



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2020 – 02:31 PM EST

PDB ID : 7K4W  
Title : Crystal structure of Kemp Eliminase HG3.17 in the inactive state  
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Deposited on : 2020-09-16  
Resolution : 1.90 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

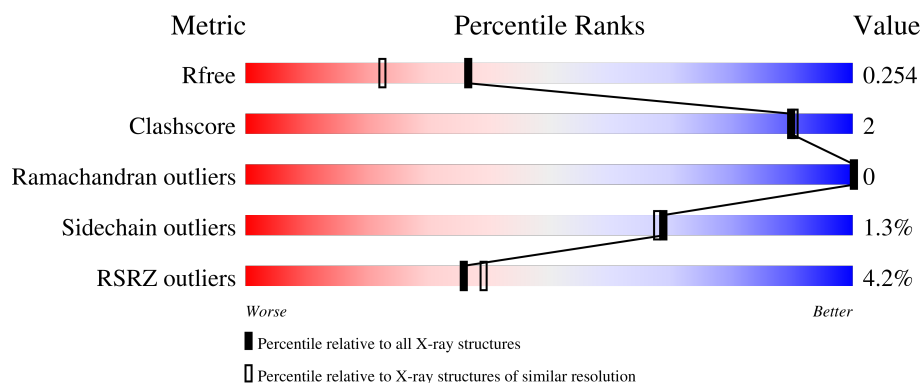
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on the lower 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  $\leq 5\%$ . 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	308	<div> <div>4%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4619 atoms, of which 2203 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	H	N	O	S	0	11	0
			4462	1428	2203	390	430	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P23360
A	-3	SER	-	expression tag	UNP P23360
A	-2	GLY	-	expression tag	UNP P23360
A	-1	MET	-	expression tag	UNP P23360
A	0	ALA	-	expression tag	UNP P23360
A	1	GLU	-	expression tag	UNP P23360
A	6	ILE	VAL	conflict	UNP P23360
A	37	LYS	GLN	conflict	UNP P23360
A	42	MET	GLN	conflict	UNP P23360
A	44	TRP	THR	conflict	UNP P23360
A	47	GLU	ASN	engineered mutation	UNP P23360
A	50	GLN	LYS	conflict	UNP P23360
A	81	GLY	ARG	conflict	UNP P23360
A	82	ALA	GLY	conflict	UNP P23360
A	83	GLY	HIS	conflict	UNP P23360
A	84	CYS	THR	conflict	UNP P23360
A	89	ASN	SER	conflict	UNP P23360
A	90	PHE	GLN	conflict	UNP P23360
A	105	ILE	THR	conflict	UNP P23360
A	125	THR	ALA	conflict	UNP P23360
A	130	GLY	ASN	conflict	UNP P23360
A	142	ASN	THR	conflict	UNP P23360
A	172	MET	ASN	conflict	UNP P23360
A	208	MET	THR	conflict	UNP P23360
A	234	SER	ALA	conflict	UNP P23360
A	236	LEU	THR	conflict	UNP P23360
A	237	MET	GLU	conflict	UNP P23360

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Chain	Residue	Modelled	Actual	Comment	Reference
A	267	MET	TRP	conflict	UNP P23360
A	275	ALA	TRP	conflict	UNP P23360
A	276	PHE	ARG	conflict	UNP P23360
A	279	SER	THR	conflict	UNP P23360
A	300	ASN	ASP	engineered mutation	UNP P23360

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

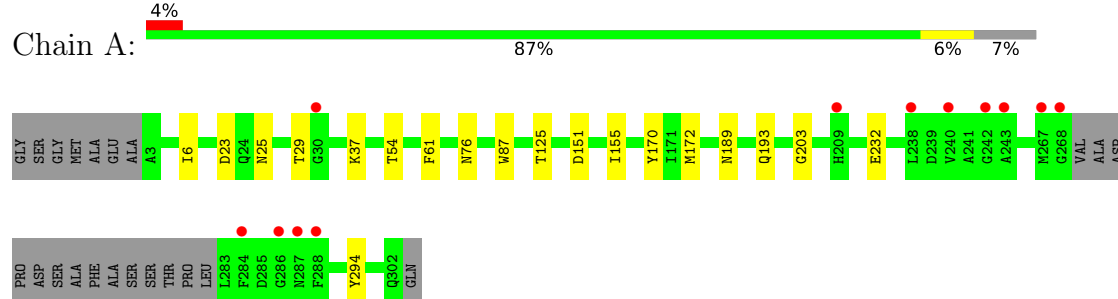
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	156	Total O 156 156	0	0



- Molecule 1: Endo-1,4-beta-xylanase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.39Å 67.39Å 74.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.04 – 1.90 50.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.04-1.90) 84.0 (50.04-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.64 (at 1.90Å)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, $R_{free}$	0.210 , 0.255 0.210 , 0.254	Depositor DCC
$R_{free}$ test set	1999 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% 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

### 5.1 Standard geometry

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

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	0.41	0/2310	0.60	0/3148

There are no bond length outliers.

There are no bond angle outliers.

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	2259	2203	2190	8	0
2	A	1	0	0	0	0
3	A	156	0	0	0	0
All	All	2416	2203	2190	8	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 2.

All (8) 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:6:ILE:HD11	1:A:294:TYR:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:O	1:A:61:PHE:HA	2.09	0.52
1:A:203:GLY:HA2	1:A:232:GLU:O	2.12	0.49
1:A:37:LYS:HE3	1:A:76:ASN:OD1	2.12	0.49
1:A:25:ASN:O	1:A:29:THR:HG23	2.14	0.48
1:A:125:THR:HG23	1:A:170:TYR:CD1	2.49	0.47
1:A:151:ASP:OD2	1:A:155:ILE:HD11	2.20	0.41
1:A:189:ASN:O	1:A:193:GLN:HG3	2.21	0.41

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 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	293/308 (95%)	290 (99%)	3 (1%)	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	Rotameric	Outliers	Percentiles	
1	A	239/246 (97%)	235 (98%)	4 (2%)	60	57

All (4) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	23	ASP
1	A	87[A]	TRP
1	A	87[B]	TRP
1	A	172	MET

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

Mol	Chain	Res	Type
1	A	24	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 1 ligands modelled in this entry, 1 is 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	286/308 (92%)	0.44	12 (4%) 36 39	14, 21, 50, 87	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	ALA	6.0
1	A	287	ASN	4.9
1	A	30	GLY	4.9
1	A	288	PHE	4.6
1	A	240	VAL	3.2
1	A	286	GLY	3.0
1	A	209[A]	HIS	2.5
1	A	267	MET	2.5
1	A	238	LEU	2.4
1	A	284	PHE	2.1
1	A	242	GLY	2.1
1	A	268	GLY	2.0

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	401	1/1	0.93	0.09	27,27,27,27	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.