



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:00 PM GMT

PDB ID : 2BCE
Title : CHOLESTEROL ESTERASE FROM BOS TAURUS
Authors : Chen, J.C.-H.; Miercke, L.J.W.; Krucinski, J.; Starr, J.R.; Saenz, G.; Wang, X.; Spilburg, C.A.; Lange, L.G.; Ellsworth, J.L.; Stroud, R.M.
Deposited on : 1998-01-28
Resolution : 1.60 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

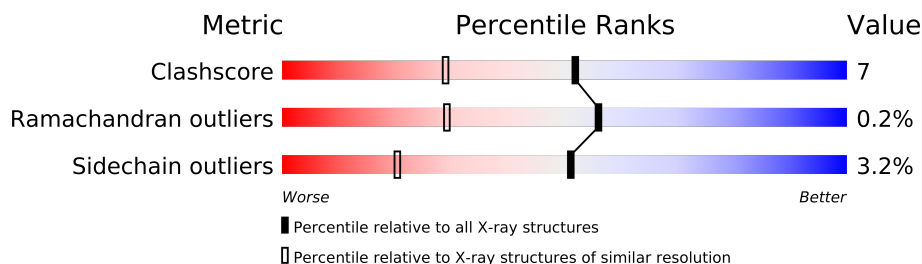
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.60 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	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	579	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4351 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CHOLESTEROL ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4132	2651	680	784	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	VAL	ILE	CONFLICT	UNP P30122
A	187	GLN	ASN	MUTATION	UNP P30122
A	361	GLN	ASN	MUTATION	UNP P30122

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	219	Total	O	0	0
			219	219		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.42Å 54.25Å 106.34Å 90.00° 104.12° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60	Depositor
% Data completeness (in resolution range)	89.1 (40.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.211 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4351	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.36	0/4244	0.63	0/5783

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4132	0	3981	58	0
2	A	219	0	0	1	0
All	All	4351	0	3981	58	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:GLU:HG2	1:A:439:LEU:HD21	1.42	1.00
1:A:74:THR:HG23	1:A:268:LEU:HD22	1.75	0.69
1:A:344:PHE:O	1:A:348:VAL:HG12	1.93	0.67
1:A:103:TRP:CZ3	1:A:192:GLY:HA2	2.31	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:PRO:HG3	1:A:351:LEU:HD23	1.77	0.64
1:A:168:HIS:HD2	1:A:209:ASN:OD1	1.84	0.60
1:A:341:GLU:HB3	1:A:364:TYR:OH	2.04	0.57
1:A:575:VAL:HG13	2:A:1062:HOH:O	2.05	0.56
1:A:193:GLU:HG2	1:A:439:LEU:CD2	2.28	0.56
1:A:365:GLU:O	1:A:369:GLU:HG3	2.05	0.56
1:A:293:GLY:HA2	1:A:297:PRO:HA	1.88	0.56
1:A:494:GLU:H	1:A:494:GLU:CD	2.09	0.56
1:A:123:TYR:HB3	1:A:124:LEU:HD22	1.89	0.54
1:A:520:GLN:O	1:A:524:GLN:HB2	2.08	0.54
1:A:282:LEU:HD13	1:A:285:LEU:HD12	1.91	0.53
1:A:175:LYS:HE3	1:A:212:LEU:HA	1.90	0.53
1:A:446:PRO:HA	1:A:453:TYR:CD2	2.43	0.53
1:A:282:LEU:HD21	1:A:324:PHE:CD1	2.44	0.53
1:A:110:LEU:HB3	1:A:576:VAL:HG12	1.92	0.52
1:A:395:ILE:O	1:A:399:ILE:HG22	2.10	0.52
1:A:427:TYR:HB3	1:A:431:MET:HG3	1.92	0.51
1:A:135:ASN:O	1:A:473:ARG:NH2	2.44	0.50
1:A:318:ASP:HB2	1:A:419:SER:HA	1.94	0.50
1:A:193:GLU:HA	1:A:219:GLN:O	2.11	0.49
1:A:163:GLY:O	1:A:167:GLN:HG3	2.13	0.49
1:A:23:PHE:HD1	1:A:23:PHE:H	1.61	0.48
1:A:80:CYS:O	1:A:142:ASN:HB2	2.14	0.47
1:A:315:GLY:HA3	1:A:416:TYR:CE1	2.49	0.47
1:A:71:GLN:OE1	1:A:271:LYS:HA	2.14	0.47
1:A:63:ARG:HH22	1:A:121:SER:HB2	1.80	0.46
1:A:153:THR:HG23	1:A:158:LEU:HB2	1.98	0.46
1:A:418:PHE:CZ	1:A:420:GLN:HB3	2.50	0.46
1:A:428:PRO:O	1:A:431:MET:HB2	2.16	0.46
1:A:366:VAL:HG21	1:A:521:PHE:CD1	2.52	0.45
1:A:444:GLY:HA2	1:A:461:SER:OG	2.17	0.45
1:A:288:VAL:HG12	1:A:579:PHE:HB2	1.99	0.45
1:A:427:TYR:HB3	1:A:428:PRO:HD2	1.98	0.44
1:A:313:ILE:HG12	1:A:414:TYR:HB2	1.98	0.44
1:A:272:LEU:HD13	1:A:285:LEU:HD21	1.99	0.44
1:A:45:PRO:HD2	1:A:165:TRP:HB3	1.99	0.44
1:A:460:VAL:O	1:A:464:MET:HG3	2.18	0.44
1:A:308:ALA:HB1	1:A:409:LYS:HG3	1.98	0.44
1:A:456:GLN:OE1	1:A:503:LYS:HD3	2.17	0.44
1:A:175:LYS:HG2	1:A:212:LEU:HD22	1.99	0.44
1:A:369:GLU:N	1:A:370:PRO:HD2	2.33	0.44
1:A:445:LYS:N	1:A:446:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:LEU:HD21	1:A:132:THR:HG21	2.00	0.43
1:A:498:TYR:CE1	1:A:514:LEU:HB2	2.53	0.43
1:A:111:MET:HE3	1:A:577:ILE:HG12	2.00	0.43
1:A:150:PHE:HE1	1:A:164:LEU:HG	1.83	0.43
1:A:415:THR:HG23	1:A:498:TYR:HB3	2.01	0.43
1:A:23:PHE:N	1:A:23:PHE:CD1	2.88	0.42
1:A:196:GLY:O	1:A:200:VAL:HG23	2.20	0.41
1:A:105:TYR:CZ	1:A:576:VAL:HG22	2.55	0.41
1:A:368:THR:O	1:A:371:TRP:HB2	2.20	0.41
1:A:67:ALA:O	1:A:109:PHE:HA	2.20	0.41
1:A:111:MET:CE	1:A:577:ILE:HG12	2.51	0.40
1:A:103:TRP:CE3	1:A:192:GLY:HA2	2.57	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	526/579 (91%)	505 (96%)	20 (4%)	1 (0%)	56	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASP

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	436/480 (91%)	422 (97%)	14 (3%)	51 20

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	23	PHE
1	A	110	LEU
1	A	111	MET
1	A	210	LYS
1	A	249	ASP
1	A	266	LEU
1	A	268	LEU
1	A	320	ASP
1	A	348	VAL
1	A	399	ILE
1	A	454	ARG
1	A	468	TRP
1	A	524	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	168	HIS
1	A	403	GLN
1	A	407	HIS
1	A	520	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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 ⓘ

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.