



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1AQL
Title : CRYSTAL STRUCTURE OF BOVINE BILE-SALT ACTIVATED LIPASE
COMPLEXED WITH TAUROCHOLATE
Authors : Wang, X.; Zhang, X.
Deposited on : 1997-07-30
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

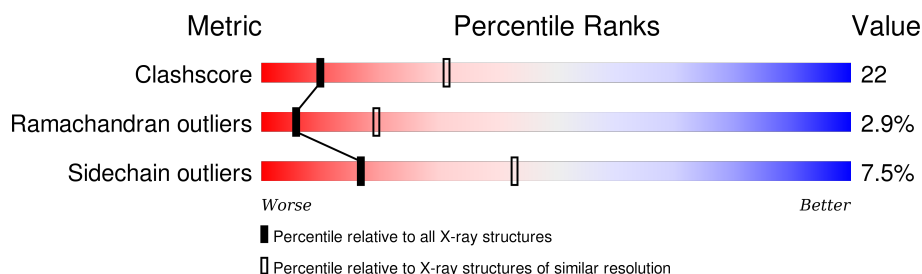
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 ≥ 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	532	
1	B	532	

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
3	TCH	A	601	X	-	-	-
3	TCH	A	602	X	-	-	-
3	TCH	B	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TCH	B	602	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8498 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.

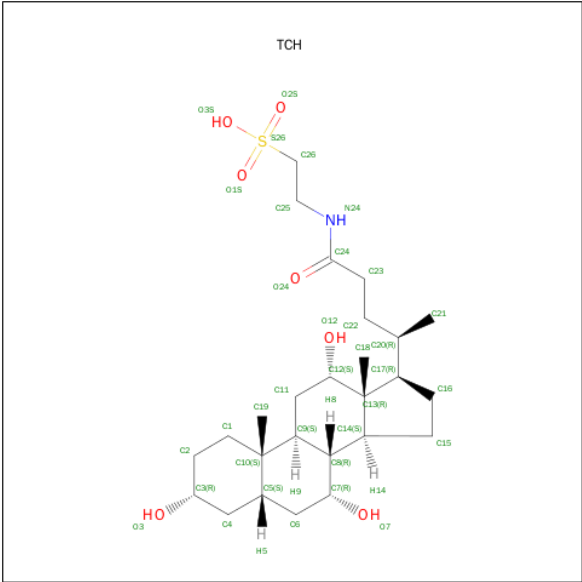
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			
1	B	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is TAUROCHOLIC ACID (three-letter code: TCH) (formula: $C_{26}H_{45}NO_7S$).



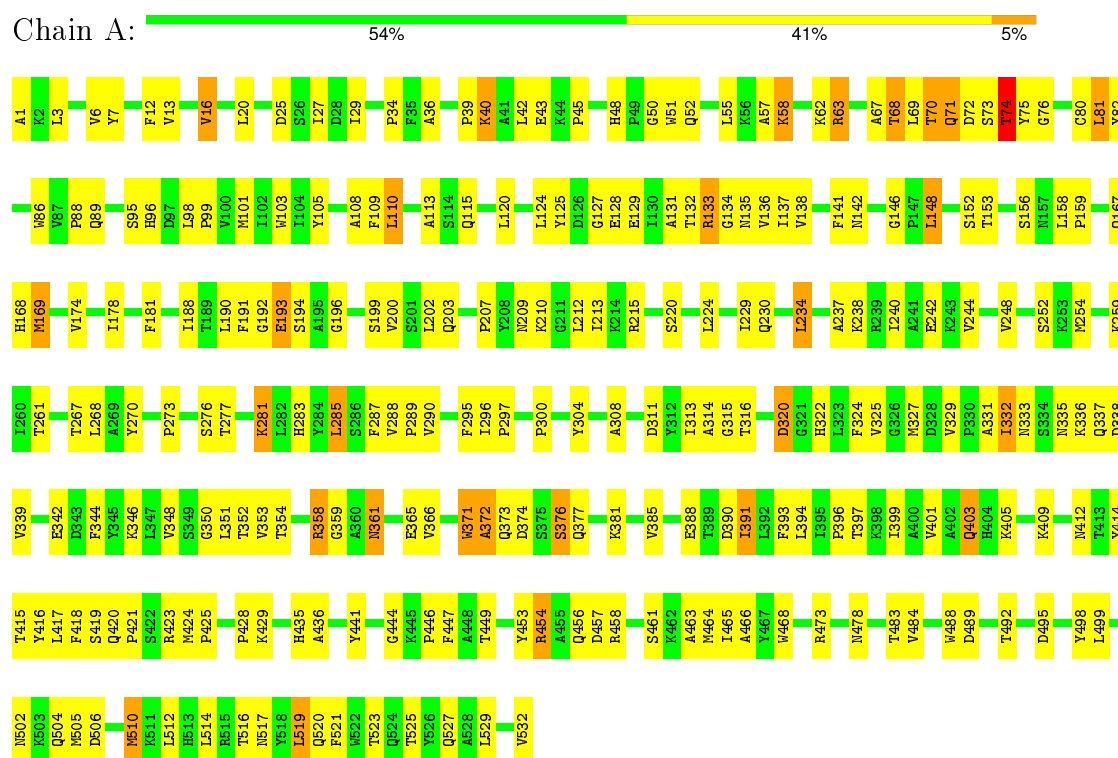
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		

3 Residue-property plots

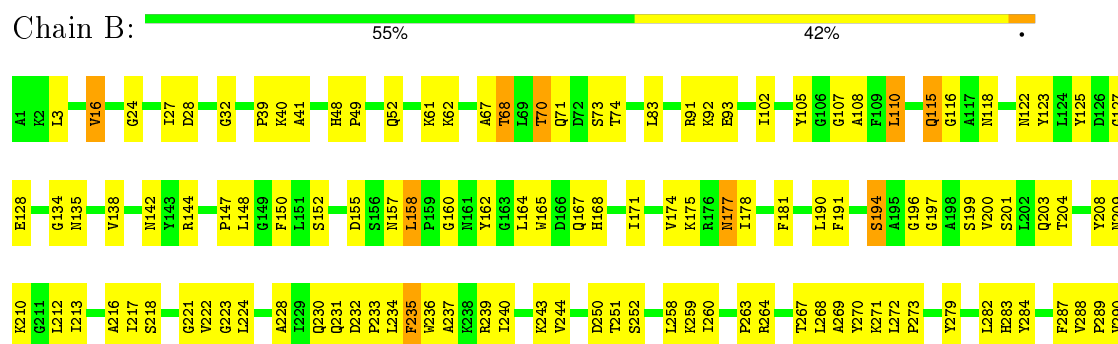
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 1: BILE-SALT ACTIVATED LIPASE



T525	T526	Q527	P530	T531	V532	Q440	Y441	V442	F443	Q444	K445	P446	F447	A448	T449	P450	L451	G452	Y453	R454	A455	Q456	D457	R458	T459	V460	S461	K462	I465	W468	T469	R473	T474	T483	D489	P490	E494	D495	D496	N497	Y498	K503	Q504	S507	N510	K511	L512	H513	L514	R515	L519	Q520	F521	H522	E365	E369	P370	W371	A372	Q373	D374	Q377	R380	K381	K382	T383	V385	D386	L387	E388	T389	D390	I391	L392	F393	L394	I395	P396	T397	K398	I399	A400	V401	H404	A408	K409	N412	T413	Y414	T415	Y416	L417	R423	M424	Y427	P428	K429	W430	M431	H435	A436	D437	D438	L439	I291	D294	F295	I296	P297	D298	D299	P300	V301	N302	L303	Y304	A308	D309	V310	I313	A314	D318	I319	D320	G321	H322	V325	P330	A331	I332	I333	S334	I335	K336	I337	D338	V339	T340	E341	E342	D343	K346	G350	L351	T352	K355	G356	L357	R358	G359	A360	I361	A362	T363	Y364
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	130.23Å 104.09Å 120.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	79.5 (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.211 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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: NAG, TCH

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	0.46	0/4278	0.71	0/5824
1	B	0.44	0/4278	0.69	1/5824 (0.0%)
All	All	0.45	0/8556	0.70	1/11648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	LEU	CA-CB-CG	5.61	128.19	115.30

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	4165	0	4055	196	0
1	B	4165	0	4055	170	0
2	A	14	0	13	2	0
2	B	14	0	13	1	0
3	A	70	0	82	9	0
3	B	70	0	82	11	0
All	All	8498	0	8300	369	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 22.

The worst 5 of 369 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:B:67:ALA:HA	1:B:73:SER:HA	1.37	1.04
1:B:115:GLN:HE21	1:B:115:GLN:H	1.11	0.96
1:B:325:VAL:HB	1:B:388:GLU:HG3	1.50	0.92
1:A:336:LYS:HG3	1:A:337:GLN:H	1.34	0.92
1:A:336:LYS:HE2	1:A:337:GLN:HG2	1.52	0.91

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	530/532 (100%)	451 (85%)	63 (12%)	16 (3%)	5	18
1	B	530/532 (100%)	456 (86%)	59 (11%)	15 (3%)	6	21
All	All	1060/1064 (100%)	907 (86%)	122 (12%)	31 (3%)	6	19

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	VAL
1	B	52	GLN
1	B	68	THR
1	B	158	LEU
1	A	70	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	444/444 (100%)	403 (91%)	41 (9%)	11	32
1	B	444/444 (100%)	418 (94%)	26 (6%)	24	57
All	All	888/888 (100%)	821 (92%)	67 (8%)	17	43

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	ARG
1	A	516	THR
1	B	468	TRP
1	A	454	ARG
1	A	504	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	ASN
1	B	115	GLN
1	B	230	GLN
1	A	524	GLN
1	B	283	HIS

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 ⓘ

6 ligands are modelled in this entry.

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
2	NAG	A	600	1	14,14,15	0.69	0	15,19,21	1.00	1 (6%)
3	TCH	A	601	-	37,38,38	2.09	11 (29%)	59,60,60	4.85	37 (62%)
3	TCH	A	602	-	37,38,38	2.20	12 (32%)	59,60,60	4.96	37 (62%)
2	NAG	B	600	1	14,14,15	0.70	0	15,19,21	1.11	2 (13%)
3	TCH	B	601	-	37,38,38	2.07	11 (29%)	59,60,60	4.75	35 (59%)
3	TCH	B	602	-	37,38,38	1.97	10 (27%)	59,60,60	4.75	36 (61%)

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
2	NAG	A	600	1	-	0/6/23/26	0/1/1/1
3	TCH	A	601	-	4/4/13/14	0/16/81/81	0/4/4/4
3	TCH	A	602	-	4/4/13/14	0/16/81/81	0/4/4/4
2	NAG	B	600	1	-	0/6/23/26	0/1/1/1
3	TCH	B	601	-	4/4/13/14	0/16/81/81	0/4/4/4
3	TCH	B	602	-	4/4/13/14	0/16/81/81	0/4/4/4

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	TCH	C6-C5	-5.28	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	TCH	C6-C5	-5.06	1.45	1.53
3	A	602	TCH	C10-C5	-5.00	1.46	1.55
3	B	602	TCH	C11-C9	-4.71	1.46	1.53
3	B	602	TCH	C10-C5	-4.41	1.47	1.55

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TCH	C9-C11-C12	-11.27	100.12	114.36
3	A	601	TCH	C9-C11-C12	-10.88	100.62	114.36
3	A	602	TCH	C9-C11-C12	-10.06	101.65	114.36
3	B	601	TCH	C9-C11-C12	-8.66	103.42	114.36
3	A	602	TCH	C5-C6-C7	-8.26	105.22	114.44

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	602	TCH	C5
3	B	602	TCH	C3
3	B	602	TCH	C20
3	B	602	TCH	C9
3	A	602	TCH	C5

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NAG	2	0
3	A	601	TCH	1	0
3	A	602	TCH	8	0
2	B	600	NAG	1	0
3	B	601	TCH	7	0
3	B	602	TCH	4	0

5.7 Other polymers [i](#)

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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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