WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 02:19 am GMT

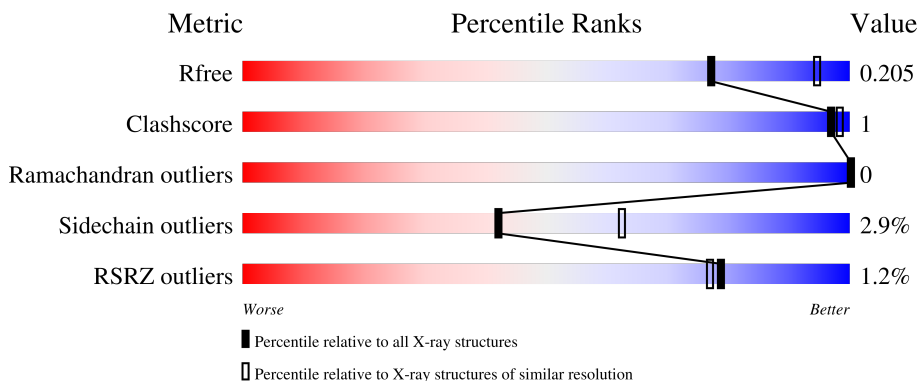|		
PDB ID	:	5FV4
Title	:	Pig liver esterase 5 (PLE5)
Authors	:	Werten, S.; Palm, G.J.; Berndt, L.; Hinrichs, W.
Deposited on	:	2016-02-03
Resolution	:	2.40 Å(reported)

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 2.40 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.
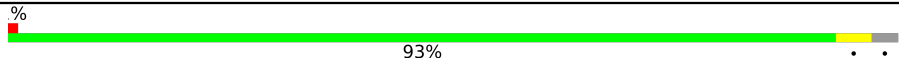
Metric	Percentile Ranks	Value
Rfree		0.205
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		2.9%
RSRZ outliers		1.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	544	92% 5% ·
1	B	544	.% 93% · ·
1	C	544	92% 5% ·
1	D	544	2% 91% 6% · ·
1	E	544	3% 92% 5% ·

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Mol	Chain	Length	Quality of chain
1	F	544	

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 25087 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 CARBOXYLIC ESTER HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	B	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	C	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	D	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	E	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			
1	F	530	Total	C	N	O	S	0	0	0
			4095	2636	682	760	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ASP	GLU	conflict	UNP A9GYW6
A	75	VAL	ILE	conflict	UNP A9GYW6
A	76	ALA	GLY	conflict	UNP A9GYW6
A	80	THR	LEU	conflict	UNP A9GYW6
A	459	ALA	PHE	conflict	UNP A9GYW6
A	461	PHE	LEU	conflict	UNP A9GYW6
A	463	ARG	LYS	conflict	UNP A9GYW6
B	73	ASP	GLU	conflict	UNP A9GYW6
B	75	VAL	ILE	conflict	UNP A9GYW6
B	76	ALA	GLY	conflict	UNP A9GYW6
B	80	THR	LEU	conflict	UNP A9GYW6
B	459	ALA	PHE	conflict	UNP A9GYW6
B	461	PHE	LEU	conflict	UNP A9GYW6
B	463	ARG	LYS	conflict	UNP A9GYW6
C	73	ASP	GLU	conflict	UNP A9GYW6
C	75	VAL	ILE	conflict	UNP A9GYW6
C	76	ALA	GLY	conflict	UNP A9GYW6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	80	THR	LEU	conflict	UNP A9GYW6
C	459	ALA	PHE	conflict	UNP A9GYW6
C	461	PHE	LEU	conflict	UNP A9GYW6
C	463	ARG	LYS	conflict	UNP A9GYW6
D	73	ASP	GLU	conflict	UNP A9GYW6
D	75	VAL	ILE	conflict	UNP A9GYW6
D	76	ALA	GLY	conflict	UNP A9GYW6
D	80	THR	LEU	conflict	UNP A9GYW6
D	459	ALA	PHE	conflict	UNP A9GYW6
D	461	PHE	LEU	conflict	UNP A9GYW6
D	463	ARG	LYS	conflict	UNP A9GYW6
E	73	ASP	GLU	conflict	UNP A9GYW6
E	75	VAL	ILE	conflict	UNP A9GYW6
E	76	ALA	GLY	conflict	UNP A9GYW6
E	80	THR	LEU	conflict	UNP A9GYW6
E	459	ALA	PHE	conflict	UNP A9GYW6
E	461	PHE	LEU	conflict	UNP A9GYW6
E	463	ARG	LYS	conflict	UNP A9GYW6
F	73	ASP	GLU	conflict	UNP A9GYW6
F	75	VAL	ILE	conflict	UNP A9GYW6
F	76	ALA	GLY	conflict	UNP A9GYW6
F	80	THR	LEU	conflict	UNP A9GYW6
F	459	ALA	PHE	conflict	UNP A9GYW6
F	461	PHE	LEU	conflict	UNP A9GYW6
F	463	ARG	LYS	conflict	UNP A9GYW6

- Molecule 2 is water.

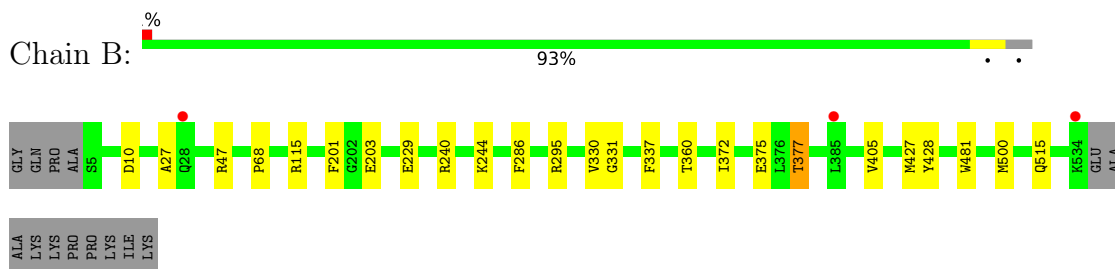| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total 92	O 92	0	0
2	B	103	Total 103	O 103	0	0
2	C	124	Total 124	O 124	0	0
2	D	34	Total 34	O 34	0	0
2	E	54	Total 54	O 54	0	0
2	F	110	Total 110	O 110	0	0

3 Residue-property plots ⓘ

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.
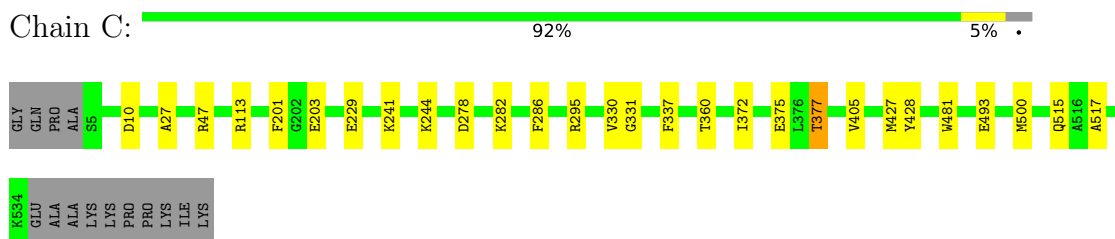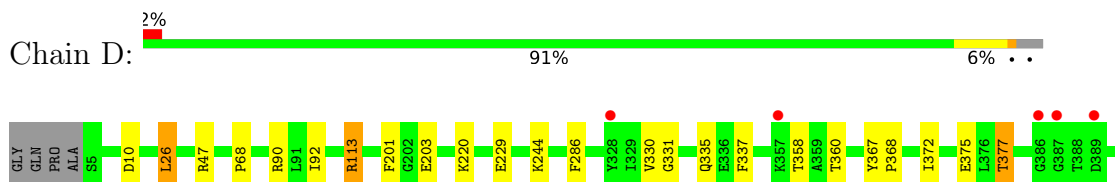
• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain A:

• Molecule 1: CARBOXYLIC ESTER HYDROLASE
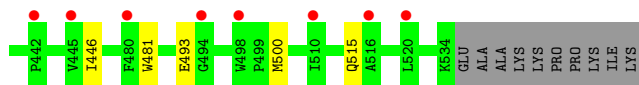
Chain B:

• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain C:

• Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain D:

K393 L397 V405 V414 M427 Y428 Q431 I446 E468 W481 G492 L495 M500 Q515 S533 K534 GLU ALA ALA LYS LYS PRO PRO LYS ILE LYS

● Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain E:

3%

92%

5%

GLY GLN PRO ALA S5 D10 R47 L83 R113 F201 G202 E203 E229 T235 A236 K241 K244 F286 V330 G331 F337 L349 S350 E351 G352 K353 L354 T360 Y367 P368 I372 E375 L376 T377 D389 D390 P391 V405 M427 Y428

P42 V445 I446 F480 W481 E493 G494 W498 P499 M500 I510 Q515 A516 L520 K534 GLU ALA ALA LYS LYS PRO PRO LYS ILE LYS

● Molecule 1: CARBOXYLIC ESTER HYDROLASE

Chain F:

%

93%

GLY GLN PRO ALA S5 D10 E24 G25 R47 W57 K61 E186 F201 G202 E203 E229 K244 F286 V330 G331 Q335 E336 F337 T360 I372 E375 L376 T377 V405 M427 Y428 G464 D465 W481 M500 Q515 S533 K534

GLU ALA ALA LYS LYS PRO PRO LYS ILE LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.86Å 188.02Å 109.50Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	71.14 – 2.40 71.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.14-2.40) 99.7 (71.14-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.205 0.181 , 0.205	Depositor DCC
R_{free} test set	7248 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 30.4	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25087	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.75	0/4207	0.77	1/5724 (0.0%)
1	B	0.70	0/4207	0.78	5/5724 (0.1%)
1	C	0.67	0/4207	0.77	3/5724 (0.1%)
1	D	0.66	0/4207	0.78	3/5724 (0.1%)
1	E	0.61	0/4207	0.74	2/5724 (0.0%)
1	F	0.69	0/4207	0.78	4/5724 (0.1%)
All	All	0.68	0/25242	0.77	18/34344 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	465	ASP	CB-CG-OD2	9.25	126.62	118.30
1	D	26	LEU	CB-CG-CD1	8.28	125.08	111.00
1	C	295	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	47	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	B	295	ARG	NE-CZ-NH1	6.95	123.77	120.30

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	4095	0	4041	12	0
1	B	4095	0	4041	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4095	0	4041	10	0
1	D	4095	0	4041	15	2
1	E	4095	0	4041	8	2
1	F	4095	0	4041	6	0
2	A	92	0	0	0	0
2	B	103	0	0	0	0
2	C	124	0	0	0	0
2	D	34	0	0	0	0
2	E	54	0	0	0	0
2	F	110	0	0	0	0
All	All	25087	0	24246	46	2

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 1.

The worst 5 of 46 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:350:SER:C	1:D:90:ARG:HH12	1.96	0.69
1:A:350:SER:O	1:D:90:ARG:NH1	2.33	0.62
1:A:351:GLU:HG2	1:D:92:ILE:HD11	1.92	0.51
1:A:360:THR:HG23	1:A:377:THR:HG23	1.93	0.51
1:B:360:THR:HG23	1:B:377:THR:HG23	1.93	0.50

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:GLY:O	1:E:493:GLU:OE1[1_455]	1.85	0.35
1:D:495:LEU:O	1:E:493:GLU:OE2[1_455]	1.91	0.29

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	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	B	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	C	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	D	528/544 (97%)	508 (96%)	20 (4%)	0	100	100
1	E	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
1	F	528/544 (97%)	509 (96%)	19 (4%)	0	100	100
All	All	3168/3264 (97%)	3053 (96%)	115 (4%)	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	440/450 (98%)	428 (97%)	12 (3%)	44	65
1	B	440/450 (98%)	428 (97%)	12 (3%)	44	65
1	C	440/450 (98%)	428 (97%)	12 (3%)	44	65
1	D	440/450 (98%)	423 (96%)	17 (4%)	32	50
1	E	440/450 (98%)	428 (97%)	12 (3%)	44	65
1	F	440/450 (98%)	428 (97%)	12 (3%)	44	65
All	All	2640/2700 (98%)	2563 (97%)	77 (3%)	42	62

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	244	LYS
1	F	337	PHE
1	E	337	PHE
1	F	10	ASP
1	F	500	MET

Sometimes 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 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 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, 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(Å²)	Q<0.9
1	A	530/544 (97%)	-0.48	1 (0%)	95	94	36, 52, 87, 133	0
1	B	530/544 (97%)	-0.39	3 (0%)	89	88	38, 59, 99, 154	0
1	C	530/544 (97%)	-0.44	0	100	100	36, 57, 95, 141	0
1	D	530/544 (97%)	-0.20	9 (1%)	70	68	38, 70, 127, 159	0
1	E	530/544 (97%)	-0.03	18 (3%)	45	44	43, 80, 127, 151	0
1	F	530/544 (97%)	-0.41	6 (1%)	80	79	38, 58, 113, 142	0
All	All	3180/3264 (97%)	-0.33	37 (1%)	79	77	36, 61, 116, 159	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	494	GLY	5.7
1	E	498	TRP	4.8
1	E	391	PRO	4.5
1	E	389	ASP	4.5
1	F	24	GLU	4.5

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 monosaccharides 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.