



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2020 – 02:37 PM EST

PDB ID : 7K4P  
Title : Crystal structure of Kemp Eliminase HG3  
Authors : Padua, R.A.P.; Otten, R.; Bunzel, A.; Nguyen, V.; Pitsawong, W.; Patterson, M.; Sui, S.; Perry, S.L.; Cohen, A.E.; Hilvert, D.; Kern, D.  
Deposited on : 2020-09-16  
Resolution : 1.08 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.

---

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

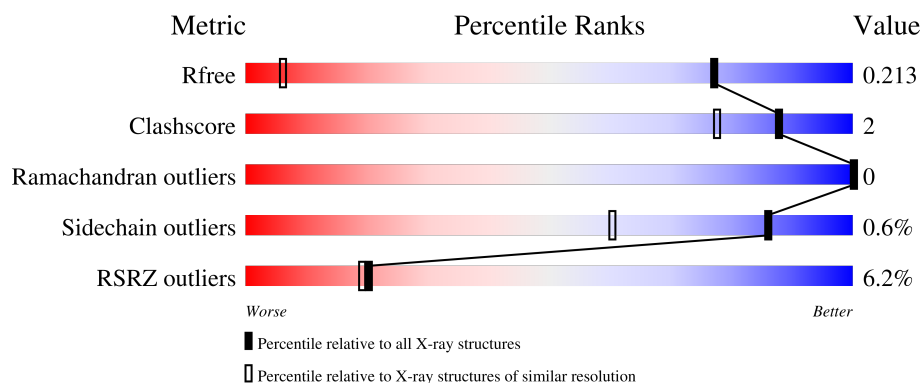
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.08 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	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)
RSRZ outliers	127900	1359 (1.12-1.04)

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>6%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	308	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12290 atoms, of which 6009 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	299	Total	C	H	N	O	S	0	125	0
			5875	1858	3017	459	525	16			
1	B	294	Total	C	H	N	O	S	0	125	0
			5808	1834	2992	448	515	19			

There are 34 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	42	MET	GLN	conflict	UNP P23360
A	44	TRP	THR	conflict	UNP P23360
A	81	GLY	ARG	conflict	UNP P23360
A	83	GLY	HIS	conflict	UNP P23360
A	84	MET	THR	conflict	UNP P23360
A	130	GLY	ASN	conflict	UNP P23360
A	172	MET	ASN	conflict	UNP P23360
A	234	SER	ALA	conflict	UNP P23360
A	236	LEU	THR	conflict	UNP P23360
A	237	MET	GLU	conflict	UNP P23360
A	267	PHE	TRP	conflict	UNP P23360
B	-4	GLY	-	expression tag	UNP P23360
B	-3	SER	-	expression tag	UNP P23360
B	-2	GLY	-	expression tag	UNP P23360
B	-1	MET	-	expression tag	UNP P23360
B	0	ALA	-	expression tag	UNP P23360
B	1	GLU	-	expression tag	UNP P23360
B	42	MET	GLN	conflict	UNP P23360
B	44	TRP	THR	conflict	UNP P23360

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	81	GLY	ARG	conflict	UNP P23360
B	83	GLY	HIS	conflict	UNP P23360
B	84	MET	THR	conflict	UNP P23360
B	130	GLY	ASN	conflict	UNP P23360
B	172	MET	ASN	conflict	UNP P23360
B	234	SER	ALA	conflict	UNP P23360
B	236	LEU	THR	conflict	UNP P23360
B	237	MET	GLU	conflict	UNP P23360
B	267	PHE	TRP	conflict	UNP P23360

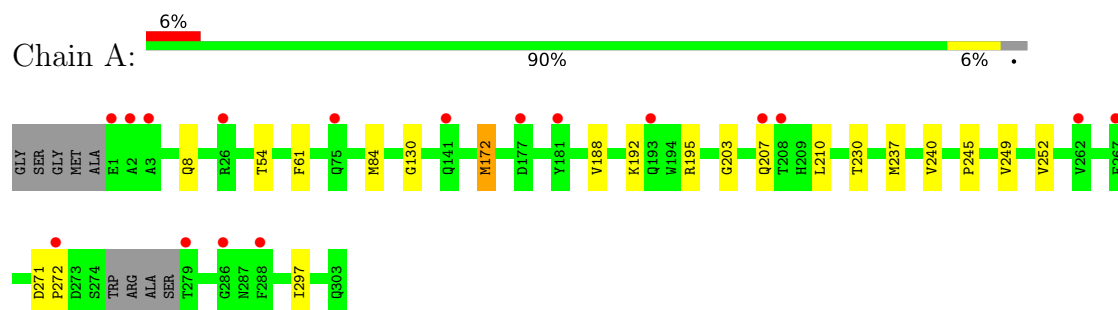
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	324	Total O 332 332	0	14
2	B	271	Total O 275 275	0	12

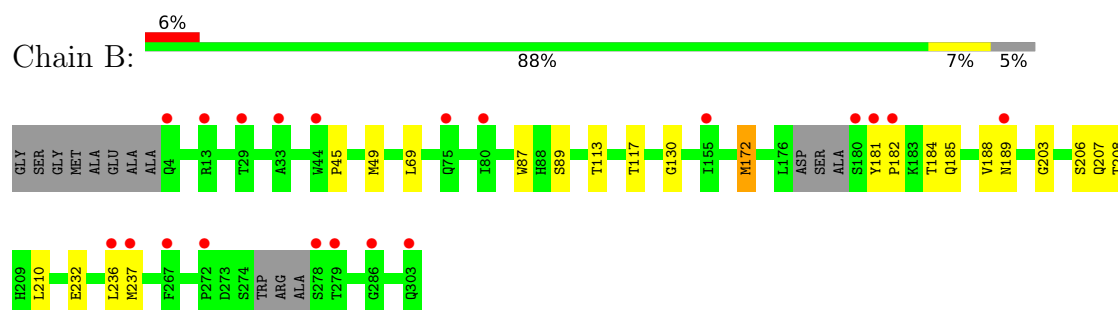
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Endo-1,4-beta-xylanase



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.61Å 58.03Å 81.61Å 90.00° 101.42° 90.00°	Depositor
Resolution (Å)	32.93 – 1.08 32.93 – 1.08	Depositor EDS
% Data completeness (in resolution range)	95.2 (32.93-1.08) 91.2 (32.93-1.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 1.08Å)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, $R_{free}$	0.193 , 0.213 0.194 , 0.213	Depositor DCC
$R_{free}$ test set	1997 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.0	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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 55.38 % 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 3.1873e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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](#)

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	0.36	0/3381	0.64	0/4604
1	B	0.34	0/3329	0.60	0/4525
All	All	0.35	0/6710	0.62	0/9129

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 [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	2858	3017	2801	11	0
1	B	2816	2992	2764	12	0
2	A	332	0	0	1	0
2	B	275	0	0	0	0
All	All	6281	6009	5565	23	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 (23) 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:84[A]:MET:SD	1:A:130:GLY:HA3	2.43	0.59

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLY:HA2	1:B:172[B]:MET:HG3	1.89	0.53
1:A:172[A]:MET:SD	1:A:207[A]:GLN:NE2	2.82	0.52
1:B:208[B]:THR:HG22	1:B:210[B]:LEU:HG	1.92	0.51
1:B:181[A]:TYR:CD1	1:B:182:PRO:HD3	2.49	0.48
1:B:207[B]:GLN:HG3	1:B:237[B]:MET:HB2	1.95	0.48
1:B:87:TRP:CE2	1:B:89:SER:HB2	2.49	0.48
1:A:237[B]:MET:HG2	2:A:690[B]:HOH:O	2.15	0.46
1:A:210[A]:LEU:HB2	1:A:240[A]:VAL:HG22	1.98	0.46
1:A:188:VAL:HG12	1:A:192[C]:LYS:HE3	1.98	0.46
1:A:245[A]:PRO:O	1:A:249[A]:VAL:HG23	2.16	0.45
1:B:45:PRO:HB3	1:B:69[B]:LEU:HD22	1.96	0.45
1:B:113:THR:O	1:B:117[A]:THR:HG23	2.16	0.45
1:B:185:GLN:O	1:B:189[A]:ASN:OD1	2.38	0.42
1:B:45:PRO:HG3	1:B:49[A]:MET:SD	2.60	0.42
1:A:252:VAL:HG21	1:A:297[B]:ILE:HG12	2.02	0.41
1:A:271:ASP:N	1:A:272[B]:PRO:HD2	2.36	0.41
1:A:54:THR:O	1:A:61:PHE:HA	2.19	0.41
1:B:206:SER:C	1:B:236[B]:LEU:HD23	2.41	0.41
1:B:203:GLY:HA2	1:B:232[A]:GLU:O	2.21	0.41
1:A:195[B]:ARG:HD2	1:A:230[B]:THR:HG22	2.04	0.40
1:B:184:THR:O	1:B:188[A]:VAL:HG23	2.21	0.40

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 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	419/308 (136%)	408 (97%)	11 (3%)	0	100	100
1	B	409/308 (133%)	401 (98%)	8 (2%)	0	100	100
All	All	828/616 (134%)	809 (98%)	19 (2%)	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	364/246 (148%)	360 (99%)	4 (1%)	73	39
1	B	361/246 (147%)	358 (99%)	3 (1%)	81	50
All	All	725/492 (147%)	718 (99%)	7 (1%)	86	43

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8[A]	GLN
1	A	8[B]	GLN
1	A	172[A]	MET
1	A	172[C]	MET
1	B	172[A]	MET
1	B	172[B]	MET
1	B	172[C]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

There are no ligands in this entry.

## 5.7 Other polymers

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	299/308 (97%)	0.91	17 (5%)	23 21	7, 10, 18, 31	1 (0%)
1	B	294/308 (95%)	0.93	20 (6%)	17 17	9, 13, 23, 52	0
All	All	593/616 (96%)	0.92	37 (6%)	20 19	7, 12, 21, 52	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	SER	5.2
1	B	236[A]	LEU	5.1
1	B	303	GLN	4.5
1	A	2	ALA	4.2
1	A	3	ALA	4.2
1	B	181[A]	TYR	3.8
1	B	182	PRO	3.7
1	A	1	GLU	3.5
1	A	181[A]	TYR	3.3
1	A	141[A]	GLN	3.3
1	B	180	SER	3.2
1	B	267[A]	PHE	3.2
1	A	272[A]	PRO	3.1
1	A	267[A]	PHE	3.1
1	A	75[A]	GLN	2.9
1	B	44[A]	TRP	2.9
1	A	288[A]	PHE	2.9
1	B	272	PRO	2.8
1	B	189[A]	ASN	2.8
1	B	75[A]	GLN	2.7
1	A	207[A]	GLN	2.6
1	B	237[A]	MET	2.6
1	A	279	THR	2.6
1	B	279[A]	THR	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	4[A]	GLN	2.5
1	B	29[A]	THR	2.4
1	B	80[A]	ILE	2.4
1	A	177[A]	ASP	2.3
1	A	286	GLY	2.3
1	B	286	GLY	2.3
1	B	155[A]	ILE	2.2
1	A	193[A]	GLN	2.2
1	A	26[B]	ARG	2.1
1	B	13[A]	ARG	2.1
1	A	208[A]	THR	2.1
1	B	33	ALA	2.1
1	A	262	VAL	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.