



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:29 AM GMT

PDB ID : 2QZP
Title : Crystal structure of mutation of an acylptide hydrolase/esterase from Aeropyrum pernix K1
Authors : Zhang, H.F.; Zheng, B.S.; Rao, Z.
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
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

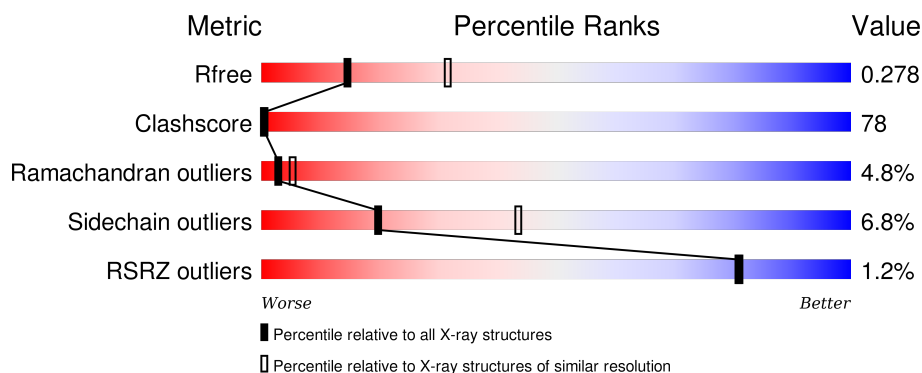
1 Overall quality at a glance

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	562	<div> <div>22%</div> <div>70%</div> <div>7%</div> </div>
1	B	562	<div> <div>20%</div> <div>72%</div> <div>8%</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			

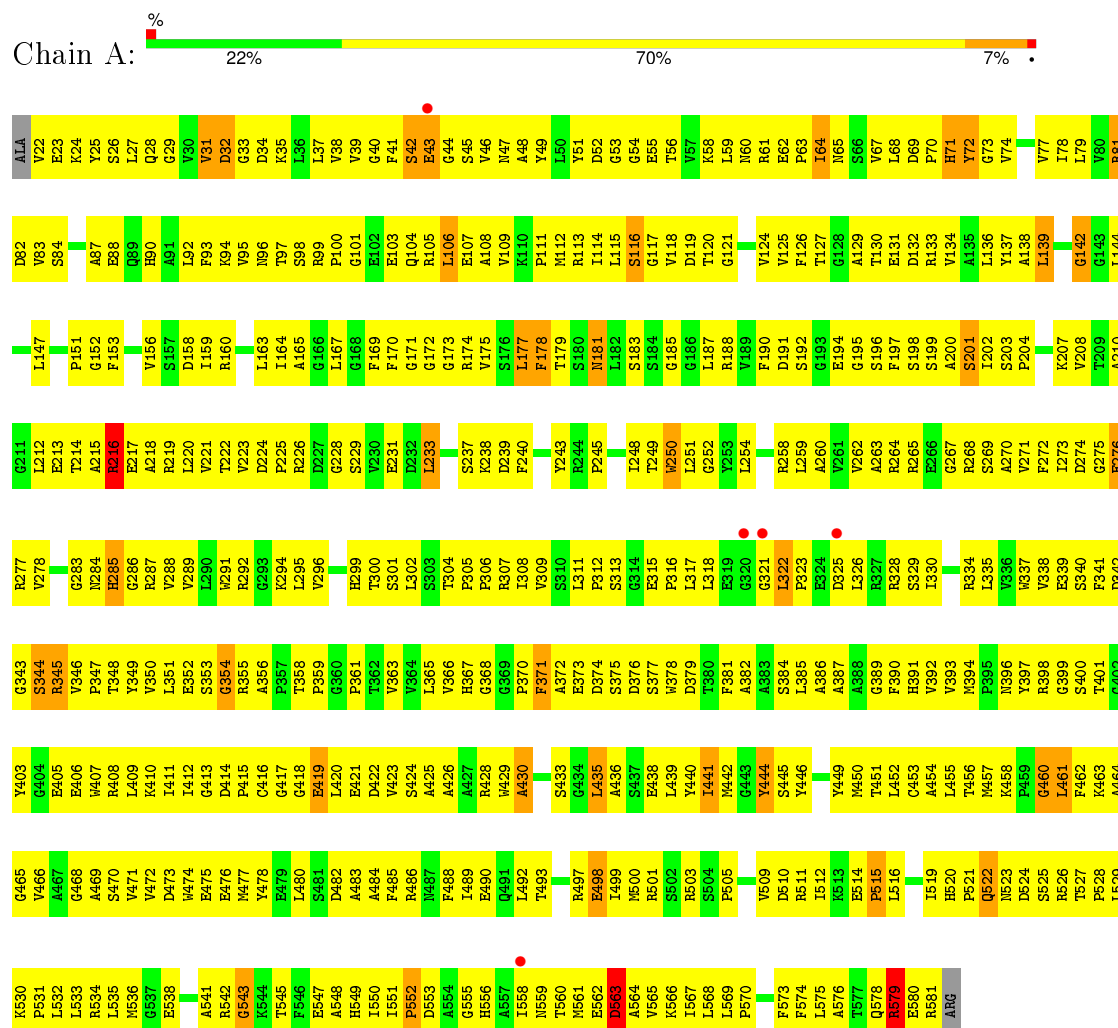
- Molecule 2 is water.

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 errors 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



R526	T527	G465	Y403	D342	A280	A218	E146	S84
P528	G404	V466	E405	G343	F281	R219	L147	R85
L529	E406	A467	E406	S344	Q282	R220	A148	G86
K530	G407	G468	E407	G283	Q283	V221	R149	A87
P531	K408	A469	W407	V346	N284	T222	L150	E88
L532	S470	S471	R408	P347	H285	V223	D89	H90
L533	V471	V472	L409	G286	G286	D224	F153	L92
R534	D473	D473	K410	V350	R287	P225	V156	F93
L535	W474	W474	L411	L351	V288	D227	S157	K94
M536	E475	E475	D414	E352	V289		D158	V95
G537	E476	E476	P415	S353	L290		I159	I96
E538	M477	M477	G416	G355	W291	V230	R160	
L539	Y478	Y478	G417	A356	G293	D232	G161	R99
L540	E479	E479	G418	P357	K294	L233	D162	P100
A541	L480	L480	E419	T358	L295	E234	L163	G101
R542	S481	S481	L420	P359	V296	L235	I164	E102
G543	D482	D482	E421	G360		P236		E103
K544	A483	A483	D422	P361	H299		G168	E104
T545	A484	A484	V423	T362	T300	D239	F169	Q105
F546	F485	F485	W424	V363	S301	F240	F170	L106
E547	R486	R486	A425	V364	L302	S241	G171	G172
A548	N487	N487		L365	S303	S242	G172	E107
H549	F488	F488	R428	V366	T304	Y243	G173	A108
I550	L489	L489	W429	H367	P305	R244	R174	V109
I551	E490	E490	A430	G368	P306	P245	V175	K110
P552	Q491	Q491	R431	G369	R307	T246	S176	P111
D553	L492	L492	E432	F371	T308	A247	L177	M112
A554	T493	T493	S433	A372	V309	L248	F178	R113
G555	G494	G494	G434	E373	L311	T249	T179	L114
H556	G495	G495	L435	D374	P312	W250	S180	L115
A557	S496	S496	A436	S375	S313	L251	N181	S116
L558	R497	R497	S437	D376	G314	G252	L182	G117
N559	E498	E498	E438	S377	E315	Y253		V118
M561	M500	M500	Y440	W378	P316	L254	G185	D119
E562	R501	R501	L441	D379	L317	D256	G186	T120
D563	S502	S502	W442	T380	L318	G257	L187	G121
A564	R503	R503	G443	F381	E319	R258	R188	E122
V565	S504	S504	Y444	A382		L259	V189	A123
K566	P505	P505	S445	A383	L322	A260	G195	V125
I567	I506	I506	Y446	S384	P323	V261	F196	F126
L568	N507	N507	Q447	L385	E324	A263	F197	T127
L569	H508	H508	Q448	A386	D325	R264	S198	
P570	V509	V509	Y449	A387	L326	R265	S199	T130
A571	D510	D510	W450	A388	R327	E266	S201	E131
V572	R511	R511	T451	G389	R328	R266	I201	D132
F573	I512	I512	L452	F390	S329	G267	I202	R133
F574	K513	K513	Q453	H391	T330	R268	S203	V134
	E514	E514	A454	V392	A331	S269	P204	A135
	P515	P515	L455	V393	G332	A270	G205	L136
T577	L516	L516	W456	M394	S333	V271	M206	Y137
Q578	A517	A517	W457	P395	R334	F272	K207	A138
R579	L518	L518	K458	N396	L335	L273	V208	L139
E580	I519	I519	Q459	Y397	V336	D274	T209	D140
R581	H520	H520	Q460	R398	W337	G275	A210	G141
ARG	P521	P521	L461	G399	V338	E276	G211	G142
	Q522	Q522	F462	S400	E339	R277	L212	G143
	N523	N523	K463	T401	S340	V278	E213	L144
			A464	G402	F341	E279		R145

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.277 0.226 , 0.278	Depositor DCC
R_{free} test set	1393 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 35151 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8881	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	7
1	B	559/562 (100%)	432 (77%)	96 (17%)	31 (6%)	2	4
All	All	1117/1124 (99%)	877 (78%)	186 (17%)	54 (5%)	3	5

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%)	20	44
1	B	448/449 (100%)	417 (93%)	31 (7%)	19	43
All	All	896/898 (100%)	835 (93%)	61 (7%)	20	43

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, 95th 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 ²)	Q<0.9
1	A	560/562 (99%)	-0.07	5 (0%) 85 86	7, 26, 44, 73	0
1	B	561/562 (99%)	0.16	9 (1%) 74 75	9, 32, 51, 71	0
All	All	1121/1124 (99%)	0.05	14 (1%) 81 81	7, 28, 49, 73	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	ILE	3.9
1	B	295	LEU	3.9
1	A	325	ASP	3.0
1	B	261	VAL	2.8
1	B	558	ILE	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.