Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2023 – 04:03 PM EDT

PDB ID	:	1LKS
Title	:	HEN EGG WHITE LYSOZYME NITRATE
Authors	:	Steinrauf, L.K.
Deposited on	:	1997-10-09
Resolution	:	1.10 Å(reported)

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

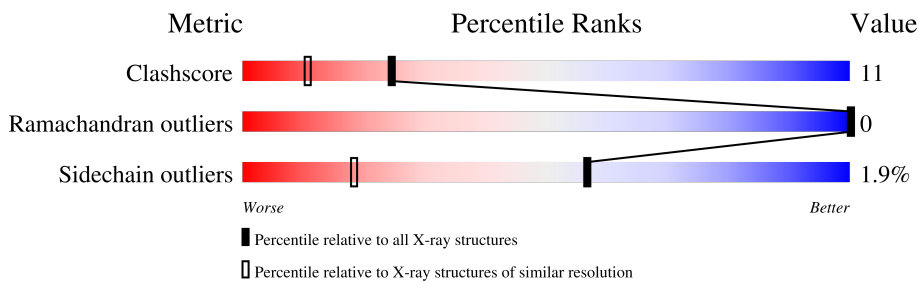|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.10 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		1.9%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)

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 <=5%

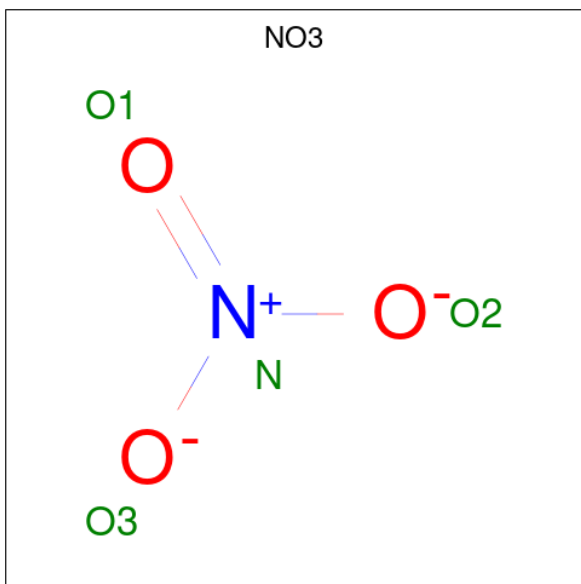| Mol	Chain	Length	Quality of chain
1	A	129	84% 11% 5% •

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 1235 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 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	6	0
			1014	618	197	189	10			

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO_3).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	N 1	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total 197	O 197	0	0

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. 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. 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: LYSOZYME

Chain A:

84%   11%   5% ·

K1 V2 F3 G4 R5 R14 D18 N19 Y20 R21 Y53 R61 W62 R68 R73 V99 G102 N103 G104 M105 N106 R112 R125 G126 C127 R128 L129
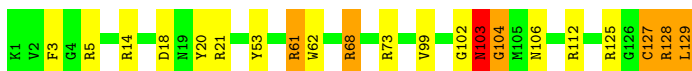
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	31.97Å 65.08Å 27.25Å 94.57° 111.56° 82.98°	Depositor
Resolution (Å)	20.00 – 1.10 64.55 – 1.75	Depositor EDS
% Data completeness (in resolution range)	78.8 (20.00-1.10) 77.0 (64.55-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 1.74Å)	Xtriage
Refinement program	SHELXL-93	Depositor
R, R_{free}	(Not available) , (Not available) 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 69.4	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	1235	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 99.79 % 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 2.0206e-14. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NO3

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	1.22	7/1064 (0.7%)	1.82	28/1435 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	TRP	CD1-NE1	9.38	1.53	1.38
1	A	62	TRP	CG-CD1	-8.15	1.25	1.36
1	A	127	CYS	C-N	-6.22	1.19	1.34
1	A	5	ARG	CB-CG	-5.94	1.36	1.52
1	A	104	GLY	N-CA	5.47	1.54	1.46
1	A	61[A]	ARG	CZ-NH2	5.02	1.39	1.33
1	A	61[B]	ARG	CZ-NH2	5.02	1.39	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61[A]	ARG	CD-NE-CZ	24.25	157.55	123.60
1	A	61[B]	ARG	CD-NE-CZ	24.25	157.55	123.60
1	A	112	ARG	CD-NE-CZ	19.83	151.37	123.60
1	A	128	ARG	O-C-N	10.86	140.08	122.70
1	A	112	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	A	128	ARG	CA-C-N	-8.43	98.65	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61[A]	ARG	NH1-CZ-NH2	-8.36	110.20	119.40
1	A	61[B]	ARG	NH1-CZ-NH2	-8.36	110.20	119.40
1	A	73	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	68	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	20	TYR	CZ-CE2-CD2	7.07	126.16	119.80
1	A	62	TRP	CB-CG-CD2	-6.70	117.89	126.60
1	A	125	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	5	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	21	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	103	ASN	C-N-CA	-6.07	109.55	122.30
1	A	21	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	103	ASN	CB-CA-C	5.88	122.17	110.40
1	A	62	TRP	CD1-CG-CD2	5.88	111.01	106.30
1	A	128	ARG	CB-CA-C	-5.87	98.67	110.40
1	A	5	ARG	CA-CB-CG	5.86	126.28	113.40
1	A	14	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	53	TYR	CB-CG-CD1	5.66	124.40	121.00
1	A	128	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	125	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	125	ARG	NH1-CZ-NH2	5.39	125.33	119.40
1	A	3	PHE	CB-CG-CD2	5.31	124.52	120.80
1	A	18	ASP	CB-CG-OD1	5.26	123.03	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	103	ASN	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASN	Sidechain
1	A	127	CYS	Peptide
1	A	61[A]	ARG	Sidechain
1	A	61[B]	ARG	Sidechain

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	1014	0	963	20	0
2	A	24	0	0	1	0
3	A	197	0	0	4	0
All	All	1235	0	963	20	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 11.

All (20) 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:A:128:ARG:HB3	1:A:129:LEU:HG	1.16	1.13
1:A:128:ARG:HG3	1:A:129:LEU:H	1.10	1.09
1:A:128:ARG:HG3	1:A:129:LEU:N	1.73	1.03
1:A:128:ARG:CG	1:A:129:LEU:H	1.40	0.97
1:A:128:ARG:HB3	1:A:129:LEU:CG	1.99	0.93
1:A:106:ASN:OD1	3:A:228:HOH:O	1.92	0.88
1:A:128:ARG:CG	1:A:129:LEU:N	2.22	0.83
1:A:106:ASN:ND2	2:A:133:NO3:N	2.29	0.80
1:A:102[B]:GLY:O	1:A:103:ASN:HB3	1.98	0.63
1:A:128:ARG:HG3	1:A:129:LEU:CA	2.31	0.59
1:A:128:ARG:O	1:A:129:LEU:O	2.26	0.54
1:A:128:ARG:HG2	1:A:129:LEU:HD23	1.91	0.52
1:A:104:GLY:N	3:A:213:HOH:O	2.44	0.47
1:A:99:VAL:HA	1:A:103:ASN:O	2.15	0.46
1:A:68:ARG:NH2	3:A:173:HOH:O	2.45	0.45
1:A:68:ARG:HG3	1:A:68:ARG:HH11	1.82	0.44
1:A:128:ARG:CG	1:A:129:LEU:HD23	2.48	0.43
1:A:128:ARG:HG3	1:A:129:LEU:HA	1.99	0.43
1:A:106:ASN:HB2	3:A:213:HOH:O	2.19	0.41
1:A:128:ARG:C	1:A:129:LEU:O	2.60	0.41

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

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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	132/129 (102%)	130 (98%)	2 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	110/105 (105%)	108 (98%)	2 (2%)	59	21

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	129	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	NO3	A	133	1	1,3,3	0.34	0	0,3,3	-	-
2	NO3	A	132	-	1,3,3	0.12	0	0,3,3	-	-
2	NO3	A	130	-	1,3,3	1.14	0	0,3,3	-	-
2	NO3	A	131	-	1,3,3	0.68	0	0,3,3	-	-
2	NO3	A	134	-	1,3,3	0.71	0	0,3,3	-	-
2	NO3	A	135	-	1,3,3	0.26	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	133	NO3	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

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5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	127:CYS	C	128:ARG	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.