



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:15 PM GMT

PDB ID : 1ESC  
Title : THE MOLECULAR MECHANISM OF ENANTIORECOGNITION BY ESTERASES  
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Deposited on : 1994-10-07  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/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	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
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

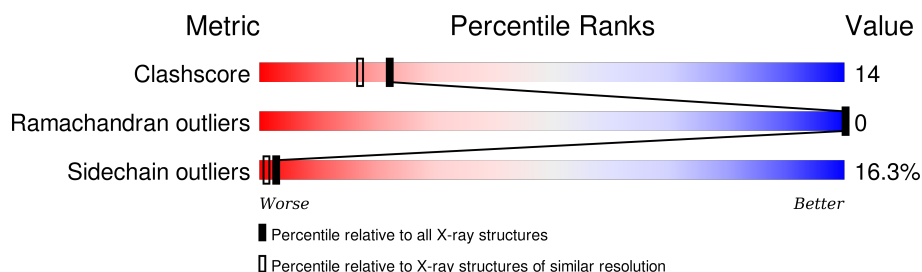
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	 55% 31% 10% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2518 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 ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2295	1442	390	456	7			

- Molecule 2 is water.

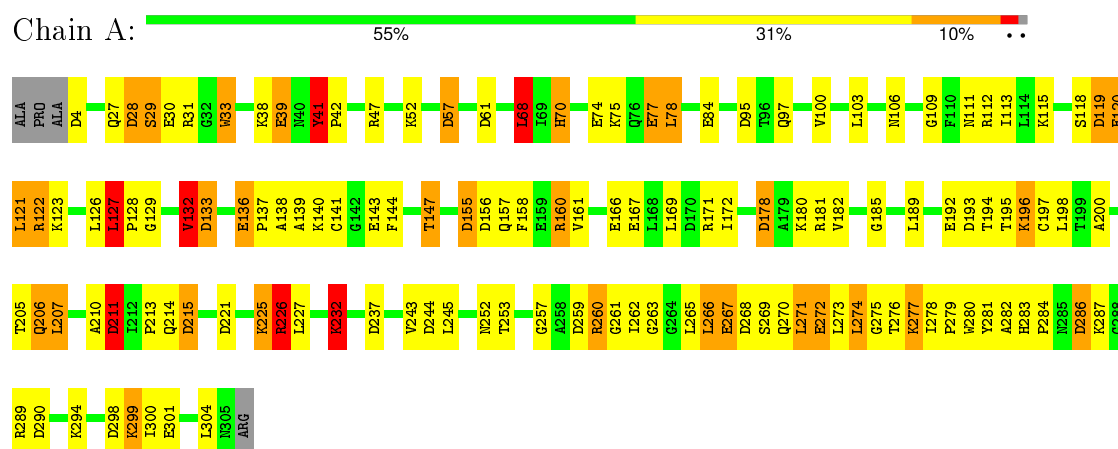
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	223	Total	O	0	0
			223	223		

### 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: ESTERASE



## 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, $\alpha$ , $\beta$ , $\gamma$	131.03Å 48.50Å 70.31Å 90.00° 118.09° 90.00°	Depositor
Resolution (Å)	7.50 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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	0.83	2/2344 (0.1%)	2.03	70/3185 (2.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	GLU	CD-OE1	7.70	1.34	1.25
1	A	272	GLU	CD-OE2	7.13	1.33	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	CD-NE-CZ	20.91	152.87	123.60
1	A	31	ARG	NE-CZ-NH2	-18.36	111.12	120.30
1	A	31	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	A	160	ARG	CD-NE-CZ	14.07	143.30	123.60
1	A	160	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	289	ARG	NE-CZ-NH1	10.81	125.71	120.30
1	A	171	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	A	289	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	A	226	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	192	GLU	CA-CB-CG	8.60	132.33	113.40
1	A	122	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	A	221	ASP	CB-CG-OD1	-8.38	110.75	118.30
1	A	28	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	A	232	LYS	CA-CB-CG	8.13	131.29	113.40
1	A	28	ASP	N-CA-CB	-7.96	96.27	110.60
1	A	226	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	237	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	274	LEU	CB-CA-C	7.75	124.92	110.20
1	A	112	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	A	178	ASP	CB-CG-OD1	7.66	125.19	118.30
1	A	27	GLN	CA-CB-CG	7.65	130.24	113.40
1	A	136	GLU	CB-CA-C	7.55	125.51	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLU	OE1-CD-OE2	7.42	132.20	123.30
1	A	28	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	206	GLN	CA-CB-CG	-7.26	97.42	113.40
1	A	286	ASP	CB-CG-OD2	7.24	124.81	118.30
1	A	270	GLN	CG-CD-OE1	7.09	135.78	121.60
1	A	57	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	156	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	61	ASP	N-CA-C	-6.97	92.17	111.00
1	A	215	ASP	CA-CB-CG	6.94	128.66	113.40
1	A	259	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	268	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	178	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	133	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	95	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	61	ASP	N-CA-CB	6.42	122.16	110.60
1	A	147	THR	N-CA-CB	-6.28	98.36	110.30
1	A	132	VAL	CB-CA-C	6.19	123.16	111.40
1	A	260	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	267	GLU	OE1-CD-OE2	6.12	130.64	123.30
1	A	211	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	127	LEU	O-C-N	5.93	132.36	121.10
1	A	68	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	275	GLY	N-CA-C	-5.79	98.63	113.10
1	A	252	ASN	N-CA-CB	5.64	120.76	110.60
1	A	120	GLU	CG-CD-OE2	-5.63	107.03	118.30
1	A	206	GLN	N-CA-CB	5.58	120.65	110.60
1	A	57	ASP	CB-CA-C	5.53	121.46	110.40
1	A	33	TRP	CA-CB-CG	-5.52	103.21	113.70
1	A	133	ASP	N-CA-CB	5.52	120.54	110.60
1	A	84	GLU	CA-CB-CG	5.51	125.53	113.40
1	A	290	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	160	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	39	GLU	CA-CB-CG	5.46	125.42	113.40
1	A	155	ASP	N-CA-CB	5.46	120.43	110.60
1	A	167	GLU	CG-CD-OE2	-5.36	107.57	118.30
1	A	119	ASP	N-CA-CB	5.36	120.25	110.60
1	A	277	LYS	O-C-N	5.33	131.23	122.70
1	A	74	GLU	CG-CD-OE1	5.32	128.93	118.30
1	A	143	GLU	CG-CD-OE2	5.32	128.93	118.30
1	A	178	ASP	N-CA-CB	-5.25	101.16	110.60
1	A	262	ILE	CA-C-N	5.25	126.69	116.20
1	A	41	TYR	CB-CA-C	5.15	120.69	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLU	CA-CB-CG	5.12	124.65	113.40
1	A	97	GLN	CA-CB-CG	5.05	124.51	113.40
1	A	77	GLU	CA-CB-CG	5.03	124.47	113.40
1	A	283	HIS	N-CA-CB	5.03	119.64	110.60
1	A	290	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	143	GLU	OE1-CD-OE2	-5.01	117.29	123.30

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	2295	0	2211	62	0
2	A	223	0	0	8	0
All	All	2518	0	2211	62	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 14.

All (62) 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:272:GLU:HA	1:A:276:THR:O	1.77	0.82
1:A:195:THR:HA	1:A:198:LEU:HD12	1.69	0.74
1:A:172:ILE:HG21	1:A:181:ARG:HG2	1.79	0.64
1:A:158:PHE:CZ	1:A:226:ARG:HD2	2.37	0.60
1:A:225:LYS:HD3	2:A:437:HOH:O	2.02	0.58
1:A:257:GLY:O	1:A:260:ARG:NH1	2.31	0.58
1:A:169:LEU:O	1:A:181:ARG:NH1	2.37	0.58
1:A:263:GLY:HA3	1:A:280:TRP:CD1	2.38	0.58
1:A:121:LEU:HD22	1:A:265:LEU:HD21	1.85	0.57
1:A:133:ASP:HB3	1:A:136:GLU:HB2	1.86	0.57
1:A:70:HIS:ND1	2:A:589:HOH:O	2.33	0.55
1:A:300:ILE:O	1:A:304:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:O	1:A:196:LYS:HG3	2.07	0.53
1:A:200:ALA:HB3	2:A:621:HOH:O	2.08	0.53
1:A:195:THR:O	1:A:198:LEU:HB2	2.10	0.52
1:A:267:GLU:O	1:A:279:PRO:HA	2.09	0.52
1:A:29:SER:HA	2:A:573:HOH:O	2.10	0.52
1:A:269:SER:OG	1:A:271:LEU:HB2	2.10	0.52
1:A:178:ASP:HB2	2:A:500:HOH:O	2.09	0.52
1:A:194:THR:HG22	1:A:214:GLN:OE1	2.11	0.50
1:A:197:CYS:O	1:A:207:LEU:HD13	2.12	0.50
1:A:115:LYS:NZ	1:A:127:LEU:O	2.38	0.50
1:A:158:PHE:CE2	1:A:226:ARG:HD2	2.47	0.49
1:A:185:GLY:O	1:A:245:LEU:HD12	2.11	0.49
1:A:111:ASN:HD22	1:A:129:GLY:HA3	1.76	0.49
1:A:41:TYR:CG	1:A:42:PRO:HD3	2.48	0.49
1:A:33:TRP:HB2	1:A:78:LEU:HG	1.93	0.49
1:A:158:PHE:CZ	1:A:226:ARG:HB3	2.49	0.48
1:A:226:ARG:HD3	2:A:609:HOH:O	2.14	0.47
1:A:276:THR:HG22	1:A:277:LYS:O	2.15	0.47
1:A:193:ASP:OD1	1:A:195:THR:OG1	2.29	0.47
1:A:120:GLU:HB2	1:A:211:ASP:OD2	2.15	0.46
1:A:39:GLU:OE1	1:A:47:ARG:NH2	2.48	0.46
1:A:206:GLN:HG2	1:A:207:LEU:H	1.81	0.45
1:A:119:ASP:HA	1:A:122:ARG:HG3	1.98	0.45
1:A:263:GLY:HA3	1:A:280:TRP:CG	2.52	0.45
1:A:133:ASP:HB2	1:A:144:PHE:CE1	2.52	0.45
1:A:132:VAL:HG22	1:A:144:PHE:CZ	2.51	0.45
1:A:68:LEU:HD22	1:A:106:ASN:HB3	1.99	0.45
1:A:126:LEU:HD12	1:A:278:ILE:HD12	1.98	0.45
1:A:157:GLN:O	1:A:161:VAL:HG23	2.18	0.44
1:A:139:ALA:HA	1:A:213:PRO:HG3	1.99	0.44
1:A:157:GLN:NE2	2:A:512:HOH:O	2.47	0.44
1:A:115:LYS:NZ	1:A:129:GLY:O	2.46	0.43
1:A:243:VAL:HG22	1:A:299:LYS:HG2	2.01	0.43
1:A:137:PRO:O	1:A:138:ALA:C	2.58	0.42
1:A:298:ASP:O	1:A:301:GLU:HB3	2.20	0.42
1:A:52:LYS:HD2	2:A:552:HOH:O	2.20	0.41
1:A:120:GLU:HG2	1:A:266:LEU:HD21	2.02	0.41
1:A:232:LYS:NZ	1:A:244:ASP:OD2	2.53	0.41
1:A:210:ALA:HB2	1:A:266:LEU:CD2	2.51	0.41
1:A:127:LEU:HD22	1:A:128:PRO:HD2	2.03	0.41
1:A:158:PHE:HE1	1:A:227:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:O	1:A:282:ALA:HB3	2.21	0.40
1:A:261:GLY:O	1:A:284:PRO:HA	2.21	0.40
1:A:140:LYS:HB3	1:A:140:LYS:HE3	1.94	0.40
1:A:70:HIS:CD2	1:A:70:HIS:C	2.95	0.40
1:A:210:ALA:HB2	1:A:266:LEU:HD22	2.02	0.40
1:A:109:GLY:O	1:A:113:ILE:HG13	2.20	0.40
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.95	0.40
1:A:253:THR:O	1:A:260:ARG:HA	2.22	0.40
1:A:100:VAL:HG22	1:A:182:VAL:HB	2.02	0.40

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	300/306 (98%)	275 (92%)	25 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	239/241 (99%)	200 (84%)	39 (16%)	3	1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	28	ASP
1	A	29	SER
1	A	38	LYS
1	A	41	TYR
1	A	57	ASP
1	A	68	LEU
1	A	70	HIS
1	A	75	LYS
1	A	77	GLU
1	A	78	LEU
1	A	118	SER
1	A	121	LEU
1	A	123	LYS
1	A	127	LEU
1	A	132	VAL
1	A	141	CYS
1	A	147	THR
1	A	155	ASP
1	A	160	ARG
1	A	166	GLU
1	A	180	LYS
1	A	189	LEU
1	A	196	LYS
1	A	205	THR
1	A	207	LEU
1	A	211	ASP
1	A	215	ASP
1	A	225	LYS
1	A	226	ARG
1	A	232	LYS
1	A	266	LEU
1	A	271	LEU
1	A	273	LEU
1	A	274	LEU
1	A	286	ASP
1	A	287	LYS
1	A	294	LYS
1	A	299	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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