

wwPDB X-ray Structure Validation Summary Report (i)

Aug 19, 2023 – 06:26 PM EDT

PDB ID : 2FBB

Title : Crystal Structure Analysis of Hexagonal Lysozyme

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Deposited on : 2005-12-09

Resolution : 1.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) 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 : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

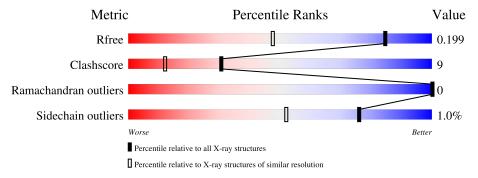
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.46 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)

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	85%	13%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	A	150	-	-	X	-
3	NO3	A	158	-	-	X	-
3	NO3	A	163[B]	-	-	X	-



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.

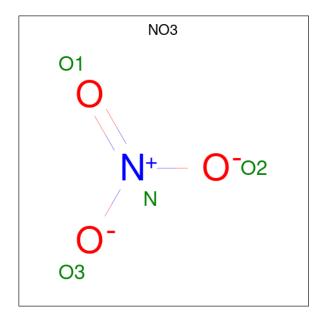
• Molecule 1 is a protein called Lysozyme C.

\mathbf{N}	Iol	Chain	Residues		\mathbf{A}_{1}	toms			ZeroOcc	AltConf	Trace
	1	A	129	Total 1010	C 617	N 195	O 188	S 10	0	3	0

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

• Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

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

• Molecule 4 is water.

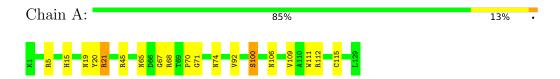
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	165	Total O 165 165	0	0



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. 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 C





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	85.64Å 85.64Å 67.93Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.00 - 1.46	Depositor
rtesolution (A)	42.82 - 1.46	EDS
% Data completeness	98.1 (70.00-1.46)	Depositor
(in resolution range)	98.1 (42.82-1.46)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.39 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
P. P.	0.183 , 0.198	Depositor
R, R_{free}	0.192 , 0.199	DCC
R_{free} test set	503 reflections $(1.97%)$	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.43, 42.3	EDS
L-test for twinning ²	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1252	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage'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.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.92	0/1046	1.00	1/1412 (0.1%)	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	5	ARG	NE-CZ-NH1	5.48	123.04	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	SER	Peptide

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	1010	0	955	18	0
2	A	5	0	0	0	0
3	A	72	0	0	3	6
4	A	165	0	0	11	1
All	All	1252	0	955	19	7

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 9.

The worst 5 of 19 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:106:ASN:ND2	4:A:1091:HOH:O	2.11	0.83
1:A:15:HIS:HD2	4:A:1165:HOH:O	1.74	0.70
1:A:19[A]:ASN:OD1	4:A:1039:HOH:O	2.11	0.69
1:A:71:GLY:HA2	4:A:1148:HOH:O	1.99	0.62
3:A:156:NO3:O1	4:A:1038:HOH:O	2.16	0.62

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
3:A:150:NO3:O1	3:A:150:NO3:O2[8_556]	0.07	2.13
3:A:150:NO3:N	3:A:150:NO3:O2[8_556]	1.33	0.87
3:A:158:NO3:N	3:A:158:NO3:O3[8_556]	1.34	0.86
3:A:158:NO3:N	3:A:158:NO3:O1[8_556]	1.37	0.83
3:A:150:NO3:N	3:A:150:NO3:O1[8_556]	1.40	0.80

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	129/129 (100%)	125 (97%)	4 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	Analysed Rotameric		Percentiles	
1	A	108/105 (103%)	107 (99%)	1 (1%)	78 57	

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	65	ASN
1	A	93	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 monosaccharides in this entry.



5.6 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	Trno	Chain	Res	Link	В	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	NO3	A	160	-	1,3,3	2.66	1 (100%)	0,3,3	-	-	
3	NO3	A	152	2	1,3,3	3.86	1 (100%)	0,3,3	-	-	
3	NO3	A	154	-	1,3,3	0.41	0	0,3,3	-	=	
3	NO3	A	163[A]	-	1,3,3	3.57	1 (100%)	0,3,3	-	-	
3	NO3	A	153	2	1,3,3	2.85	1 (100%)	0,3,3	_	-	
3	NO3	A	156	2	1,3,3	3.36	1 (100%)	0,3,3	-	-	
3	NO3	A	150	2	1,3,3	3.45	1 (100%)	0,3,3	-	-	
3	NO3	A	161	2	1,3,3	2.93	1 (100%)	0,3,3	-	-	
3	NO3	A	165	-	1,3,3	4.59	1 (100%)	0,3,3	-	-	
3	NO3	A	155	-	1,3,3	2.78	1 (100%)	0,3,3	-	-	
3	NO3	A	164	-	1,3,3	4.18	1 (100%)	0,3,3	-	-	
3	NO3	A	151	-	1,3,3	0.98	0	0,3,3	-	-	
3	NO3	A	162	-	1,3,3	3.61	1 (100%)	0,3,3	_	-	
3	NO3	A	163[B]	-	1,3,3	3.72	1 (100%)	0,3,3	_	-	
3	NO3	A	157	-	1,3,3	3.70	1 (100%)	0,3,3	-	-	
3	NO3	A	159[B]	-	1,3,3	2.78	1 (100%)	0,3,3	-	-	
3	NO3	A	158	-	1,3,3	2.87	1 (100%)	0,3,3	-	-	
3	NO3	A	159[A]	-	1,3,3	3.65	1 (100%)	0,3,3	-	-	

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
3	A	165	NO3	O1-N	4.59	1.45	1.24
3	A	164	NO3	O1-N	4.18	1.43	1.24
3	A	152	NO3	O1-N	3.86	1.41	1.24
3	A	163[B]	NO3	O1-N	3.72	1.41	1.24
3	A	157	NO3	O1-N	3.70	1.41	1.24



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	156	NO3	1	0
3	A	150	NO3	0	3
3	A	163[B]	NO3	2	0
3	A	158	NO3	0	3

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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

