



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2019 – 08:56 PM EDT

PDB ID : 6H0T  
Title : Crystal structure of native recombinant human bile salt activated lipase  
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Deposited on : 2018-07-10  
Resolution : 1.90 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

<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  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

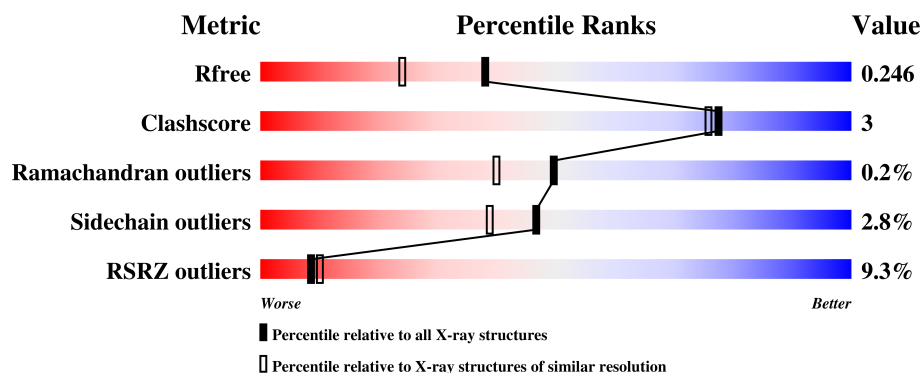
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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.

Mol	Chain	Length	Quality of chain
1	A	547	<div> <div>9%</div> <div>85%</div> <div>8% • 6%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4161 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 Bile salt-activated lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4019	2586	674	744	15			

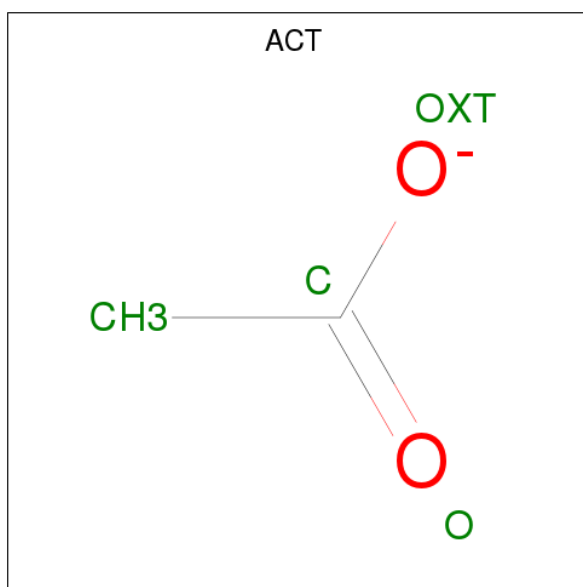
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP P19835
A	-12	HIS	-	expression tag	UNP P19835
A	-11	HIS	-	expression tag	UNP P19835
A	-10	HIS	-	expression tag	UNP P19835
A	-9	HIS	-	expression tag	UNP P19835
A	-8	HIS	-	expression tag	UNP P19835
A	-7	HIS	-	expression tag	UNP P19835
A	-6	HIS	-	expression tag	UNP P19835
A	-5	GLU	-	expression tag	UNP P19835
A	-4	ASN	-	expression tag	UNP P19835
A	-3	LEU	-	expression tag	UNP P19835
A	-2	TYR	-	expression tag	UNP P19835
A	-1	PHE	-	expression tag	UNP P19835
A	0	GLN	-	expression tag	UNP P19835
A	1	SER	-	expression tag	UNP P19835
A	186	ASP	ASN	engineered mutation	UNP P19835
A	298	ASP	ALA	engineered mutation	UNP P19835

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

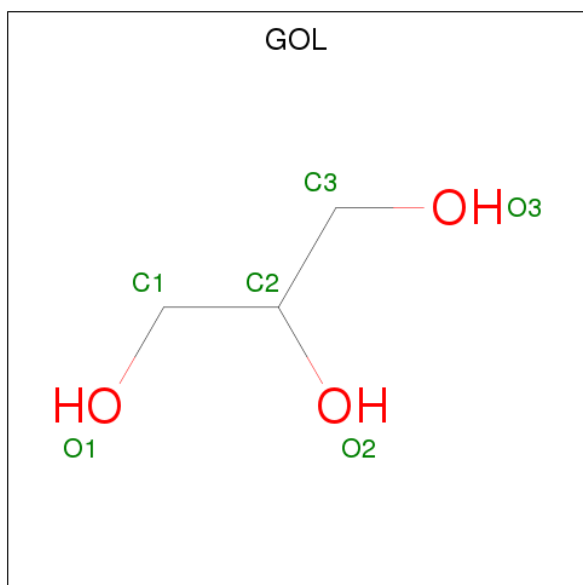
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	Zn	0	0
			8	8		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.27Å 97.68Å 109.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 1.90 44.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.93-1.90) 99.5 (44.61-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.210 , 0.246 0.210 , 0.246	Depositor DCC
$R_{free}$ test set	2389 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4161	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, ACT

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	0.41	0/4127	0.58	3/5612 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	176	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	510	MET	CG-SD-CE	5.18	108.49	100.20

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	4019	0	3962	26	0
2	A	8	0	0	0	0
3	A	16	0	12	0	0
4	A	6	0	7	0	0
5	A	112	0	0	2	0
All	All	4161	0	3981	26	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 3.

All (26) 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:323:ILE:HD13	1:A:434:ASP:CG	2.13	0.68
1:A:319:MET:HG3	1:A:432:GLY:HA3	1.82	0.62
1:A:62:LYS:HA	1:A:63:ARG:NH1	2.17	0.60
1:A:285:VAL:O	5:A:701:HOH:O	2.16	0.59
1:A:308:ALA:HB1	1:A:409:LYS:HG3	1.87	0.56
1:A:68:THR:OG1	1:A:69:ILE:N	2.39	0.55
1:A:235:PHE:O	1:A:239:LYS:HG2	2.07	0.54
1:A:241:ALA:HB1	1:A:246:CYS:HB2	1.89	0.54
1:A:215:ARG:NH1	1:A:472:ALA:O	2.43	0.52
1:A:193:GLU:OE2	5:A:702:HOH:O	2.19	0.50
1:A:72:ASP:OD2	1:A:72:ASP:N	2.40	0.49
1:A:355:LYS:HG3	1:A:526:TYR:CZ	2.50	0.47
1:A:247:PRO:O	1:A:254:MET:HB2	2.16	0.46
1:A:250:ASP:HB3	1:A:253:ARG:HB2	1.96	0.46
1:A:288:VAL:HB	1:A:289:PRO:HD2	1.98	0.46
1:A:69:ILE:HD12	1:A:69:ILE:H	1.81	0.45
1:A:210:LYS:HA	1:A:210:LYS:HD3	1.83	0.45
1:A:323:ILE:HD13	1:A:434:ASP:OD1	2.17	0.45
1:A:486:THR:HG21	1:A:506:GLY:O	2.19	0.43
1:A:527:LEU:HA	1:A:527:LEU:HD12	1.80	0.42
1:A:2:LYS:HE2	1:A:2:LYS:HB3	1.72	0.42
1:A:215:ARG:HA	1:A:310:ILE:HG23	2.02	0.40
1:A:495:ASN:OD1	1:A:496:SER:N	2.54	0.40
1:A:485:PRO:HB2	1:A:505:MET:HB2	2.04	0.40
1:A:63:ARG:CZ	1:A:63:ARG:H	2.33	0.40
1:A:70:THR:OG1	1:A:72:ASP:OD2	2.23	0.40

There are no symmetry-related clashes.

## 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	508/547 (93%)	491 (97%)	16 (3%)	1 (0%)	49 40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	THR

### 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	424/452 (94%)	412 (97%)	12 (3%)	47 39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	92	LYS
1	A	148	LEU
1	A	191	PHE
1	A	210	LYS
1	A	215	ARG
1	A	231	LYS
1	A	358	ARG
1	A	417	LEU
1	A	423	ARG
1	A	468	TRP
1	A	505	MET

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 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 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	A	609	2	1,3,3	8.38	1 (100%)	0,3,3	0.00	-
3	ACT	A	610	2	1,3,3	7.60	1 (100%)	0,3,3	0.00	-
3	ACT	A	611	2	1,3,3	7.42	1 (100%)	0,3,3	0.00	-
3	ACT	A	612	2	1,3,3	6.15	1 (100%)	0,3,3	0.00	-
4	GOL	A	613	-	5,5,5	1.27	0	5,5,5	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	609	2	-	0/0/0/0	0/0/0/0
3	ACT	A	610	2	-	0/0/0/0	0/0/0/0
3	ACT	A	611	2	-	0/0/0/0	0/0/0/0
3	ACT	A	612	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	613	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	ACT	CH3-C	6.15	1.56	1.48
3	A	611	ACT	CH3-C	7.42	1.58	1.48
3	A	610	ACT	CH3-C	7.60	1.58	1.48
3	A	609	ACT	CH3-C	8.38	1.59	1.48

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 [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 ⓘ

### 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	514/547 (93%)	0.48	48 (9%) 8 10	29, 43, 73, 96	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	9.0
1	A	284	TYR	8.8
1	A	69	ILE	7.0
1	A	426	VAL	7.0
1	A	424	MET	6.2
1	A	427	TYR	5.0
1	A	428	PRO	4.8
1	A	270	TYR	4.8
1	A	430	TRP	4.4
1	A	429	LYS	4.2
1	A	164	LEU	4.1
1	A	92	LYS	3.9
1	A	423	ARG	3.9
1	A	336	ASN	3.6
1	A	279	TYR	3.6
1	A	104	ILE	3.4
1	A	425	PRO	3.3
1	A	533	THR	3.1
1	A	217	ILE	2.9
1	A	93	GLN	2.9
1	A	249	GLY	2.8
1	A	200	VAL	2.8
1	A	271	LYS	2.7
1	A	235	PHE	2.7
1	A	253	ARG	2.7
1	A	282	LEU	2.6
1	A	72	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	285	VAL	2.6
1	A	190	LEU	2.5
1	A	432	GLY	2.5
1	A	250	ASP	2.5
1	A	70	THR	2.5
1	A	123	TYR	2.4
1	A	102	ILE	2.4
1	A	22	LEU	2.3
1	A	530	PRO	2.3
1	A	334	LYS	2.3
1	A	295	PHE	2.2
1	A	248	VAL	2.2
1	A	256	GLN	2.2
1	A	195	ALA	2.2
1	A	527	LEU	2.2
1	A	337	LYS	2.2
1	A	493	THR	2.2
1	A	171	ILE	2.1
1	A	68	THR	2.1
1	A	143	TYR	2.1
1	A	141	PHE	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	606	1/1	0.88	0.10	82,82,82,82	0
4	GOL	A	613	6/6	0.90	0.35	41,45,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	A	610	4/4	0.92	0.14	46,51,54,55	0
3	ACT	A	612	4/4	0.95	0.21	73,73,73,74	0
2	ZN	A	607	1/1	0.96	0.09	67,67,67,67	1
3	ACT	A	611	4/4	0.96	0.10	35,37,42,44	0
2	ZN	A	601	1/1	0.98	0.10	47,47,47,47	0
2	ZN	A	608	1/1	0.98	0.12	47,47,47,47	1
2	ZN	A	604	1/1	0.98	0.09	64,64,64,64	1
2	ZN	A	603	1/1	0.99	0.11	35,35,35,35	0
3	ACT	A	609	4/4	0.99	0.07	36,37,39,41	0
2	ZN	A	602	1/1	0.99	0.11	35,35,35,35	0
2	ZN	A	605	1/1	1.00	0.09	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.