



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:46 PM GMT

PDB ID : 1LZH
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
<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 (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

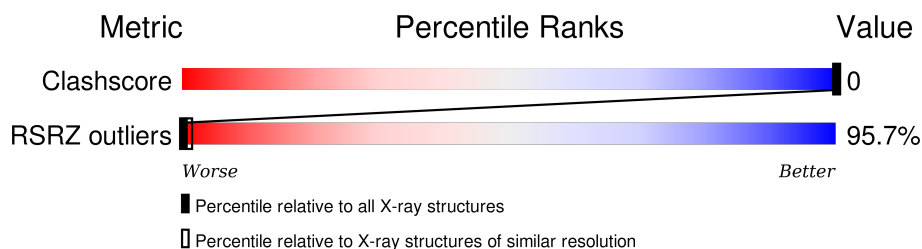
1 Overall quality at a glance

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 ≥ 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	 94% 100%
1	B	129	 98% 100%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 258 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.

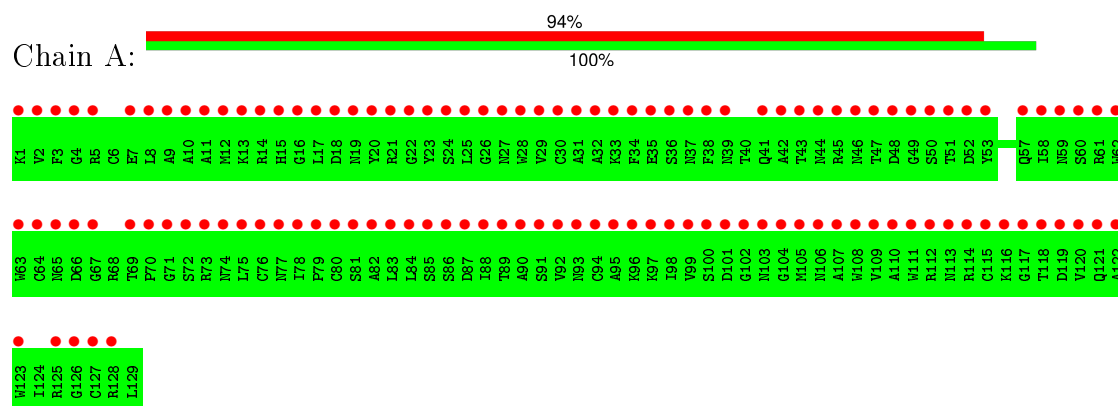
- Molecule 1 is a protein called HEN EGG WHITE LYSOZYME.

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

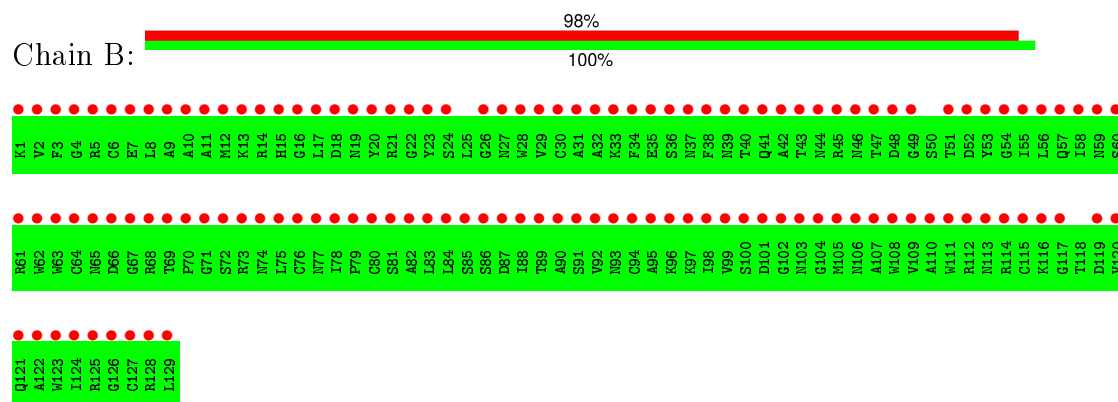
3 Residue-property plots

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



• Molecule 1: HEN EGG WHITE LYSOZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	28.12Å 63.61Å 60.52Å 90.00° 91.05° 90.00°	Depositor
Resolution (Å)	(Not available) – 6.00 27.32 – 5.92	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-6.00) 97.9 (27.32-5.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	36.04 (at 6.05Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.503 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	-0.1	Xtriage
Anisotropy	-30.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.6	EDS
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.137 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 571 reflections	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	258	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8009e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [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
1	B	129	0	0	0	0
All	All	258	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 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, 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%)	9.33	121 (93%) 0 1	0, 0, 0, 0	0
1	B	129/129 (100%)	8.76	126 (97%) 0 1	0, 0, 0, 0	0
All	All	258/258 (100%)	9.04	247 (95%) 0 1	0, 0, 0, 0	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	THR	24.3
1	A	65	ASN	24.0
1	A	45	ARG	23.1
1	A	3	PHE	22.7
1	A	35	GLU	20.8
1	A	30	CYS	19.1
1	A	73	ARG	18.9
1	B	106	ASN	18.5
1	A	90	ALA	18.3
1	B	95	ALA	18.2
1	A	13	LYS	17.6
1	B	18	ASP	17.5
1	B	19	ASN	17.2
1	A	17	LEU	17.2
1	A	80	CYS	17.0
1	B	74	ASN	16.5
1	A	44	ASN	16.2
1	A	12	MET	15.7
1	A	28	TRP	15.5
1	B	14	ARG	15.5
1	B	43	THR	15.5
1	B	80	CYS	15.2
1	B	62	TRP	15.0
1	B	89	THR	14.9

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Mol	Chain	Res	Type	RSRZ
1	A	119	ASP	14.8
1	A	74	ASN	14.6
1	A	66	ASP	14.4
1	B	59	ASN	14.3
1	A	2	VAL	14.2
1	B	39	ASN	14.1
1	A	4	GLY	14.0
1	A	34	PHE	13.9
1	B	125	ARG	13.9
1	B	57	GLN	13.8
1	A	105	MET	13.8
1	A	18	ASP	13.8
1	A	104	GLY	13.6
1	B	73	ARG	13.6
1	B	46	ASN	13.6
1	B	13	LYS	13.5
1	A	77	ASN	13.5
1	A	48	ASP	13.4
1	B	64	CYS	13.3
1	A	19	ASN	13.2
1	A	75	LEU	13.1
1	B	109	VAL	13.1
1	A	59	ASN	13.0
1	B	30	CYS	12.9
1	A	42	ALA	12.8
1	B	47	THR	12.7
1	A	92	VAL	12.7
1	B	88	ILE	12.6
1	B	29	VAL	12.6
1	A	29	VAL	12.5
1	B	52	ASP	12.5
1	A	43	THR	12.4
1	A	64	CYS	12.4
1	A	20	TYR	12.4
1	B	45	ARG	12.4
1	A	11	ALA	12.1
1	A	22	GLY	12.1
1	B	122	ALA	12.1
1	B	87	ASP	12.0
1	B	48	ASP	12.0
1	A	106	ASN	12.0
1	B	79	PRO	11.8

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Mol	Chain	Res	Type	RSRZ
1	B	115	CYS	11.7
1	B	23	TYR	11.7
1	A	24	SER	11.7
1	A	62	TRP	11.7
1	B	104	GLY	11.6
1	A	85	SER	11.5
1	B	75	LEU	11.4
1	A	63	TRP	11.4
1	B	72	SER	11.4
1	A	93	ASN	11.3
1	B	65	ASN	11.2
1	B	1	LYS	11.2
1	A	94	CYS	11.2
1	A	21	ARG	11.1
1	B	86	SER	11.1
1	B	105	MET	11.1
1	B	44	ASN	11.0
1	B	35	GLU	11.0
1	B	112	ARG	10.9
1	B	101	ASP	10.9
1	B	92	VAL	10.9
1	B	58	ILE	10.9
1	A	41	GLN	10.8
1	B	27	ASN	10.7
1	A	102	GLY	10.6
1	B	33	LYS	10.6
1	A	122	ALA	10.6
1	A	81	SER	10.5
1	A	96	LYS	10.5
1	B	16	GLY	10.5
1	B	96	LYS	10.5
1	B	93	ASN	10.5
1	B	110	ALA	10.4
1	B	107	ALA	10.3
1	A	51	THR	10.3
1	B	77	ASN	10.3
1	A	101	ASP	10.2
1	B	22	GLY	10.2
1	B	51	THR	10.2
1	B	9	ALA	10.1
1	A	33	LYS	10.0
1	B	17	LEU	10.0

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Mol	Chain	Res	Type	RSRZ
1	B	53	TYR	10.0
1	B	7	GLU	10.0
1	B	28	TRP	9.7
1	A	100	SER	9.5
1	A	112	ARG	9.5
1	A	107	ALA	9.4
1	A	36	SER	9.3
1	A	97	LYS	9.3
1	A	91	SER	9.3
1	A	31	ALA	9.2
1	B	63	TRP	9.2
1	A	27	ASN	9.1
1	B	15	HIS	9.1
1	A	23	TYR	9.1
1	B	70	PRO	9.0
1	A	61	ARG	8.9
1	B	116	LYS	8.8
1	B	124	ILE	8.8
1	B	8	LEU	8.8
1	A	9	ALA	8.7
1	B	121	GLN	8.7
1	A	76	CYS	8.6
1	A	110	ALA	8.6
1	A	116	LYS	8.5
1	A	46	ASN	8.5
1	A	115	CYS	8.4
1	A	127	CYS	8.4
1	B	85	SER	8.3
1	A	117	GLY	8.3
1	A	114	ARG	8.3
1	A	32	ALA	8.2
1	A	95	ALA	8.1
1	B	10	ALA	8.1
1	B	20	TYR	8.0
1	B	128	ARG	8.0
1	A	86	SER	8.0
1	A	10	ALA	7.9
1	B	3	PHE	7.9
1	B	83	LEU	7.9
1	A	70	PRO	7.9
1	A	60	SER	7.8
1	B	24	SER	7.8

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Mol	Chain	Res	Type	RSRZ
1	A	49	GLY	7.8
1	A	84	LEU	7.8
1	B	103	ASN	7.7
1	B	26	GLY	7.7
1	A	25	LEU	7.6
1	A	50	SER	7.4
1	A	98	ILE	7.4
1	A	113	ASN	7.2
1	B	97	LYS	7.2
1	A	5	ARG	7.2
1	B	71	GLY	7.1
1	B	91	SER	7.1
1	A	72	SER	7.0
1	A	14	ARG	7.0
1	B	32	ALA	7.0
1	B	2	VAL	7.0
1	B	21	ARG	6.9
1	A	123	TRP	6.9
1	A	111	TRP	6.8
1	B	98	ILE	6.8
1	B	37	ASN	6.7
1	A	103	ASN	6.7
1	B	90	ALA	6.6
1	B	127	CYS	6.6
1	B	102	GLY	6.6
1	A	109	VAL	6.6
1	A	39	ASN	6.6
1	A	52	ASP	6.5
1	A	47	THR	6.5
1	B	6	CYS	6.5
1	A	15	HIS	6.4
1	B	82	ALA	6.3
1	B	108	TRP	6.3
1	B	113	ASN	6.3
1	B	81	SER	6.3
1	A	126	GLY	6.3
1	B	60	SER	6.2
1	A	120	VAL	6.0
1	B	76	CYS	6.0
1	B	41	GLN	6.0
1	B	56	LEU	6.0
1	B	111	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	87	ASP	5.9
1	B	40	THR	5.8
1	B	100	SER	5.8
1	B	11	ALA	5.8
1	B	31	ALA	5.6
1	A	26	GLY	5.6
1	A	88	ILE	5.6
1	B	94	CYS	5.6
1	B	42	ALA	5.5
1	A	1	LYS	5.5
1	B	4	GLY	5.3
1	A	58	ILE	5.2
1	A	71	GLY	5.1
1	B	34	PHE	5.1
1	B	36	SER	5.0
1	A	121	GLN	5.0
1	A	69	THR	4.8
1	A	8	LEU	4.8
1	A	53	TYR	4.8
1	B	114	ARG	4.8
1	A	83	LEU	4.6
1	B	78	ILE	4.6
1	B	69	THR	4.5
1	A	125	ARG	4.4
1	B	68	ARG	4.4
1	B	66	ASP	4.3
1	B	61	ARG	4.3
1	A	128	ARG	4.2
1	A	118	THR	4.1
1	A	37	ASN	4.1
1	A	108	TRP	4.0
1	A	16	GLY	3.9
1	B	12	MET	3.9
1	B	117	GLY	3.9
1	B	67	GLY	3.8
1	B	126	GLY	3.8
1	A	57	GLN	3.6
1	B	119	ASP	3.6
1	B	84	LEU	3.5
1	A	99	VAL	3.4
1	A	78	ILE	3.4
1	A	67	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	38	PHE	3.2
1	B	54	GLY	3.2
1	A	82	ALA	3.0
1	B	99	VAL	2.9
1	B	123	TRP	2.8
1	B	55	ILE	2.7
1	B	49	GLY	2.7
1	A	38	PHE	2.6
1	B	120	VAL	2.5
1	A	7	GLU	2.4
1	B	129	LEU	2.3
1	A	79	PRO	2.2
1	B	5	ARG	2.1

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.