



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6H0T / pdb_00006h0t
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

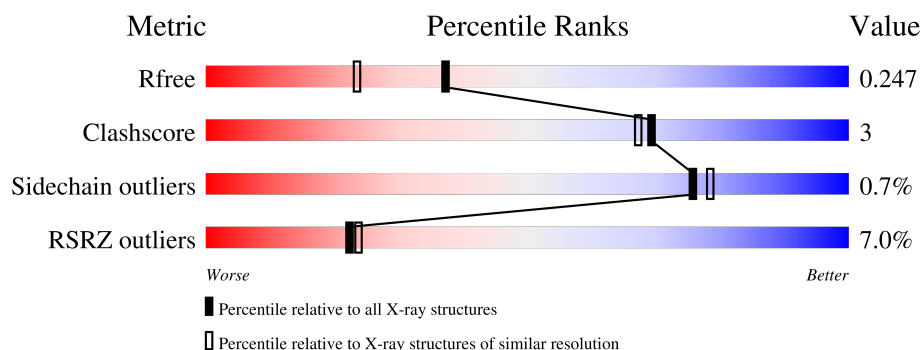
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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 $\leq 5\%$. 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	

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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 (CCD ID: GOL) (formula: C₃H₈O₃).



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		

- Molecule 1: Bile salt-activated lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.27Å 97.68Å 109.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 1.90 39.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.93-1.90) 99.5 (39.93-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.246 0.211 , 0.247	Depositor DCC
R_{free} test set	2389 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.34	0/4127	0.50	0/5612

There are no bond length outliers.

There are no bond angle outliers.

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	4019	0	3962	28	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	28	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 (28) 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	0.74
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:238:LYS:HG2	1:A:254:MET:HE1	1.88	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:70:THR:OG1	1:A:72:ASP:OD2	2.23	0.51
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:HD3	1:A:210:LYS:HA	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:505:MET:HE3	1:A:505:MET:HB3	1.83	0.41
1:A:215:ARG:HA	1:A:310:ILE:HG23	2.02	0.40
1:A:485:PRO:HB2	1:A:505:MET:HB2	2.04	0.40
1:A:495:ASN:OD1	1:A:496:SER:N	2.54	0.40
1:A:63:ARG:H	1:A:63:ARG:CZ	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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%)	421 (99%)	3 (1%)	76	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	417	LEU
1	A	505	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	71	GLN
1	A	157	ASN
1	A	333	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 oligosaccharides 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	611	2	3,3,3	1.50	1 (33%)	3,3,3	1.32	0
3	ACT	A	609	2	3,3,3	1.71	1 (33%)	3,3,3	1.17	0
3	ACT	A	610	2	3,3,3	1.55	1 (33%)	3,3,3	1.39	0
4	GOL	A	613	-	5,5,5	1.30	0	5,5,5	0.99	0
3	ACT	A	612	2	3,3,3	1.34	0	3,3,3	1.35	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
4	GOL	A	613	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	609	ACT	CH3-C	2.62	1.59	1.49
3	A	610	ACT	CH3-C	2.37	1.58	1.49
3	A	611	ACT	CH3-C	2.31	1.58	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	613	GOL	O1-C1-C2-C3
4	A	613	GOL	O1-C1-C2-O2

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

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(Å ²)	Q<0.9
1	A	514/547 (93%)	0.56	36 (7%) 22 24	29, 43, 73, 96	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	6.7
1	A	284	TYR	5.4
1	A	123	TYR	5.2
1	A	426	VAL	4.5
1	A	69	ILE	3.9
1	A	424	MET	3.9
1	A	430	TRP	3.8
1	A	427	TYR	3.6
1	A	428	PRO	3.4
1	A	425	PRO	3.1
1	A	283	HIS	3.1
1	A	432	GLY	3.0
1	A	282	LEU	3.0
1	A	351	PHE	3.0
1	A	124	LEU	2.9
1	A	423	ARG	2.8
1	A	533	THR	2.8
1	A	1	SER	2.7
1	A	279	TYR	2.7
1	A	285	VAL	2.6
1	A	270	TYR	2.6
1	A	110	LEU	2.5
1	A	280	PRO	2.4
1	A	429	LYS	2.4
1	A	335	GLY	2.3
1	A	68	THR	2.3
1	A	331	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	2.2
1	A	422	SER	2.2
1	A	256	GLN	2.2
1	A	187	ASN	2.1
1	A	332	ILE	2.1
1	A	333	ASN	2.1
1	A	22	LEU	2.0
1	A	527	LEU	2.0
1	A	451	THR	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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(Å ²)	Q<0.9
3	ACT	A	612	4/4	0.83	0.13	73,73,73,74	0
2	ZN	A	606	1/1	0.84	0.10	82,82,82,82	0
3	ACT	A	610	4/4	0.85	0.20	46,51,54,55	0
4	GOL	A	613	6/6	0.88	0.13	41,45,49,51	0
3	ACT	A	611	4/4	0.91	0.10	35,37,42,44	0
2	ZN	A	604	1/1	0.96	0.08	64,64,64,64	1
2	ZN	A	608	1/1	0.97	0.06	47,47,47,47	1
3	ACT	A	609	4/4	0.97	0.06	36,37,39,41	0
2	ZN	A	607	1/1	0.97	0.06	67,67,67,67	1
2	ZN	A	601	1/1	0.98	0.04	47,47,47,47	0
2	ZN	A	603	1/1	0.99	0.03	35,35,35,35	0
2	ZN	A	602	1/1	1.00	0.02	35,35,35,35	0
2	ZN	A	605	1/1	1.00	0.01	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.