



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 01:28 PM EST

PDB ID : 1XO1  
Title : T5 5'-EXONUCLEASE MUTANT K83A  
Authors : Ceska, T.A.; Suck, D.; Sayers, J.R.  
Deposited on : 1998-11-19  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

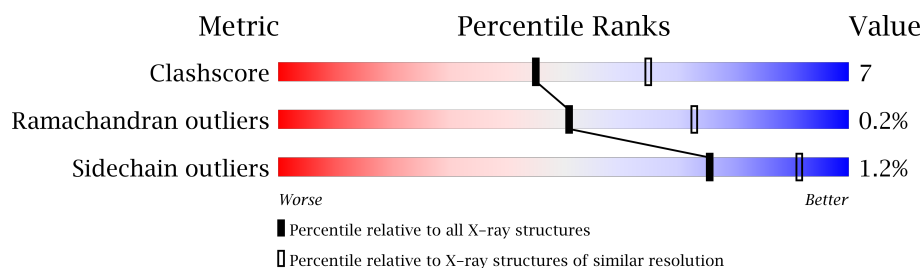
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	291	
1	B	291	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4264 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 5'-EXONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1974	1269	329	370	6			
1	B	245	Total	C	N	O	S	0	0	0
			1974	1269	329	370	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	LYS	ENGINEERED MUTATION	UNP P06229
B	83	ALA	LYS	ENGINEERED MUTATION	UNP P06229

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	152	Total	O	0	0
			152	152		
2	B	164	Total	O	0	0
			164	164		



Note EDS was not executed.

Chain A:

Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. A bar at the top shows the percentage of conserved residues: 70% (green), 14% (yellow), and 16% (grey).

Position	Amino Acid	Information Content (bits)
1	THR	0.05
2	GLU	0.05
3	GLU	0.05
4	GLU	0.05
5	LYS	0.05
6	ALA	0.05
7	LEU	0.05
8	ASP	0.05
9	GLN	0.05
10	P104	0.05
11	F105	0.05
12	E106	0.05
13	K109	0.05
14	G115	0.05
15	K116	0.05
16	P120	0.05
17	T121	0.05
18	E128	0.05
19	L139	0.05
20	H142	0.05
21	D145	0.05
22	L159	0.05
23	S168	0.05
24	F169	0.05
25	H185	0.05
26	L195	0.05
27	M199	0.05
28	L202	0.05
29	G208	0.05
30	A214	0.05
31	I231	0.05
32	L234	0.05
33	Q240	0.05
34	L262	0.05
35	P263	0.05
36	I270	0.05
37	V273	0.05

Chain B:

Position	Conservation Level	Most Conserved Amino Acid(s)
1	High (Yellow)	Met
2	High (Yellow)	Ser
3	High (Yellow)	Lys
4	High (Yellow)	Ser
5	High (Yellow)	Trp
6	High (Yellow)	Gly
7	High (Yellow)	Phe
8	High (Yellow)	Leu
9	High (Yellow)	Asp
10	High (Yellow)	Asn
11	High (Yellow)	Glu
12	High (Yellow)	Glu
13	High (Yellow)	Glu
14	High (Yellow)	Ala
15	High (Yellow)	Ser
16	High (Yellow)	R19
17	High (Yellow)	R20
18	High (Yellow)	R33
19	High (Yellow)	F34
20	High (Yellow)	Lys
21	High (Yellow)	His
22	High (Yellow)	Asn
23	High (Yellow)	Asn
24	High (Yellow)	Ser
25	High (Yellow)	Lys
26	High (Yellow)	Lys
27	High (Yellow)	F42
28	High (Yellow)	S49
29	High (Yellow)	O52
30	High (Yellow)	S53
31	High (Yellow)	S54
32	High (Yellow)	R61
33	High (Yellow)	T62
34	High (Yellow)	T63
35	High (Yellow)	T64
36	High (Yellow)	V65
37	High (Yellow)	R69
38	High (Yellow)	S72
39	High (Yellow)	E81
40	High (Yellow)	T82
41	High (Yellow)	A83
42	High (Yellow)	Gly
43	High (Yellow)	Asn
44	High (Yellow)	Arg
45	High (Yellow)	Asp
46	High (Yellow)	Glu
47	High (Yellow)	Lys
48	High (Yellow)	Tyr
49	High (Yellow)	Ala
50	High (Yellow)	Gln
51	High (Yellow)	Arg
52	High (Yellow)	Thr
53	High (Yellow)	Glu
54	High (Yellow)	Glu
55	High (Yellow)	Lys
56	High (Yellow)	Ala
57	High (Yellow)	Leu
58	High (Yellow)	Asp
59	High (Yellow)	Glu
60	High (Yellow)	Gln
61	High (Yellow)	F104
62	High (Yellow)	C115
63	High (Yellow)	K116
64	High (Yellow)	P120
65	High (Yellow)	T121
66	High (Yellow)	R125
67	High (Yellow)	E128
68	High (Yellow)	M132
69	High (Yellow)	I136
70	High (Yellow)	V137
71	High (Yellow)	K138
72	High (Yellow)	T152
73	High (Yellow)	L159
74	High (Yellow)	F169
75	High (Yellow)	T170
76	High (Yellow)	T171
77	High (Yellow)	R172
78	High (Yellow)	R178
79	High (Yellow)	M185
80	High (Yellow)	D188
81	High (Yellow)	F192
82	High (Yellow)	K196
83	High (Yellow)	D204
84	High (Yellow)	R207
85	High (Yellow)	N226
86	High (Yellow)	V227
87	High (Yellow)	L228
88	High (Yellow)	I231
89	High (Yellow)	L234
90	High (Yellow)	Q240
91	High (Yellow)	Q244
92	High (Yellow)	E250
93	High (Yellow)	N256
94	High (Yellow)	L257
95	High (Yellow)	L258
96	High (Yellow)	L259
97	High (Yellow)	V260
98	High (Yellow)	P263
99	High (Yellow)	T264
100	High (Yellow)	Y265
101	High (Yellow)	C266
102	High (Yellow)	A271
103	High (Yellow)	Q275
104	High (Yellow)	D276
105	High (Yellow)	V277
106	High (Yellow)	L278
107	High (Yellow)	F281
108	High (Yellow)	I285
109	High (Yellow)	E290
110	High (Yellow)	Gln

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.89 Å 76.81 Å 120.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.6 (6.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	8.20	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.226 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.32	0/2013	0.57	0/2720
1	B	0.32	0/2013	0.57	0/2720
All	All	0.32	0/4026	0.57	0/5440

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	1974	0	1956	24	0
1	B	1974	0	1956	35	0
2	A	152	0	0	5	0
2	B	164	0	0	8	0
All	All	4264	0	3912	58	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 7.

The worst 5 of 58 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:B:227:VAL:HG21	1:B:257:LEU:HD13	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ALA:HA	1:B:204:ASP:HA	1.67	0.75
1:B:72:SER:HB2	1:B:128:GLU:HG3	1.71	0.73
1:A:72:SER:HB2	1:A:128:GLU:HG3	1.76	0.67
1:B:116:LYS:HG2	1:B:121:THR:HB	1.77	0.65

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	239/291 (82%)	235 (98%)	3 (1%)	1 (0%)	38	59
1	B	239/291 (82%)	238 (100%)	1 (0%)	0	100	100
All	All	478/582 (82%)	473 (99%)	4 (1%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	SER

### 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	214/254 (84%)	211 (99%)	3 (1%)	71	90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	214/254 (84%)	212 (99%)	2 (1%)	82	94
All	All	428/508 (84%)	423 (99%)	5 (1%)	75	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	106	GLU
1	A	202	LEU
1	B	81	GLU
1	B	227	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	B	245	ASN
1	B	52	GLN
1	A	142	HIS
1	B	142	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.



## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.