



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 02:01 am BST

PDB ID : 2QZP  
Title : Crystal structure of mutation of an acylptide hydrolase/esterase from Aeropyrum pernix K1  
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Deposited on : 2007-08-17  
Resolution : 2.70 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

<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	:	2.11
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)	:	2.11

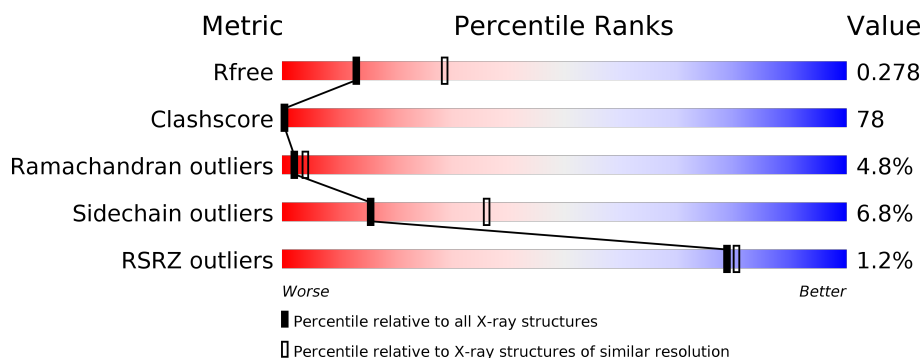
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	562	<div> <div> <div></div> <div>22%</div> <div>70%</div> <div>7%</div> </div> <div> <div></div> <div>2%</div> </div> </div>
1	B	562	<div> <div> <div></div> <div>20%</div> <div>72%</div> <div>8%</div> </div> <div> <div></div> <div>2%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8881 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 Acylamino-acid-releasing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4255	2685	750	808	12			
1	B	561	Total	C	N	O	S	0	0	0
			4260	2688	751	809	12			

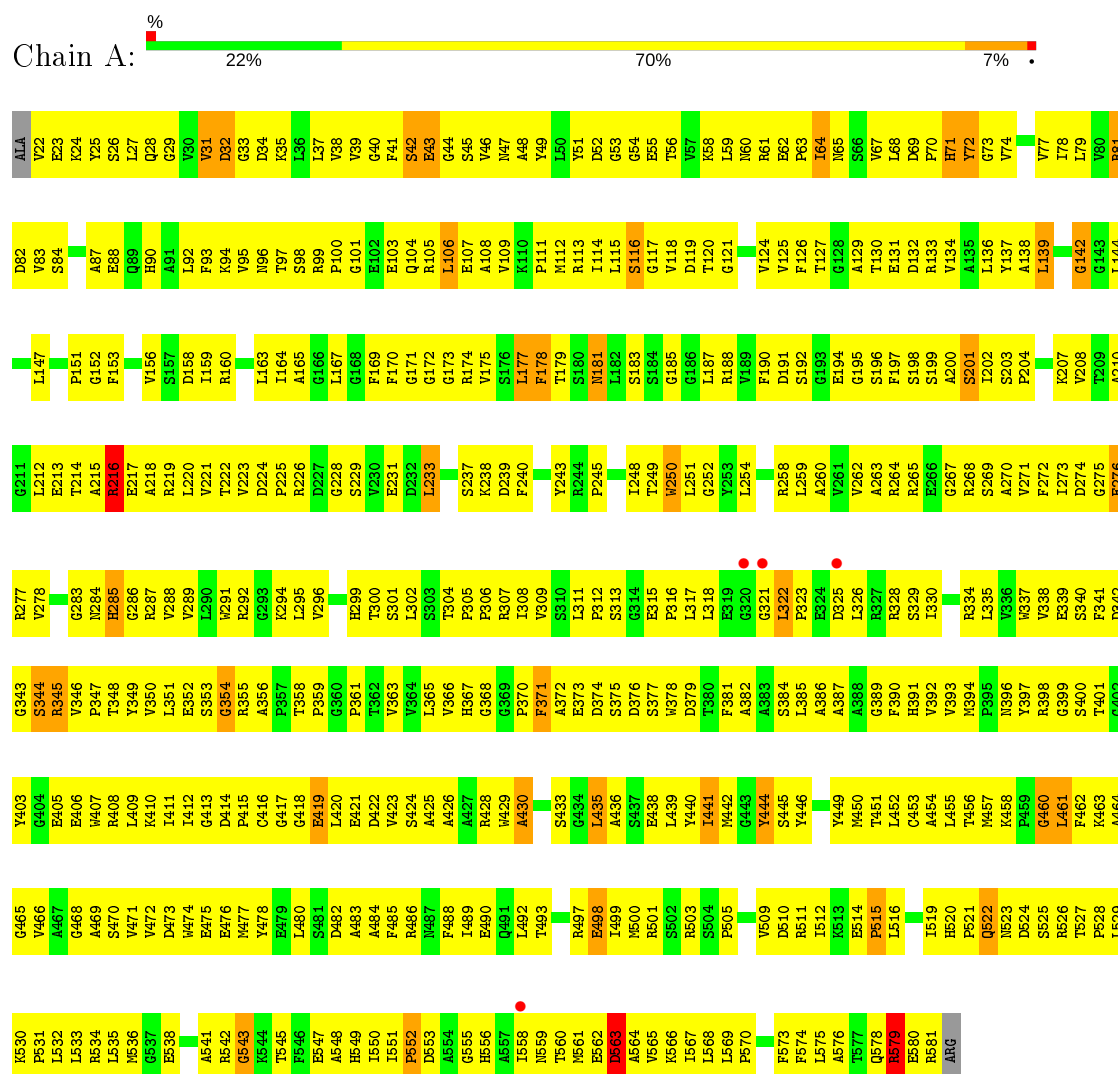
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total	O	0	0
			154	154		
2	B	212	Total	O	0	0
			212	212		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Acylamino-acid-releasing enzyme



#### • Molecule 1: Acylamino-acid-releasing enzyme



R526	G465	Y403	D342	A280	A218	E146	S84	A21
T527	V466	G404	G343	P281	R219	L147	R85	S26
P528	A467	E405	S344	Q282	L220	A148	G86	L27
L529	G468	E406	R345	G283	V221	R149	A87	Q28
K530	A469	W407	V346	N284	T222	L150	E88	G29
P531	S470	R408	P347	H285	V223	F153	R89	V30
L532	V471	L409	V350	G286	D224	V156	R90	V31
L533	D472	K410	L351	R287	P225	G157	A91	D32
R534	D473	I411	E352	V288	D227	D158	L92	G33
L535	W474	D414	S353	L290		D162	F93	D34
M536	E475	P415	G354	W291	V230	R160	K94	D35
G537	E476	C416	R355	R292	E231	G161	P95	K35
E538	W477	G417	A356	G293	D232	D163	N96	L36
L539	Y478	G418	P357	K294	E234	I164	L37	V38
L540	E479	L419	T358	L295	L235	G168	R99	V39
A541	L480	E420	P359	V296	P236	F169	P100	G40
R542	S481	L421	G360			F170	G101	
G543	D482	E422	P361	H299	D239	G171	E102	F41
K544	A483	D423	T362	T300	F240	F176	E103	S42
T545	A484	V423	V363	S301	F249	S176	Q104	E43
F546	F485	S424	V364	S302	S241	L177	R105	G44
E547	R486	A425	L365	S303	S242	G172	L106	S45
A548	M487		V366	T304	Y243	G173	E107	V46
H549	F488	R428	H367	P305	R244	R174	A108	N47
I550	I489	W429	G368	P306	P245	V175	V109	A48
I551	E490	A430	G369	R307	T246	S176	K110	Y49
P552	Q491	R431	G370	R308	L247	G185	P111	L50
D553	L492	E432	P370	P310	A247	G186	M12	Y51
A554	T493	S433	F371	V309	L248	L187	G121	N60
G494	G494	G434	A372	S310	T249	E122	E122	R61
G495	G495	L435	E373	L311	W250	A123	V124	S62
S496	S496	A436	D374	P312	L251	G195	F126	N65
R497	R497	S437	S375	S313	G252	F197	T127	S66
E498	E498	L439	D376	G314	Y253	S198		V67
N500	N500	Y440	S377	E315	L254	G199	T130	L68
R501	R501	I441	D378	P316	P255	S198	D132	D69
S502	S502	M442	T380	L317	D256	A200	P70	H71
R503	R503	G443	F381	E319	G257	S201	R133	Y72
S504	S504	Y444	A382		R258	I202	V134	G73
P505	P505	S445	A383	L322	V261	G195	A135	V74
I506	I506	Y446	S384	P323	V262	F197	L136	G75
N507	N507	G447	L385	E324	A263	S198	Y137	R76
H508	H508	G448	A386	D325	R264	S199	A138	R77
V509	V509	Y449	A387	L326	R265	A200	L139	V78
D510	D510	M450	A388	R327	E266	S202	D140	L79
R511	R511	T451	G389	R328	G267	I202	G142	F80
I512	I512	L452	F390	S329	R268	S203	G143	D82
K513	K513	C453	H391	I330	S269	G204	L144	R81
E514	E514	A454	V392	A331	A270	G205	L136	
P515	P515	L455	V393	G332	V271	M206	Y137	
L516	L516	T456	M394	S333	A263	K207	A138	
A517	A517	M457	P395	R334	R264	S199	L139	
K458	K458	L458	N396	F272	E266	A200	V208	
I519	I519	P459	Y397	L335	G267	I202	D140	
G460	G460	P460	R398	V336	D274	S203	G141	
L461	L461	L461	G399	V337	G275	G211	G142	
F462	F462	K462	S400	V338	E276	L212	G143	
N523	N523	A464	T401	E339	R277	E213	L144	
			G402	F341	E279		R145	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.12Å 102.18Å 163.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.70 48.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.11-2.70) 90.3 (48.11-2.50)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.226 , 0.277 0.226 , 0.278	Depositor DCC
$R_{free}$ test set	1393 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 81.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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](#)

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	0.47	0/4346	0.76	0/5892
1	B	0.46	0/4351	0.75	1/5899 (0.0%)
All	All	0.46	0/8697	0.75	1/11791 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	ASP	N-CA-C	-5.06	97.33	111.00

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	4255	0	4219	642	0
1	B	4260	0	4224	704	0
2	A	154	0	0	93	0
2	B	212	0	0	137	0
All	All	8881	0	8443	1329	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 78.

The worst 5 of 1329 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:497:ARG:HH11	1:B:497:ARG:HB2	0.94	1.11
1:A:552:PRO:HD3	1:B:547:GLU:HB2	1.30	1.11
1:A:346:VAL:HG21	1:A:422:ASP:HB3	1.32	1.09
1:B:334:ARG:HH21	1:B:350:VAL:HG11	1.03	1.09
1:A:547:GLU:HB3	1:B:552:PRO:HD3	1.18	1.07

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	558/562 (99%)	445 (80%)	90 (16%)	23 (4%)	3	6
1	B	559/562 (100%)	432 (77%)	96 (17%)	31 (6%)	2	3
All	All	1117/1124 (99%)	877 (78%)	186 (17%)	54 (5%)	2	4

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	72	TYR
1	A	563	ASP
1	B	206	MET
1	B	232	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 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	448/449 (100%)	418 (93%)	30 (7%)	16	37
1	B	448/449 (100%)	417 (93%)	31 (7%)	15	35
All	All	896/898 (100%)	835 (93%)	61 (7%)	16	36

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	559	ASN
1	B	133	ARG
1	B	482	ASP
1	A	563	ASP
1	B	41	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	HIS
1	B	96	ASN
1	B	507	ASN
1	B	28	GLN
1	B	65	ASN

### 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 [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	560/562 (99%)	-0.10	4 (0%) 87 89	7, 26, 44, 73	0
1	B	561/562 (99%)	0.13	9 (1%) 72 74	9, 32, 51, 71	0
All	All	1121/1124 (99%)	0.02	13 (1%) 79 80	7, 28, 49, 73	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	LEU	3.9
1	A	558	ILE	3.9
1	A	325	ASP	2.9
1	B	261	VAL	2.8
1	B	296	VAL	2.7

### 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 carbohydrates 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.