



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:01 PM EDT

PDB ID : 2FBB / pdb_00002fbb
Title : Crystal Structure Analysis of Hexagonal Lysozyme
Authors : Brinkmann, C.; Weiss, M.S.; Weckert, E.
Deposited on : 2005-12-09
Resolution : 1.46 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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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 1.46 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1252 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.

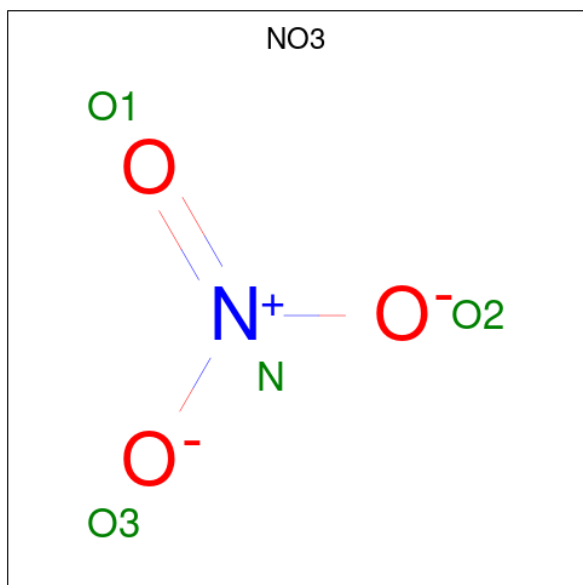
- Molecule 1 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1010	617	195	188	10	0	3	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	5	5	5	0	0

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	1
			8	2	6		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	1
			8	2	6		
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total	O	0	0
			165	165		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.64Å 85.64Å 67.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.00 – 1.46	Depositor
% Data completeness (in resolution range)	98.1 (70.00-1.46)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 1.46Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.198	Depositor
Wilson B-factor (Å ²)	20.3	Xtrriage
Anisotropy	0.069	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1252	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 for Mogul analysis.

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
3	NO3	A	151	-	1,3,3	0.87	0	0,3,3	-	-
3	NO3	A	163[B]	-	1,3,3	3.43	1 (100%)	0,3,3	-	-
3	NO3	A	159[A]	-	1,3,3	3.37	1 (100%)	0,3,3	-	-
3	NO3	A	164	-	1,3,3	3.87	1 (100%)	0,3,3	-	-
3	NO3	A	152	2	1,3,3	3.56	1 (100%)	0,3,3	-	-
3	NO3	A	155	-	1,3,3	2.56	1 (100%)	0,3,3	-	-
3	NO3	A	161	2	1,3,3	2.69	1 (100%)	0,3,3	-	-
3	NO3	A	154	-	1,3,3	0.32	0	0,3,3	-	-
3	NO3	A	158	-	1,3,3	2.64	1 (100%)	0,3,3	-	-
3	NO3	A	150	2	1,3,3	3.18	1 (100%)	0,3,3	-	-
3	NO3	A	162	-	1,3,3	3.33	1 (100%)	0,3,3	-	-
3	NO3	A	163[A]	-	1,3,3	3.29	1 (100%)	0,3,3	-	-
3	NO3	A	153	2	1,3,3	2.62	1 (100%)	0,3,3	-	-
3	NO3	A	165	-	1,3,3	4.24	1 (100%)	0,3,3	-	-
3	NO3	A	156	2	1,3,3	3.10	1 (100%)	0,3,3	-	-
3	NO3	A	160	-	1,3,3	2.43	1 (100%)	0,3,3	-	-
3	NO3	A	157	-	1,3,3	3.41	1 (100%)	0,3,3	-	-
3	NO3	A	159[B]	-	1,3,3	2.55	1 (100%)	0,3,3	-	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	165	NO3	O1-N	4.24	1.45	1.24
3	A	164	NO3	O1-N	3.87	1.43	1.24
3	A	152	NO3	O1-N	3.56	1.41	1.24
3	A	163[B]	NO3	O1-N	3.43	1.41	1.24
3	A	157	NO3	O1-N	3.41	1.41	1.24
3	A	159[A]	NO3	O1-N	3.37	1.40	1.24
3	A	162	NO3	O1-N	3.33	1.40	1.24
3	A	163[A]	NO3	O1-N	3.29	1.40	1.24
3	A	150	NO3	O1-N	3.18	1.39	1.24
3	A	156	NO3	O1-N	3.10	1.39	1.24
3	A	161	NO3	O1-N	2.69	1.37	1.24
3	A	158	NO3	O1-N	2.64	1.37	1.24
3	A	153	NO3	O1-N	2.62	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	NO3	O1-N	2.56	1.36	1.24
3	A	159[B]	NO3	O1-N	2.55	1.36	1.24
3	A	160	NO3	O1-N	2.43	1.36	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	158	NO3	0	3
3	A	150	NO3	0	3

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.