



# wwPDB X-ray Structure Validation Summary Report

May 15, 2014 – 11:37 PM EDT

PDB ID : 1C2O  
Title : ELECTROPHORUS ELECTRICUS ACETYLCHOLINESTERASE  
Authors : Bourne, Y.; Marchot, P.  
Deposited on : 1999-07-26  
Resolution : 4.20 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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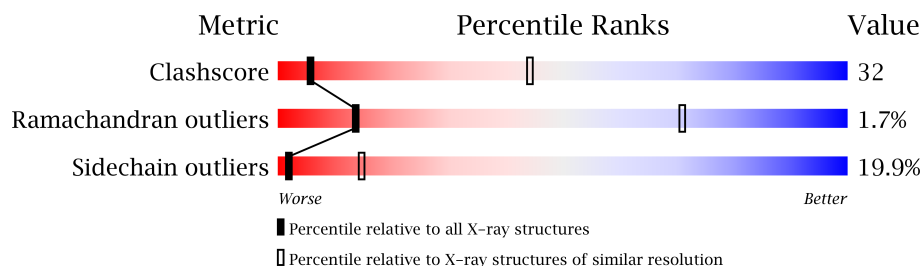
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 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) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 4.20 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	1259 (4.84-3.50)
Ramachandran outliers	78287	1192 (4.84-3.50)
Sidechain outliers	78261	1175 (4.84-3.50)

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. 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	539	
1	B	539	
1	C	539	
1	D	539	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16688 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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			
1	B	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			
1	C	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			
1	D	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			

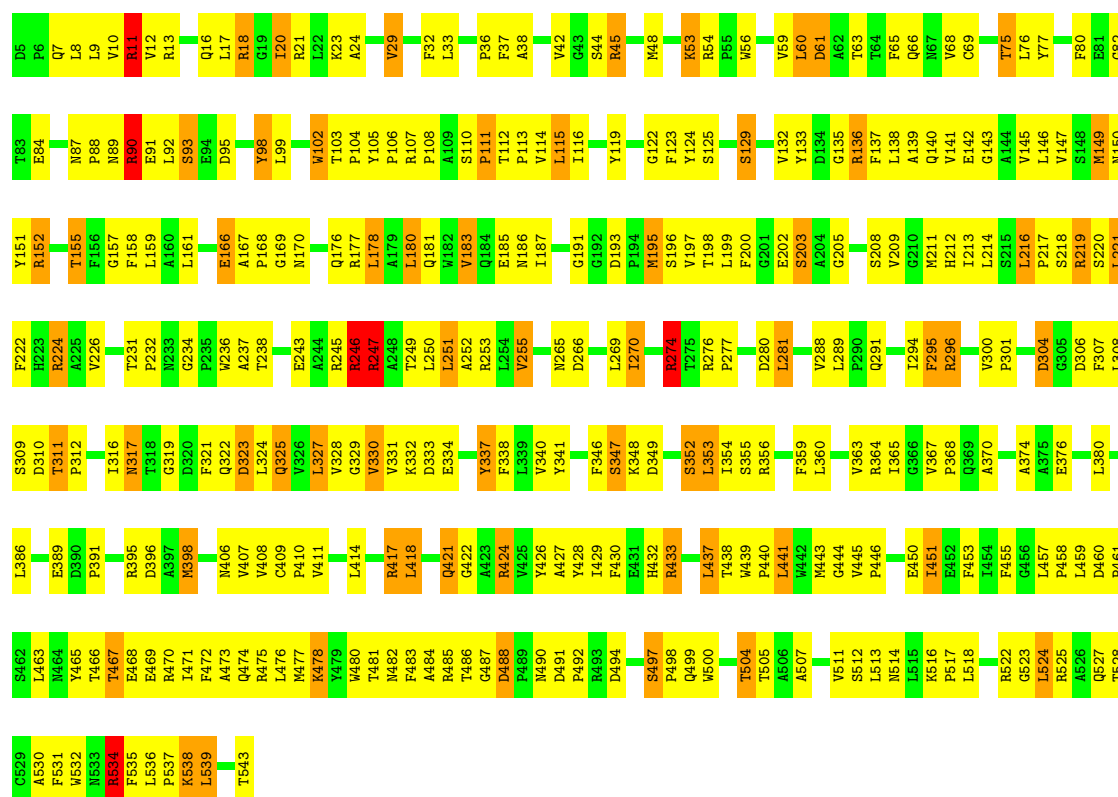
### 3 Residue-property plots

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.

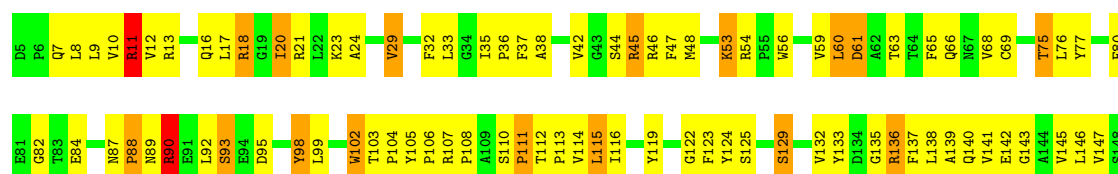
#### • Molecule 1: ACETYLCHOLINESTERASE

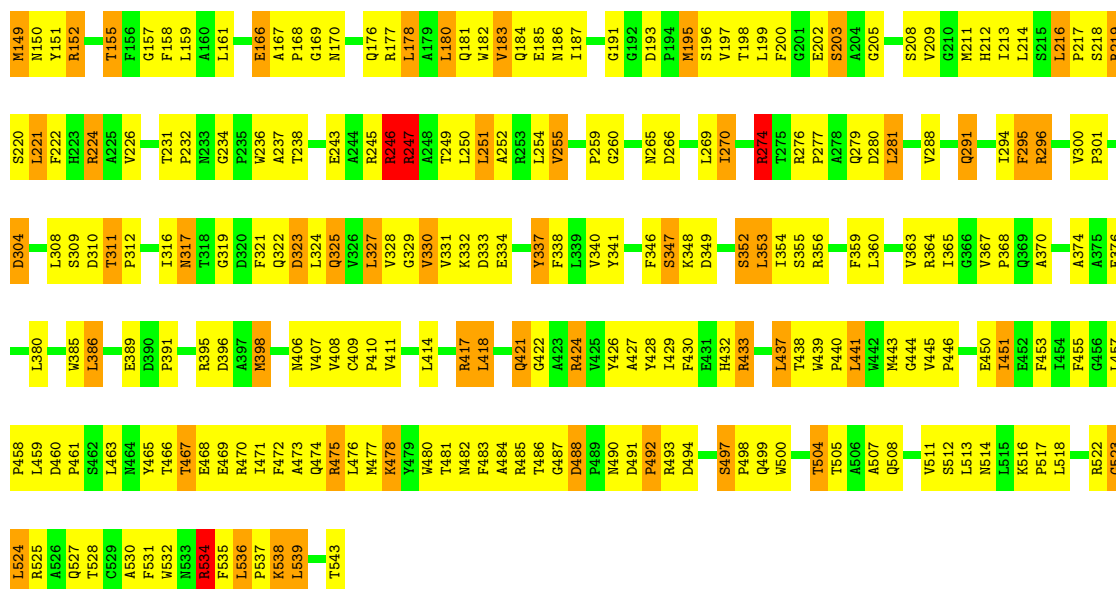
Chain A: 



#### • Molecule 1: ACETYLCHOLINESTERASE

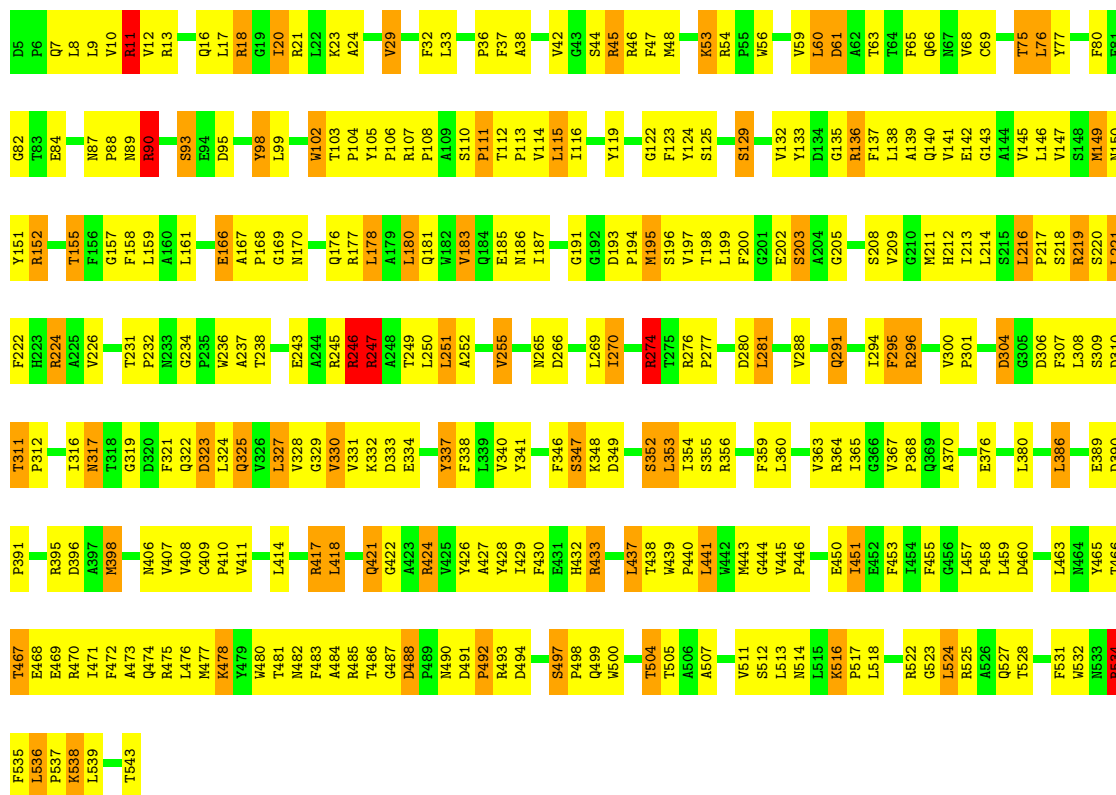
Chain B: 





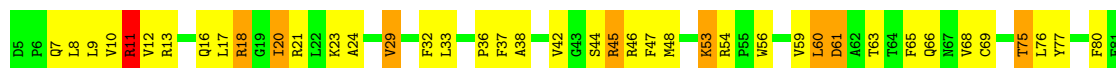
### • Molecule 1: ACETYLCHOLINESTERASE

Chain C:



### • Molecule 1: ACETYLCHOLINESTERASE

Chain D:



N533	T466	S309	L221	M150	G82
R534	T467	D310	F222	Y151	T83
L536	E468	P311	H223	R152	E84
P537	E469	P312	R224		
K538	R470			T155	N87
L539	I471	I316	A225	F156	P88
	F472	N317	V226	G157	N89
	A473	T318		F158	R30
	Q474	G319	T231	L159	E91
	R475	D320	P232	L161	L92
	L476	F321	N233		S93
	M477	Q322	G234		E94
	K478	D323	P235	E166	D95
	Y479	L324	A236	A167	
	W480	Q325	A237	P168	Y98
	T481	V326	T238	G169	L99
	N482	L414		N170	
	F483	R417	E243		W102
	A484	V328	A244	Q176	T103
	R485	G329	R245	R177	P104
	T486	V330	R246	L178	Y105
	G487	V331	R247	A179	P106
	D488	K332	A248	L180	R107
	P489	D333	T249	Q181	P108
	N490	E334	L250	W182	A109
	D491		L251	V183	S110
	P492	Y337	A252	Q184	P111
	R493	F338		E185	T112
	D494	L339	V255	N186	P113
		F340		I187	V114
		Y341	P259		L115
				G191	T116
	S497	F346	N265	G192	
	P498	S347	D266	D193	Y119
	Q499	K348		P194	
	W500	D349	L269	M195	G122
			L270	S196	F123
	T504	S352		V197	Y124
	T505	L353	R273	T198	S125
	A506	I354	T275	L199	
	A507	S355	R276	F200	S129
		R356	P277	G201	
	V511	F359	A278	E202	V132
	S512	L360	Q279	S203	Y133
	L513		D280	A204	D134
	N514	V363	L281	G205	G135
	L515	R364			R136
	K516	I365	V288	S208	F137
	P517			V209	L138
	L518	P368	Q291	G210	A139
				M211	Q140
	R522	A374	T294	H212	V141
	G523	A375	F295	I213	E142
	L524	E376	R296	L214	G143
	R525			S215	A144
	A526	L380	V300	L216	V145
	Q527		P301	P217	L146
	T528			S218	V147
	G529	L386	D304	R219	S148
	A530	E389	L308	S220	M149
	F531				
	W532				

## 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, $\alpha$ , $\beta$ , $\gamma$	211.16Å 129.75Å 195.42Å 90.00° 103.20° 90.00°	Depositor
Resolution (Å)	12.00 – 4.20	Depositor
% Data completeness (in resolution range)	66.0 (12.00-4.20)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.375 , 0.385	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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	0.66	0/4298	1.42	32/5879 (0.5%)
1	B	0.65	0/4298	1.42	33/5879 (0.6%)
1	C	0.66	0/4298	1.42	33/5879 (0.6%)
1	D	0.66	0/4298	1.42	32/5879 (0.5%)
All	All	0.66	0/17192	1.42	130/23516 (0.6%)

There are no bond length outliers.

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	D	247	ARG	NE-CZ-NH2	-13.24	113.68	120.30
1	A	247	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	C	247	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	C	274	ARG	NE-CZ-NH2	-12.34	114.13	120.30

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	4172	0	4052	257	7
1	B	4172	0	4052	272	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4172	0	4052	270	10
1	D	4172	0	4052	256	0
All	All	16688	0	16208	1039	17

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 32.

The worst 5 of 1039 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:306:ASP:OD1	1:B:259:PRO:HB2	1.47	1.11
1:A:306:ASP:OD1	1:B:259:PRO:CB	1.98	1.10
1:A:116:ILE:HD11	1:A:183:VAL:HG11	1.43	1.00
1:D:116:ILE:HD11	1:D:183:VAL:HG11	1.43	0.99
1:C:116:ILE:HD11	1:C:183:VAL:HG11	1.43	0.98

The worst 5 of 17 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:21:ARG:NH2	1:C:105:TYR:CE2[2_655]	0.66	1.54
1:A:88:PRO:O	1:A:91:GLU:CG[2_554]	1.08	1.12
1:C:21:ARG:NH2	1:C:105:TYR:CZ[2_655]	1.12	1.08
1:A:88:PRO:O	1:A:91:GLU:CD[2_554]	1.17	1.03
1:C:23:LYS:NZ	1:C:105:TYR:OH[2_655]	1.21	0.99

## 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	537/539 (100%)	470 (88%)	58 (11%)	9 (2%)	14	71
1	B	537/539 (100%)	471 (88%)	57 (11%)	9 (2%)	14	71
1	C	537/539 (100%)	470 (88%)	58 (11%)	9 (2%)	14	71
1	D	537/539 (100%)	469 (87%)	59 (11%)	9 (2%)	14	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2148/2156 (100%)	1880 (88%)	232 (11%)	36 (2%)	14	71

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	323	ASP
1	A	492	PRO
1	A	494	ASP
1	A	497	SER

### 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	434/440 (99%)	348 (80%)	86 (20%)	2	15
1	B	434/440 (99%)	347 (80%)	87 (20%)	2	14
1	C	434/440 (99%)	348 (80%)	86 (20%)	2	15
1	D	434/440 (99%)	348 (80%)	86 (20%)	2	15
All	All	1736/1760 (99%)	1391 (80%)	345 (20%)	2	15

5 of 345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	441	LEU
1	C	168	PRO
1	D	386	LEU
1	B	485	ARG
1	C	18	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	482	ASN
1	C	212	HIS

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Mol	Chain	Res	Type
1	D	464	ASN
1	C	16	GLN
1	C	291	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.