



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:12 am GMT

PDB ID : 6HU5  
Title : STRUCTURE OF HEWL BY ELECTRON DIFFRACTION AND MICRO-FOCUS DIFFRACTION  
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Deposited on : 2018-10-05  
Resolution : 2.80 Å (reported)  
Based on initial model : 1B2K

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

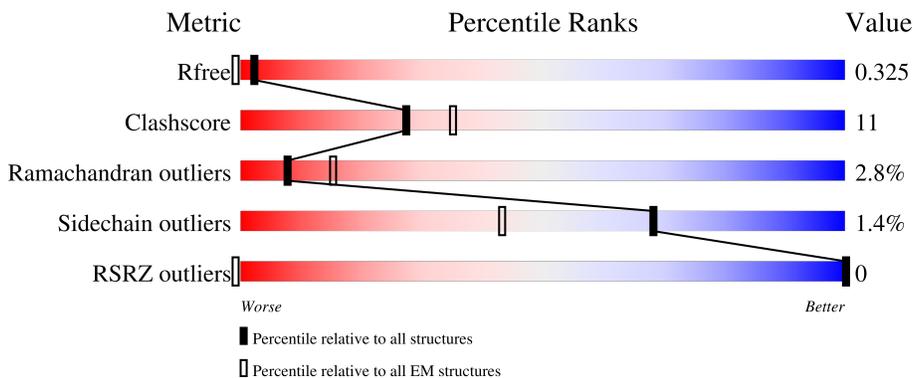
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)
$R_{free}$	130704	0
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RSRZ outliers	127900	0

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	129	 76% 22% .
1	B	129	 75% 22% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1991 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
			Total	C	N	O	S		
1	A	129	1008	618	196	184	10	1	0
1	B	128	980	602	186	182	10	0	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Cl	0
			1	1	
2	B	2	Total	Cl	0
			2	2	

### 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

Chain A:  76% 22%



- Molecule 1: Lysozyme C

Chain B:  75% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	31.85Å 54.38Å 71.79Å 90.00° 98.82° 90.00°	Depositor
Resolution (Å)	42.67 – 2.80 31.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	63.0 (42.67-2.80) 53.7 (31.47-2.80)	Depositor EDS
$R_{merge}$	0.66	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.297 , 0.339 0.306 , 0.325	Depositor DCC
$R_{free}$ test set	177 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtrriage
Anisotropy	0.747	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	1991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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](#)

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

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	0.28	0/1031	0.50	0/1393
1	B	0.29	0/1000	0.52	0/1353
All	All	0.29	0/2031	0.51	0/2746

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	46	ASN	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	1008	0	972	24	0
1	B	980	0	929	20	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
All	All	1991	0	1901	42	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.

The worst 5 of 42 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:127:CYS:HB3	1:A:129:LEU:HG	1.70	0.74
1:A:121:GLN:O	1:A:123:TRP:N	2.29	0.65
1:B:121:GLN:O	1:B:123:TRP:N	2.29	0.64
1:A:128:ARG:HA	1:A:128:ARG:HE	1.62	0.64
1:A:46:ASN:O	1:A:48:ASP:N	2.32	0.62

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	128/129 (99%)	120 (94%)	5 (4%)	3 (2%)	6	21
1	B	126/129 (98%)	117 (93%)	5 (4%)	4 (3%)	4	13
All	All	254/258 (98%)	237 (93%)	10 (4%)	7 (3%)	8	17

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	THR

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Mol	Chain	Res	Type
1	A	47	THR
1	A	71	GLY
1	A	122	ALA
1	B	48	ASP

### 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 PDB entries followed by that with respect to all EM entries.

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	106/105 (101%)	104 (98%)	2 (2%)	57	85
1	B	102/105 (97%)	101 (99%)	1 (1%)	76	93
All	All	208/210 (99%)	205 (99%)	3 (1%)	68	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	128	ARG
1	B	19	ASN

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	57	GLN
1	A	113	ASN
1	B	57	GLN

### 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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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.