



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:06 AM GMT

PDB ID : 2LZH  
Title : THE STRUCTURES OF THE MONOCLINIC AND ORTHORHOMBIC FORMS OF HEN EGG-WHITE LYSOZYME AT 6 ANGSTROMS RESOLUTION.  
Authors : Artymiuk, P.J.; Blake, C.C.F.; Rice, D.W.; Wilson, K.S.  
Deposited on : 1981-06-29  
Resolution : 6.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

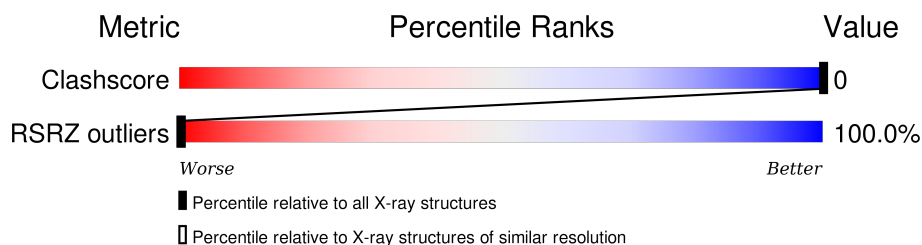
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1050 (8.30-3.70)
RSRZ outliers	91569	1001 (8.30-3.66)

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. 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	129	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 129 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.

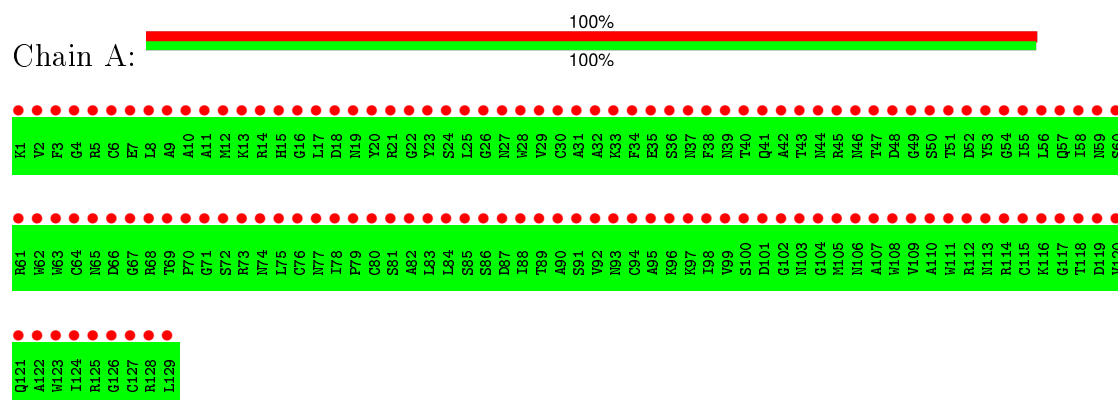
- Molecule 1 is a protein called HEN EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	129	Total 129	C 129	0	0	129

### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: HEN EGG WHITE LYSOZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.40 Å 68.70 Å 30.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 6.00 25.40 – 5.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-6.00) 99.5 (25.40-5.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	71.40 (at 6.02 Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.460 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	4.938	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 75.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 398 reflections	Xtriage
$F_o, F_c$ correlation	0.56	EDS
Total number of atoms	129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	129	0	0	0	0
All	All	129	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

### 5.3 Torsion angles

#### 5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 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	129/129 (100%)	16.53	129 (100%) 0 0	0, 0, 0, 0	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ILE	39.6
1	A	118	THR	38.8
1	A	79	PRO	38.2
1	A	44	ASN	35.6
1	A	77	ASN	34.6
1	A	113	ASN	34.3
1	A	20	TYR	33.1
1	A	4	GLY	32.5
1	A	22	GLY	28.8
1	A	16	GLY	28.1
1	A	43	THR	28.1
1	A	48	ASP	27.2
1	A	114	ARG	26.8
1	A	57	GLN	26.1
1	A	12	MET	25.7
1	A	82	ALA	25.7
1	A	36	SER	25.4
1	A	125	ARG	24.8
1	A	119	ASP	24.5
1	A	31	ALA	24.2
1	A	24	SER	23.8
1	A	120	VAL	23.7
1	A	25	LEU	23.5
1	A	9	ALA	23.5
1	A	27	ASN	23.4
1	A	45	ARG	23.0
1	A	15	HIS	22.3

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Mol	Chain	Res	Type	RSRZ
1	A	94	CYS	22.3
1	A	19	ASN	21.9
1	A	13	LYS	21.8
1	A	76	CYS	21.5
1	A	122	ALA	21.3
1	A	72	SER	21.3
1	A	32	ALA	20.9
1	A	121	GLN	20.8
1	A	51	THR	20.8
1	A	7	GLU	20.5
1	A	80	CYS	20.3
1	A	37	ASN	19.9
1	A	92	VAL	19.8
1	A	110	ALA	19.7
1	A	47	THR	19.7
1	A	5	ARG	19.3
1	A	3	PHE	19.1
1	A	40	THR	18.9
1	A	18	ASP	18.9
1	A	17	LEU	18.8
1	A	95	ALA	18.8
1	A	73	ARG	18.6
1	A	42	ALA	18.4
1	A	41	GLN	17.3
1	A	50	SER	17.0
1	A	98	ILE	17.0
1	A	23	TYR	16.8
1	A	96	LYS	16.8
1	A	34	PHE	16.8
1	A	21	ARG	16.2
1	A	30	CYS	16.2
1	A	109	VAL	16.0
1	A	123	TRP	15.9
1	A	66	ASP	15.7
1	A	71	GLY	15.7
1	A	87	ASP	15.6
1	A	85	SER	15.6
1	A	14	ARG	15.5
1	A	35	GLU	15.2
1	A	11	ALA	15.1
1	A	46	ASN	15.0
1	A	39	ASN	14.6

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Mol	Chain	Res	Type	RSRZ
1	A	65	ASN	14.3
1	A	93	ASN	14.2
1	A	126	GLY	14.1
1	A	127	CYS	14.0
1	A	28	TRP	13.8
1	A	84	LEU	13.6
1	A	33	LYS	13.5
1	A	49	GLY	13.4
1	A	117	GLY	13.3
1	A	2	VAL	12.8
1	A	10	ALA	12.8
1	A	89	THR	12.6
1	A	99	VAL	12.5
1	A	104	GLY	12.3
1	A	102	GLY	12.2
1	A	53	TYR	12.0
1	A	112	ARG	11.7
1	A	124	ILE	11.5
1	A	129	LEU	11.5
1	A	103	ASN	11.0
1	A	52	ASP	11.0
1	A	64	CYS	10.9
1	A	97	LYS	10.8
1	A	55	ILE	10.7
1	A	88	ILE	10.7
1	A	74	ASN	10.5
1	A	106	ASN	10.4
1	A	54	GLY	10.4
1	A	58	ILE	10.4
1	A	81	SER	10.2
1	A	26	GLY	10.1
1	A	111	TRP	10.1
1	A	6	CYS	10.0
1	A	91	SER	9.8
1	A	38	PHE	9.7
1	A	61	ARG	9.4
1	A	75	LEU	9.4
1	A	29	VAL	9.3
1	A	8	LEU	9.2
1	A	69	THR	8.8
1	A	59	ASN	8.8
1	A	100	SER	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	105	MET	8.6
1	A	67	GLY	8.2
1	A	128	ARG	8.2
1	A	107	ALA	8.1
1	A	56	LEU	8.1
1	A	68	ARG	8.1
1	A	60	SER	7.8
1	A	116	LYS	7.6
1	A	108	TRP	7.5
1	A	101	ASP	7.3
1	A	83	LEU	7.1
1	A	63	TRP	7.0
1	A	70	PRO	6.3
1	A	62	TRP	6.3
1	A	1	LYS	5.4
1	A	86	SER	4.9
1	A	115	CYS	4.8
1	A	90	ALA	2.8

## 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.