



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:20 am BST

PDB ID : 2HAD  
Title : CRYSTAL STRUCTURE OF HALOALKANE DEHALOGENASE: AN ENZYME TO DETOXIFY HALOGENATED ALKANES  
Authors : Verschueren, K.H.G.; Franken, S.M.; Dijkstra, B.W.  
Deposited on : 1992-08-07  
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](mailto: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.

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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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

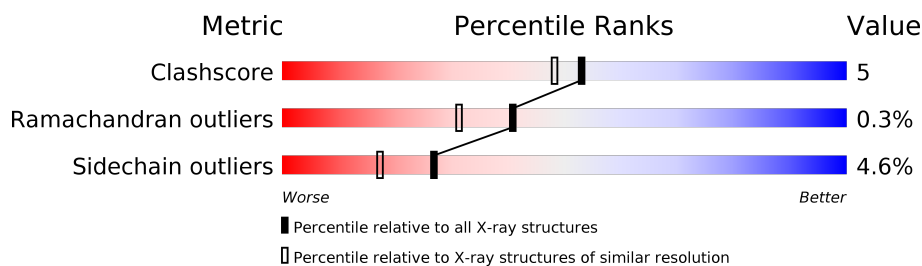
# 1 Overall quality at a glance

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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2737 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 HALOALKANE DEHALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2479	1596	406	462	15			

- Molecule 2 is water.

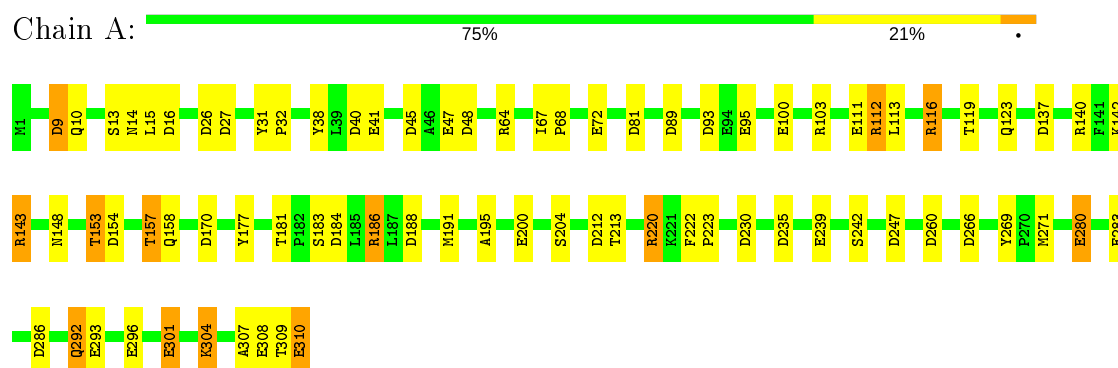
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	258	Total	O	0	0
			258	258		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: HALOALKANE DEHALOGENASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.80Å 72.80Å 41.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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	0.84	15/2552 (0.6%)	1.55	51/3470 (1.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE2	6.75	1.33	1.25
1	A	308	GLU	CD-OE2	6.63	1.32	1.25
1	A	95	GLU	CD-OE2	6.44	1.32	1.25
1	A	72	GLU	CD-OE2	6.37	1.32	1.25
1	A	200	GLU	CD-OE2	6.27	1.32	1.25
1	A	280	GLU	CD-OE2	6.25	1.32	1.25
1	A	100	GLU	CD-OE2	6.19	1.32	1.25
1	A	47	GLU	CD-OE2	6.10	1.32	1.25
1	A	301	GLU	CD-OE2	5.89	1.32	1.25
1	A	283	GLU	CD-OE2	5.89	1.32	1.25
1	A	111	GLU	CD-OE2	5.88	1.32	1.25
1	A	296	GLU	CD-OE2	5.87	1.32	1.25
1	A	310	GLU	CD-OE1	5.78	1.32	1.25
1	A	293	GLU	CD-OE2	5.12	1.31	1.25
1	A	41	GLU	CD-OE2	5.06	1.31	1.25

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ASP	CB-CG-OD2	-11.55	107.91	118.30
1	A	170	ASP	CB-CG-OD1	10.26	127.54	118.30
1	A	188	ASP	CB-CG-OD1	10.01	127.31	118.30
1	A	45	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	A	93	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	143	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	116	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	89	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	A	48	ASP	CB-CG-OD2	-7.72	111.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	212	ASP	CB-CG-OD1	7.55	125.10	118.30
1	A	26	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	230	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	116	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	143	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	93	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	9	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	45	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	184	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	212	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	A	40	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	195	ALA	CB-CA-C	6.62	120.04	110.10
1	A	235	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	27	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	48	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	89	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	247	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	286	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	153	THR	N-CA-CB	-5.81	99.26	110.30
1	A	26	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	186	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	137	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	27	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	260	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	223	PRO	N-CA-CB	5.49	109.89	103.30
1	A	170	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	40	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	220	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	81	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	293	GLU	CB-CA-C	5.40	121.20	110.40
1	A	112	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	38	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	A	191	MET	CG-SD-CE	5.25	108.60	100.20
1	A	16	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	13	SER	CB-CA-C	-5.20	100.22	110.10
1	A	260	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	64	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	269	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	A	308	GLU	CB-CA-C	5.09	120.59	110.40
1	A	140	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	119	THR	N-CA-C	-5.07	97.30	111.00

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	2479	0	2379	26	0
2	A	258	0	0	6	1
All	All	2737	0	2379	26	1

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 5.

All (26) 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:292:GLN:HE21	1:A:292:GLN:H	1.06	1.00
1:A:112:ARG:HH11	1:A:112:ARG:HG3	1.47	0.78
1:A:292:GLN:HE21	1:A:292:GLN:N	1.87	0.69
1:A:142:LYS:HG2	1:A:143:ARG:HG3	1.78	0.66
1:A:213:THR:HG23	2:A:607:HOH:O	1.94	0.65
1:A:292:GLN:H	1:A:292:GLN:NE2	1.87	0.65
1:A:309:THR:O	1:A:310:GLU:HG2	1.98	0.63
1:A:112:ARG:NH1	1:A:112:ARG:HG3	2.17	0.56
1:A:10:GLN:HG3	1:A:10:GLN:O	2.05	0.56
1:A:220:ARG:HD3	2:A:473:HOH:O	2.06	0.56
1:A:186:ARG:HD3	2:A:609:HOH:O	2.08	0.54
1:A:153:THR:HG21	1:A:158:GLN:HB2	1.90	0.54
1:A:307:ALA:C	1:A:309:THR:H	2.10	0.53
1:A:309:THR:HG22	1:A:309:THR:O	2.09	0.53
1:A:154:ASP:OD1	1:A:157:THR:HG23	2.08	0.52
1:A:204:SER:HB3	2:A:624:HOH:O	2.11	0.51
1:A:301:GLU:OE1	1:A:304:LYS:HD2	2.12	0.50
1:A:31:TYR:N	1:A:32:PRO:CD	2.75	0.49
1:A:112:ARG:NH1	1:A:112:ARG:CG	2.78	0.47
1:A:304:LYS:HE3	1:A:304:LYS:HB2	1.71	0.46
1:A:177:TYR:O	1:A:181:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HH11	1:A:103:ARG:HD3	1.62	0.45
1:A:67:ILE:HB	1:A:68:PRO:HD3	1.99	0.44
1:A:266:ASP:HB2	2:A:420:HOH:O	2.18	0.42
1:A:280:GLU:HG3	2:A:544:HOH:O	2.19	0.42
1:A:183:SER:O	1:A:213:THR:HG21	2.20	0.41

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
2:A:429:HOH:O	2:A:655:HOH:O[3_556]	1.40	0.80

## 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	308/310 (99%)	291 (94%)	16 (5%)	1 (0%)	41 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN

### 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	262/262 (100%)	250 (95%)	12 (5%)	27	17

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	14	ASN
1	A	15	LEU
1	A	113	LEU
1	A	116	ARG
1	A	123	GLN
1	A	157	THR
1	A	222	PHE
1	A	242	SER
1	A	271	MET
1	A	292	GLN
1	A	304	LYS

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	14	ASN
1	A	104	ASN
1	A	123	GLN
1	A	251	GLN
1	A	292	GLN

### 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

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.