



# wwPDB X-ray Structure Validation Summary Report i

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PDB ID : 3P2Q  
Title : Crystal structure of the fluoroacetyl-CoA-specific thioesterase, FLK  
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Deposited on : 2010-10-03  
Resolution : 1.85 Å (reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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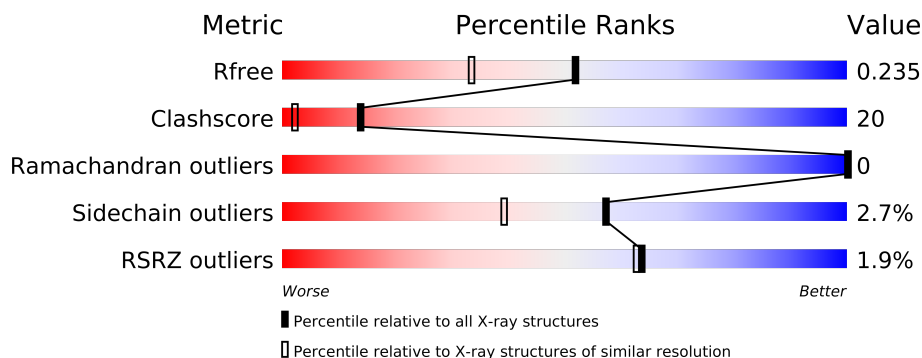
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.85 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))
$R_{free}$	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	143	
1	B	143	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2306 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Fluoroacetyl coenzyme A thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1034	656	185	187	6			
1	B	133	Total	C	N	O	S	0	0	0
			1031	654	185	187	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
A	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2
A	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
A	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2
B	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
B	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2
B	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
B	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	116	Total	O	0	0
			116	116		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.48Å 90.90Å 62.11Å 90.00° 100.99° 90.00°	Depositor
Resolution (Å)	26.96 – 1.85 25.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.7 (26.96-1.85) 91.4 (25.32-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.201 , 0.231 0.209 , 0.235	Depositor DCC
$R_{free}$ test set	1999 reflections (8.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 22397 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2306	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 7.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.70	0/1063	0.63	1/1446 (0.1%)
1	B	0.65	2/1060 (0.2%)	0.65	0/1443
All	All	0.67	2/2123 (0.1%)	0.64	1/2889 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	TYR	CE1-CZ	-6.67	1.29	1.38
1	B	56	ALA	CA-CB	-5.88	1.40	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	GLN	CB-CA-C	-6.87	96.66	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1034	0	0	31	1
1	B	1031	0	0	11	1
2	A	125	0	0	25	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	116	0	0	6	5
All	All	2306	0	0	41	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 41 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:ARG:NH1	2:A:185:HOH:O	1.70	1.23
1:A:55:ARG:NH1	2:A:188:HOH:O	1.75	1.19
1:A:96:GLU:OE1	2:A:196:HOH:O	1.71	1.07
1:A:93:ARG:NE	2:A:168:HOH:O	1.94	1.00
1:B:45:MET:SD	2:B:229:HOH:O	2.19	0.98

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:246:HOH:O	2:B:148:HOH:O[2_556]	1.12	1.08
2:B:193:HOH:O	2:B:193:HOH:O[2_556]	1.18	1.02
2:B:174:HOH:O	2:B:174:HOH:O[2_656]	1.21	0.99
2:A:245:HOH:O	2:B:148:HOH:O[2_556]	1.26	0.94
1:A:134:GLN:OE1	1:B:60:TYR:OH[4_556]	1.82	0.38

## 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	131/143 (92%)	131 (100%)	0	0	100	100
1	B	131/143 (92%)	131 (100%)	0	0	100	100
All	All	262/286 (92%)	262 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	110/114 (96%)	108 (98%)	2 (2%)	71	57
1	B	109/114 (96%)	105 (96%)	4 (4%)	45	24
All	All	219/228 (96%)	213 (97%)	6 (3%)	57	39

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	GLU
1	B	60	TYR
1	B	24	ARG
1	A	135	LYS
1	B	35	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	133/143 (93%)	0.03	1 (0%) 83 83	15, 27, 48, 61	0
1	B	133/143 (93%)	-0.06	4 (3%) 48 45	16, 25, 47, 66	0
All	All	266/286 (93%)	-0.01	5 (1%) 64 63	15, 26, 48, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	ALA	3.1
1	B	60	TYR	2.8
1	A	46	VAL	2.2
1	B	11	PHE	2.2
1	B	134	GLN	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.