



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FJ2  
Title : Crystal structure of the human acyl protein thioesterase 1 at 1.5 Å resolution  
Authors : Devedjiev, Y.; Dauter, Z.; Kuznetsov, S.; Jones, T.; Derewenda, Z.  
Deposited on : 2000-08-07  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

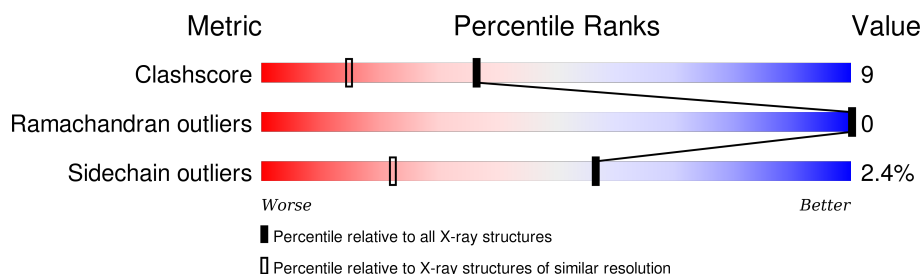
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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	232	
1	B	232	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	831	-	-	X	-
2	BR	B	839	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3959 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 PROTEIN (ACYL PROTEIN THIOESTERASE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1727	1102	292	319	14			
1	B	229	Total	C	N	O	S	0	0	0
			1727	1102	292	319	14			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	see remark 999	UNP O75608
A	-6	ALA	-	see remark 999	UNP O75608
A	-5	MET	-	see remark 999	UNP O75608
A	-4	ASP	-	see remark 999	UNP O75608
A	-3	PRO	-	see remark 999	UNP O75608
A	-2	GLU	-	see remark 999	UNP O75608
A	-1	PHE	-	see remark 999	UNP O75608

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	21	Total	Br	0	0
			21	21		
2	A	19	Total	Br	0	0
			19	19		

- Molecule 3 is water.

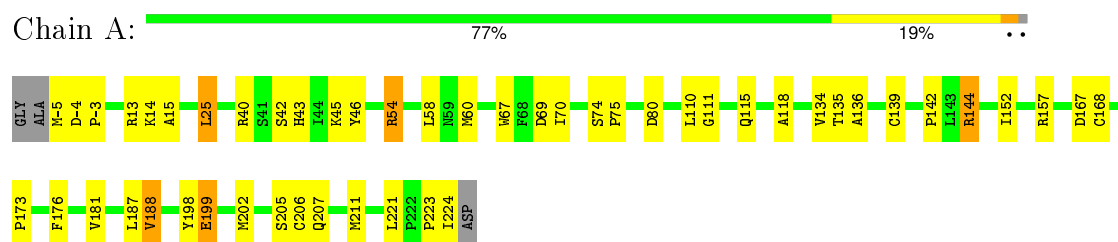
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	222	Total	O	6	0
			222	222		
3	B	243	Total	O	9	0
			243	243		

### 3 Residue-property plots

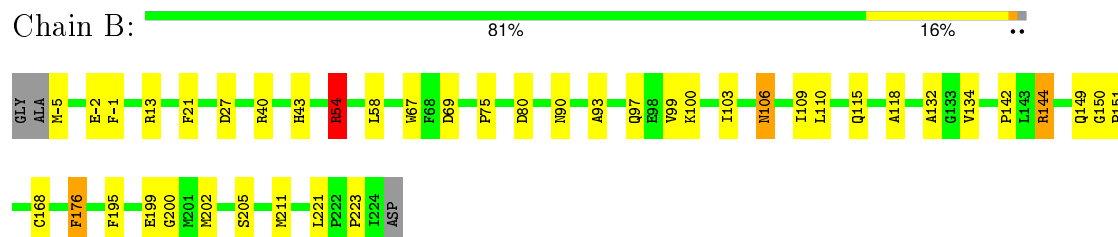
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: PROTEIN (ACYL PROTEIN THIOESTERASE 1)



#### • Molecule 1: PROTEIN (ACYL PROTEIN THIOESTERASE 1)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.59 Å   127.89 Å   39.66 Å 90.00°   102.80°   90.00°	Depositor
Resolution (Å)	20.00 – 1.50	Depositor
% Data completeness (in resolution range)	80.0 (20.00-1.50)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR

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	0.91	0/1768	1.44	22/2404 (0.9%)
1	B	0.87	0/1768	1.41	12/2404 (0.5%)
All	All	0.89	0/3536	1.43	34/4808 (0.7%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	NE-CZ-NH2	-11.81	114.40	120.30
1	A	40	ARG	NE-CZ-NH2	10.51	125.56	120.30
1	B	144	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	B	223	PRO	C-N-CA	10.05	146.82	121.70
1	A	188	VAL	N-CA-CB	-8.93	91.85	111.50
1	A	40	ARG	CG-CD-NE	8.77	130.21	111.80
1	A	40	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	B	69	ASP	CB-CG-OD1	8.43	125.89	118.30
1	A	223	PRO	C-N-CA	8.20	142.21	121.70
1	B	27	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	21	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	A	69	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	54	ARG	CA-CB-CG	6.97	128.75	113.40
1	A	188	VAL	CB-CA-C	6.87	124.45	111.40
1	A	157	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	54	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	45	LYS	CA-CB-CG	6.70	128.14	113.40
1	B	211	MET	CG-SD-CE	6.54	110.66	100.20
1	B	54	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	54	ARG	CB-CG-CD	5.97	127.12	111.60
1	A	157	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	199	GLU	OE1-CD-OE2	5.69	130.13	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	A	198	TYR	CB-CG-CD2	5.50	124.30	121.00
1	A	224	ILE	CB-CA-C	-5.29	101.01	111.60
1	A	80	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	46	TYR	CB-CG-CD1	-5.24	117.85	121.00
1	A	25	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	B	195	PHE	CB-CG-CD1	5.13	124.39	120.80
1	A	69	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	B	40	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	80	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	181	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	A	211	MET	CA-CB-CG	5.00	121.80	113.30

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	1727	0	1742	39	0
1	B	1727	0	1742	30	0
2	A	19	0	0	6	0
2	B	21	0	0	4	0
3	A	222	0	0	7	0
3	B	243	0	0	6	0
All	All	3959	0	3484	66	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 9.

All (66) 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:-4:ASP:HB2	1:A:-3:PRO:HD2	1.41	1.00
1:B:75:PRO:HB3	1:B:144:ARG:HH12	1.34	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:831:BR:BR	2:A:832:BR:BR	3.02	0.88
1:B:75:PRO:HB2	1:B:144:ARG:HH22	1.39	0.87
1:A:25:LEU:HD11	1:A:70:ILE:HG21	1.60	0.84
1:A:42:SER:OG	3:A:950:HOH:O	1.97	0.74
1:A:168:CYS:SG	2:A:831:BR:BR	3.03	0.72
1:A:-4:ASP:HB2	1:A:-3:PRO:CD	2.19	0.72
1:B:75:PRO:CB	1:B:144:ARG:HH12	2.02	0.72
1:A:70:ILE:HB	3:A:960:HOH:O	1.89	0.72
1:A:67:TRP:H	1:A:115:GLN:NE2	1.88	0.70
1:A:67:TRP:H	1:A:115:GLN:HE22	1.39	0.69
1:A:60:MET:SD	3:B:1029:HOH:O	2.52	0.68
1:B:43:HIS:HD2	3:B:898:HOH:O	1.76	0.67
2:B:839:BR:BR	3:B:851:HOH:O	2.68	0.66
1:A:144:ARG:HD2	3:A:978:HOH:O	1.97	0.65
1:B:13:ARG:NH2	2:B:803:BR:BR	2.85	0.64
1:A:202:MET:HE3	1:B:205:SER:OG	1.97	0.64
1:A:25:LEU:HD11	1:A:70:ILE:CG2	2.28	0.63
1:B:43:HIS:HE1	1:B:221:LEU:O	1.82	0.62
1:A:60:MET:HG2	3:A:1040:HOH:O	2.01	0.61
1:A:205:SER:OG	1:B:202:MET:HE3	2.01	0.60
1:A:25:LEU:CD1	1:A:70:ILE:HG21	2.30	0.59
1:A:152:ILE:HG23	1:A:187:LEU:HD22	1.83	0.59
2:A:830:BR:BR	3:A:963:HOH:O	2.72	0.58
1:B:75:PRO:HB2	1:B:144:ARG:NH2	2.14	0.58
1:A:43:HIS:HE1	1:A:221:LEU:O	1.86	0.58
1:B:202:MET:SD	3:B:958:HOH:O	2.56	0.57
1:B:67:TRP:H	1:B:115:GLN:NE2	2.02	0.57
1:B:118:ALA:HB1	1:B:142:PRO:HG3	1.86	0.56
1:B:67:TRP:H	1:B:115:GLN:HE22	1.55	0.55
1:A:173:PRO:HD2	1:A:176:PHE:CE2	2.42	0.54
1:B:110:LEU:O	1:B:134:VAL:HA	2.08	0.54
1:A:202:MET:CE	1:B:205:SER:OG	2.55	0.54
1:A:111:GLY:HA3	1:A:135:THR:HG22	1.90	0.53
1:B:106:ASN:HD22	1:B:106:ASN:C	2.11	0.53
1:A:14:LYS:HG3	3:A:1048:HOH:O	2.11	0.51
1:B:75:PRO:HB3	1:B:176:PHE:CZ	2.46	0.50
1:A:205:SER:OG	1:B:202:MET:CE	2.60	0.50
1:A:207:GLN:HE21	1:B:200:GLY:HA2	1.77	0.50
1:A:135:THR:O	1:A:135:THR:HG23	2.12	0.50
1:A:74:SER:HB2	1:A:75:PRO:HD2	1.93	0.49
1:A:13:ARG:HG3	1:A:42:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TRP:N	1:A:115:GLN:HE22	2.09	0.48
1:B:93:ALA:O	1:B:97:GLN:HG3	2.14	0.47
1:B:-2:GLU:OE1	1:B:54:ARG:NH1	2.48	0.47
1:A:43:HIS:HD2	3:A:950:HOH:O	1.98	0.46
1:A:136:ALA:HB1	1:A:139:CYS:SG	2.56	0.46
1:A:118:ALA:HB1	1:A:142:PRO:HG3	1.99	0.45
1:A:205:SER:OG	2:A:840:BR:BR	2.81	0.45
1:A:173:PRO:HD2	1:A:176:PHE:CD2	2.52	0.44
1:A:15:ALA:O	2:A:829:BR:BR	2.91	0.44
1:A:110:LEU:O	1:A:134:VAL:HA	2.18	0.44
1:B:99:VAL:HA	1:B:103:ILE:O	2.18	0.44
1:A:206:CYS:HA	1:B:202:MET:HE2	1.98	0.43
2:B:839:BR:BR	3:B:1077:HOH:O	2.76	0.43
1:B:100:LYS:HE2	2:B:839:BR:BR	2.74	0.43
1:A:206:CYS:CA	1:B:202:MET:HE2	2.49	0.42
1:B:151:PRO:HB3	3:B:1068:HOH:O	2.20	0.42
1:A:-5:MET:SD	2:A:816:BR:BR	3.33	0.42
1:B:-1:PHE:CD1	1:B:90:ASN:ND2	2.88	0.42
1:B:168:CYS:O	1:B:202:MET:HG2	2.20	0.41
1:B:150:GLY:HA2	1:B:151:PRO:HD3	1.78	0.41
1:A:167:ASP:OD2	1:A:199:GLU:HA	2.19	0.41
1:B:109:ILE:HG13	1:B:132:ALA:HB3	2.03	0.41
1:A:74:SER:HB2	1:A:75:PRO:CD	2.51	0.41

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	227/232 (98%)	220 (97%)	7 (3%)	0	100	100
1	B	227/232 (98%)	223 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	454/464 (98%)	443 (98%)	11 (2%)	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	189/190 (100%)	186 (98%)	3 (2%)	70	41
1	B	189/190 (100%)	183 (97%)	6 (3%)	46	13
All	All	378/380 (100%)	369 (98%)	9 (2%)	57	22

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	58	LEU
1	A	188	VAL
1	B	-5	MET
1	B	54	ARG
1	B	58	LEU
1	B	106	ASN
1	B	149	GLN
1	B	176	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	115	GLN
1	A	129	GLN
1	A	207	GLN
1	B	43	HIS
1	B	106	ASN

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Mol	Chain	Res	Type
1	B	115	GLN
1	B	129	GLN

### 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 ⓘ

Of 40 ligands modelled in this entry, 40 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.