



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 PM UTC

PDB ID : 2LZH / pdb_00002lzh
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

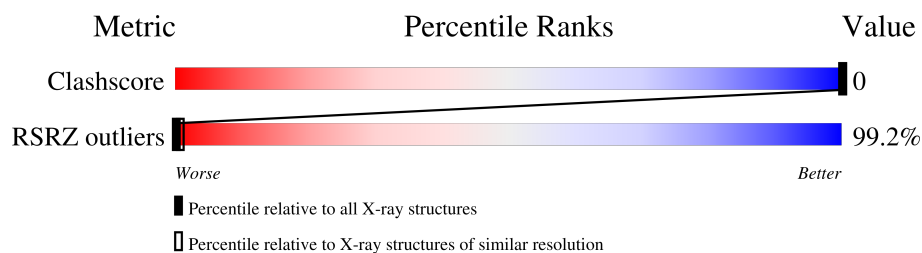
1 Overall quality at a glance

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	190562	1210 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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 $\leq 5\%$. 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	99% 100%

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.

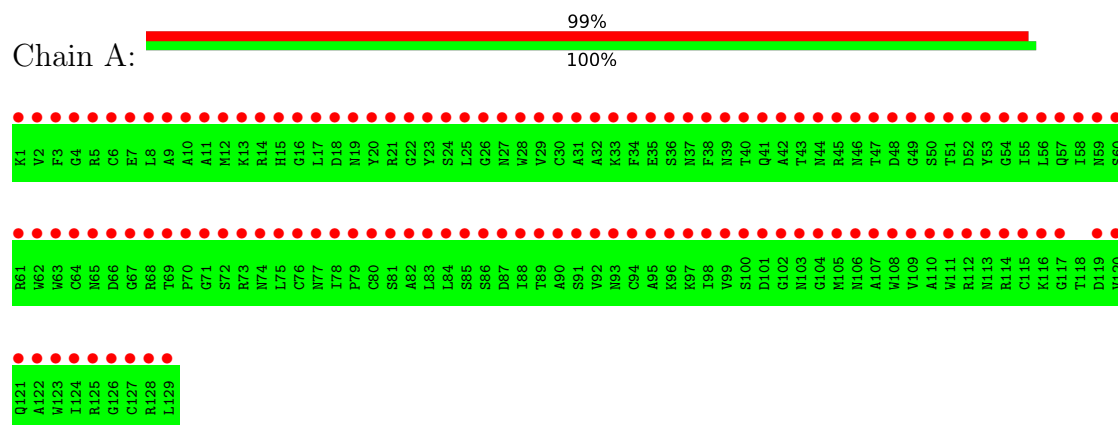
- Molecule 1 is a protein called HEN EGG WHITE LYSOZYME.

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, 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: HEN EGG WHITE LYSOZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.40Å 68.70Å 30.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 6.00 44.93 – 6.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-6.00) 97.7 (44.93-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	71.40 (at 6.02Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.370 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	4.938	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	2.37 , 914.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.48	EDS
Total number of atoms	129	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 [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	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 [i](#)

5.3.1 Protein backbone [i](#)

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 oligosaccharides 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, 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	129/129 (100%)	10.05	128 (99%) 0 1	0, 0, 0, 0	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	ASN	30.0
1	A	89	THR	29.4
1	A	90	ALA	27.4
1	A	6	CYS	20.3
1	A	7	GLU	20.2
1	A	91	SER	19.5
1	A	47	THR	19.0
1	A	11	ALA	18.5
1	A	4	GLY	16.9
1	A	127	CYS	16.1
1	A	77	ASN	15.9
1	A	117	GLY	15.8
1	A	81	SER	15.3
1	A	83	LEU	14.4
1	A	96	LYS	14.1
1	A	101	ASP	13.8
1	A	9	ALA	13.7
1	A	107	ALA	13.6
1	A	35	GLU	13.2
1	A	19	ASN	13.2
1	A	32	ALA	13.1
1	A	57	GLN	13.1
1	A	10	ALA	13.1
1	A	73	ARG	13.0
1	A	70	PRO	12.9
1	A	15	HIS	12.8
1	A	92	VAL	12.8

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASP	12.7
1	A	21	ARG	12.6
1	A	12	MET	12.5
1	A	37	ASN	12.4
1	A	31	ALA	11.8
1	A	108	TRP	11.7
1	A	68	ARG	11.7
1	A	100	SER	11.5
1	A	38	PHE	11.5
1	A	2	VAL	11.4
1	A	66	ASP	11.4
1	A	126	GLY	11.4
1	A	8	LEU	11.1
1	A	95	ALA	11.0
1	A	97	LYS	10.8
1	A	30	CYS	10.8
1	A	94	CYS	10.8
1	A	24	SER	10.8
1	A	55	ILE	10.8
1	A	85	SER	10.7
1	A	44	ASN	10.7
1	A	102	GLY	10.6
1	A	18	ASP	10.5
1	A	1	LYS	10.4
1	A	125	ARG	10.3
1	A	23	TYR	10.3
1	A	20	TYR	10.2
1	A	67	GLY	10.2
1	A	86	SER	10.1
1	A	88	ILE	10.1
1	A	34	PHE	10.0
1	A	129	LEU	9.8
1	A	58	ILE	9.8
1	A	80	CYS	9.6
1	A	104	GLY	9.6
1	A	33	LYS	9.5
1	A	56	LEU	9.4
1	A	29	VAL	9.3
1	A	41	GLN	9.2
1	A	46	ASN	9.2
1	A	49	GLY	9.1
1	A	53	TYR	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	28	TRP	9.0
1	A	98	ILE	9.0
1	A	87	ASP	9.0
1	A	122	ALA	8.8
1	A	69	THR	8.7
1	A	128	ARG	8.7
1	A	60	SER	8.7
1	A	43	THR	8.6
1	A	109	VAL	8.5
1	A	54	GLY	8.5
1	A	59	ASN	8.4
1	A	64	CYS	8.4
1	A	103	ASN	8.4
1	A	123	TRP	8.4
1	A	65	ASN	8.4
1	A	40	THR	8.3
1	A	99	VAL	8.2
1	A	36	SER	7.7
1	A	71	GLY	7.6
1	A	45	ARG	7.5
1	A	105	MET	7.5
1	A	16	GLY	7.4
1	A	25	LEU	7.4
1	A	27	ASN	7.4
1	A	79	PRO	7.4
1	A	84	LEU	7.3
1	A	106	ASN	7.3
1	A	121	GLN	7.3
1	A	50	SER	7.2
1	A	3	PHE	7.1
1	A	113	ASN	7.0
1	A	72	SER	6.9
1	A	22	GLY	6.8
1	A	51	THR	6.7
1	A	75	LEU	6.5
1	A	14	ARG	6.4
1	A	112	ARG	6.4
1	A	52	ASP	6.3
1	A	61	ARG	6.3
1	A	119	ASP	6.2
1	A	26	GLY	6.0
1	A	110	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	124	ILE	5.9
1	A	17	LEU	5.9
1	A	74	ASN	5.8
1	A	63	TRP	5.3
1	A	42	ALA	5.1
1	A	13	LYS	5.1
1	A	82	ALA	5.0
1	A	62	TRP	5.0
1	A	114	ARG	5.0
1	A	5	ARG	4.7
1	A	76	CYS	4.3
1	A	116	LYS	4.3
1	A	111	TRP	3.6
1	A	78	ILE	3.5
1	A	115	CYS	3.3
1	A	39	ASN	3.2
1	A	120	VAL	2.7

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.