B	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	263	HIS

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Mol	Chain	Res	Type
1	C	261	GLN
1	C	134	HIS
1	B	261	GLN
1	C	166	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ZER	A	300	-	24,24,24	1.27	3 (12%)	32,32,32	1.99	9 (28%)
2	ZER	B	300	-	24,24,24	1.14	2 (8%)	32,32,32	1.97	8 (25%)
2	ZER	C	300	-	24,24,24	1.32	2 (8%)	32,32,32	1.56	8 (25%)

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	ZER	A	300	-	-	0/22/22/22	1/2/2/2
2	ZER	B	300	-	-	0/22/22/22	1/2/2/2
2	ZER	C	300	-	-	0/22/22/22	1/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	ZER	O10-C12	4.20	1.43	1.34
2	C	300	ZER	C6-C1P	3.71	1.53	1.47
2	A	300	ZER	C6-C1P	3.68	1.53	1.47
2	B	300	ZER	O10-C12	3.33	1.41	1.34
2	A	300	ZER	O10-C12	3.08	1.41	1.34

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	ZER	C11-C10-C9P	-5.28	98.19	114.13
2	A	300	ZER	C4P-C5P-C6P	-5.02	101.53	114.83
2	A	300	ZER	C7P-C6P-C5P	4.54	126.28	116.93
2	A	300	ZER	C11-C10-C9P	-4.33	101.06	114.13
2	B	300	ZER	C4P-C5P-C6P	-4.26	103.54	114.83

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	ZER	C1-C10-C12-C1P-C2P-C3P-C4P-C5P-C6-C6P-C7P-C8P-C9P-O10
2	B	300	ZER	C1-C10-C12-C1P-C2P-C3P-C4P-C5P-C6-C6P-C7P-C8P-C9P-O10
2	C	300	ZER	C1-C10-C12-C1P-C2P-C3P-C4P-C5P-C6-C6P-C7P-C8P-C9P-O10

## 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<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	264/278 (94%)	-0.44	0 100 100	22, 36, 58, 73	0
1	B	264/278 (94%)	-0.41	2 (0%) 83 85	24, 39, 61, 83	0
1	C	264/278 (94%)	1.87	103 (39%) 1 1	68, 88, 128, 153	0
All	All	792/834 (94%)	0.34	105 (13%) 4 3	22, 46, 112, 153	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	TRP	10.8
1	C	155	LEU	8.7
1	C	145	GLU	8.5
1	C	24	PRO	6.7
1	C	170	ASP	6.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZER	A	300	23/23	0.24	3.74	55,64,74,78	0
2	ZER	B	300	23/23	0.23	3.05	57,64,74,78	0
2	ZER	C	300	23/23	0.32	0.81	77,86,100,106	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.