



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:39 PM EDT

PDB ID : 1LYS / pdb_00001lys
Title : X-RAY STRUCTURE OF A MONOCLINIC FORM OF HEN EGG-WHITE
LYSOZYME CRYSTALLIZED AT 313K. COMPARISON OF TWO INDE-
PENDENT MOLECULES
Authors : Harata, K.
Deposited on : 1993-12-03
Resolution : 1.72 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

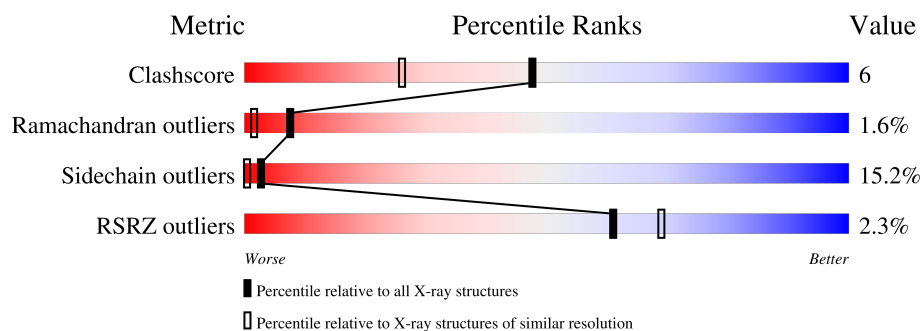
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	4% 75% 14% 10% .
1	B	129	% 71% 19% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2217 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	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	B	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

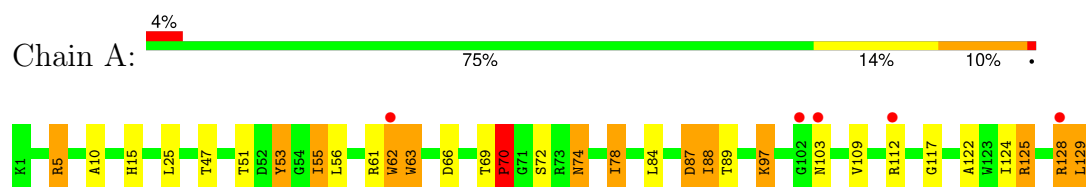
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	98	Total	O	0	0
			98	98		
2	B	117	Total	O	0	0
			117	117		

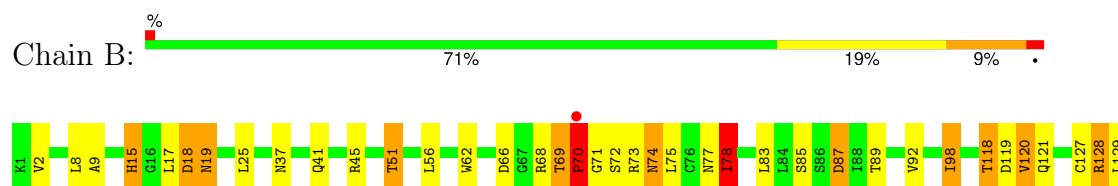
3 Residue-property plots [i](#)

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: 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	27.23Å 63.66Å 59.12Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	10.00 – 1.72 10.00 – 1.72	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.72) 84.9 (10.00-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 1.71Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available) 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 104.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2217	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 75.59 % 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 1.2263e-06. 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, 0.333 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	2/1021 (0.2%)	1.84	24/1379 (1.7%)
1	B	1.09	3/1021 (0.3%)	1.86	24/1379 (1.7%)
All	All	1.04	5/2042 (0.2%)	1.85	48/2758 (1.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	HIS	CD2-NE2	-7.60	1.29	1.37
1	A	15	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	69	THR	CA-CB	5.37	1.61	1.54
1	B	51	THR	CA-CB	5.29	1.65	1.54
1	A	15	HIS	CG-ND1	-5.10	1.32	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	THR	CA-C-N	8.55	130.52	119.84
1	B	69	THR	C-N-CA	8.55	130.52	119.84
1	B	2	VAL	N-CA-C	-8.29	95.10	107.37
1	A	55	ILE	CB-CA-C	-8.12	100.19	112.05
1	B	71	GLY	N-CA-C	-7.72	94.88	113.18
1	A	74	ASN	OD1-CG-ND2	-7.53	115.07	122.60
1	B	78	ILE	N-CA-CB	-7.07	104.08	111.64
1	A	128	ARG	N-CA-C	-7.06	98.45	109.25
1	B	127	CYS	O-C-N	7.04	130.92	122.68
1	A	62	TRP	CG-CD2-CE3	6.93	140.83	133.90
1	A	74	ASN	CB-CG-ND2	6.88	126.73	116.40
1	B	118	THR	N-CA-CB	-6.80	99.91	110.46
1	A	63	TRP	CG-CD2-CE3	6.54	140.44	133.90
1	B	120	VAL	N-CA-CB	-6.46	99.61	110.65
1	B	121	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	B	98	ILE	CB-CG1-CD1	-6.16	100.86	113.80
1	B	70	PRO	CA-N-CD	-6.14	103.40	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ILE	N-CA-C	6.03	115.83	109.01
1	B	118	THR	OG1-CB-CG2	5.90	121.10	109.30
1	A	15	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	B	41	GLN	CA-CB-CG	-5.85	102.39	114.10
1	B	19	ASN	CA-CB-CG	-5.80	106.80	112.60
1	A	88	ILE	CA-CB-CG2	5.75	120.28	110.50
1	A	62	TRP	CB-CG-CD1	-5.72	118.32	126.90
1	A	109	VAL	CB-CA-C	-5.66	104.50	112.14
1	B	15	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	B	78	ILE	CB-CA-C	5.66	114.87	109.33
1	A	87	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	62	TRP	CE2-CD2-CE3	5.63	124.43	118.80
1	A	89	THR	N-CA-C	5.55	117.78	111.11
1	A	55	ILE	N-CA-CB	5.46	119.11	110.54
1	B	89	THR	CA-C-O	-5.45	115.07	120.90
1	B	66	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	74	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	70	PRO	N-CA-C	5.43	122.57	113.78
1	B	62	TRP	CG-CD1-NE1	-5.34	103.26	110.20
1	B	18	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	88	ILE	N-CA-CB	-5.29	98.74	111.23
1	A	53	TYR	N-CA-C	5.29	117.53	108.90
1	B	87	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	69	THR	CA-C-N	5.23	124.68	119.24
1	A	69	THR	C-N-CA	5.23	124.68	119.24
1	A	5	ARG	N-CA-C	5.18	117.32	111.11
1	A	88	ILE	CA-CB-CG1	-5.17	101.61	110.40
1	B	77	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	66	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	63	TRP	CB-CG-CD1	-5.10	119.25	126.90
1	A	124	ILE	N-CA-C	-5.08	107.35	112.17

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	1001	0	959	14	0
1	B	1001	0	959	10	0
2	A	98	0	0	1	0
2	B	117	0	0	1	0
All	All	2217	0	1918	22	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 6.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:THR:HG22	1:B:70:PRO:HD2	1.49	0.92
1:B:74:ASN:HD21	1:B:78:ILE:H	1.25	0.84
1:B:69:THR:CG2	1:B:70:PRO:HD2	2.15	0.74
1:B:70:PRO:HG2	1:B:72:SER:HB3	1.74	0.69
1:A:72:SER:HB2	2:A:216:HOH:O	1.92	0.69
1:A:117:GLY:HA3	1:B:78:ILE:HD11	1.82	0.61
1:A:10:ALA:HA	1:A:129:LEU:HD11	1.84	0.59
1:A:74:ASN:HD21	1:A:78:ILE:H	1.52	0.58
1:B:15:HIS:HB3	1:B:92:VAL:HG11	1.86	0.57
1:A:62:TRP:HE3	1:A:63:TRP:HE1	1.60	0.48
1:A:62:TRP:HE3	1:A:63:TRP:NE1	2.14	0.46
1:A:122:ALA:HA	1:A:125:ARG:HH11	1.81	0.46
1:B:128:ARG:HB3	1:B:129:LEU:H	1.51	0.43
1:B:9:ALA:HB1	1:B:129:LEU:HD11	2.01	0.43
1:A:51:THR:HB	1:A:53:TYR:CE1	2.54	0.42
1:A:5:ARG:NH2	1:A:125:ARG:O	2.52	0.41
1:B:129:LEU:HB2	2:B:243:HOH:O	2.20	0.41
1:A:97:LYS:NZ	1:A:97:LYS:HB2	2.36	0.41
1:A:117:GLY:CA	1:B:78:ILE:HD11	2.48	0.40
1:A:61:ARG:HH22	1:A:70:PRO:HB2	1.86	0.40
1:A:74:ASN:HD21	1:A:78:ILE:N	2.16	0.40
1:A:74:ASN:ND2	1:A:78:ILE:H	2.16	0.40

There are no symmetry-related clashes.

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	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	5
1	B	127/129 (98%)	120 (94%)	4 (3%)	3 (2%)	4	0
All	All	254/258 (98%)	242 (95%)	8 (3%)	4 (2%)	7	1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	PRO
1	B	128	ARG
1	A	103	ASN
1	B	18	ASP

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	105/105 (100%)	92 (88%)	13 (12%)	4	0
1	B	105/105 (100%)	86 (82%)	19 (18%)	2	0
All	All	210/210 (100%)	178 (85%)	32 (15%)	3	0

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	47	THR

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Mol	Chain	Res	Type
1	A	55	ILE
1	A	56	LEU
1	A	70	PRO
1	A	84	LEU
1	A	87	ASP
1	A	88	ILE
1	A	97	LYS
1	A	112	ARG
1	A	125	ARG
1	A	128	ARG
1	A	129	LEU
1	B	8	LEU
1	B	17	LEU
1	B	19	ASN
1	B	25	LEU
1	B	37	ASN
1	B	45	ARG
1	B	51	THR
1	B	56	LEU
1	B	68	ARG
1	B	73	ARG
1	B	75	LEU
1	B	78	ILE
1	B	83	LEU
1	B	85	SER
1	B	87	ASP
1	B	98	ILE
1	B	118	THR
1	B	119	ASP
1	B	120	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	59	ASN
1	A	65	ASN
1	A	74	ASN
1	A	103	ASN
1	B	15	HIS
1	B	37	ASN
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	103	ASN

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 [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, 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%)	-0.11	5 (3%) 43 51	6, 15, 33, 47	0
1	B	129/129 (100%)	-0.39	1 (0%) 82 87	4, 11, 26, 46	0
All	All	258/258 (100%)	-0.25	6 (2%) 61 69	4, 13, 33, 47	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	GLY	6.7
1	B	70	PRO	4.5
1	A	62	TRP	3.5
1	A	112	ARG	2.4
1	A	103	ASN	2.4
1	A	128	ARG	2.3

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.