



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:44 AM UTC

PDB ID : 2HAD / pdb_00002had
Title : CRYSTAL STRUCTURE OF HALOALKANE DEHALOGENASE: AN ENZYME TO DETOXYIFY 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

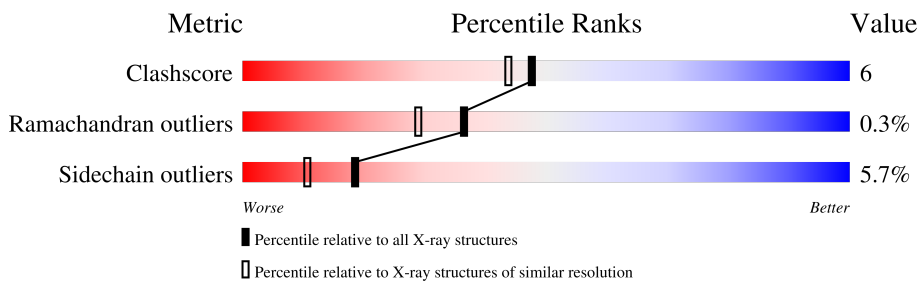
1 Overall quality at a glance

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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 75% 21% .

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		

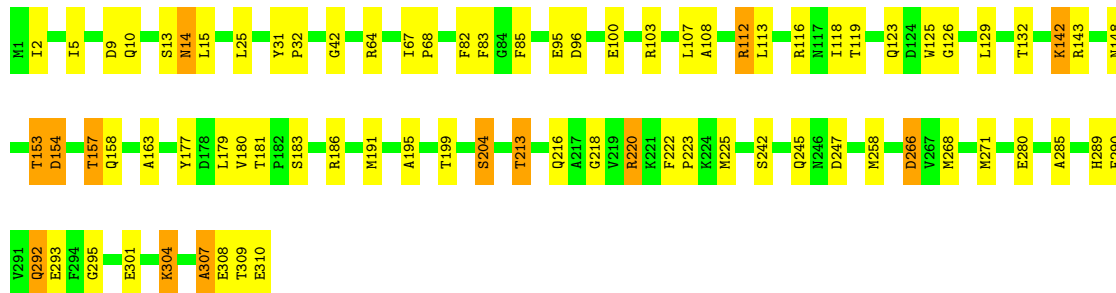
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

Chain A:  75% 21% .



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, α , β , γ	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 ²)	16.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	0.91	0/2552	1.75	50/3470 (1.4%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASP	CA-CB-CG	-10.13	102.47	112.60
1	A	216	GLN	N-CA-C	9.83	123.93	112.72
1	A	153	THR	N-CA-CB	-8.05	99.26	110.38
1	A	268	MET	N-CA-C	7.57	119.61	111.36
1	A	154	ASP	CA-CB-CG	-7.52	105.08	112.60
1	A	96	ASP	CA-CB-CG	-7.24	105.36	112.60
1	A	295	GLY	N-CA-C	7.16	122.96	113.37
1	A	14	ASN	N-CA-C	6.83	120.50	112.72
1	A	2	ILE	N-CA-C	-6.79	97.85	108.23
1	A	213	THR	N-CA-C	6.62	119.32	111.71
1	A	258	MET	N-CA-C	6.60	119.31	111.71
1	A	163	ALA	N-CA-C	6.54	118.41	111.28
1	A	13	SER	CB-CA-C	-6.37	100.22	110.79
1	A	285	ALA	N-CA-C	6.24	118.88	111.71
1	A	290	PHE	N-CA-CB	-6.08	103.11	110.53
1	A	119	THR	N-CA-C	-6.04	97.30	107.99
1	A	289	HIS	CA-CB-CG	5.99	119.79	113.80
1	A	195	ALA	CB-CA-C	5.96	120.04	111.27
1	A	223	PRO	N-CA-CB	5.96	109.89	103.33
1	A	247	ASP	N-CA-C	5.77	120.46	112.90
1	A	142	LYS	N-CA-CB	-5.76	102.29	110.81
1	A	108	ALA	CA-C-N	5.75	127.92	120.44
1	A	108	ALA	C-N-CA	5.75	127.92	120.44
1	A	204	SER	CA-CB-OG	-5.73	99.65	111.10
1	A	218	GLY	O-C-N	5.70	127.72	122.19
1	A	118	ILE	N-CA-C	5.66	116.36	108.89
1	A	179	LEU	N-CA-C	5.65	120.31	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	THR	N-CA-C	-5.58	102.49	110.59
1	A	64	ARG	N-CA-C	5.54	119.54	112.34
1	A	129	LEU	CA-C-N	5.53	126.11	119.98
1	A	129	LEU	C-N-CA	5.53	126.11	119.98
1	A	308	GLU	CB-CG-CD	5.53	121.99	112.60
1	A	245	GLN	N-CA-C	5.50	117.36	111.36
1	A	5	ILE	CB-CG1-CD1	-5.46	102.34	113.80
1	A	191	MET	N-CA-C	5.37	117.13	111.28
1	A	126	GLY	N-CA-C	-5.34	106.24	113.24
1	A	220	ARG	O-C-N	-5.28	116.13	122.15
1	A	293	GLU	CB-CA-C	5.21	121.20	110.31
1	A	85	PHE	N-CA-CB	-5.14	103.30	111.62
1	A	82	PHE	CA-C-O	-5.11	115.99	121.56
1	A	308	GLU	CB-CA-C	5.11	120.59	110.42
1	A	307	ALA	N-CA-C	-5.09	105.81	112.23
1	A	132	THR	N-CA-CB	5.07	117.99	110.49
1	A	107	LEU	CA-C-N	5.05	127.00	120.44
1	A	107	LEU	C-N-CA	5.05	127.00	120.44
1	A	25	LEU	CA-C-N	-5.05	114.06	122.08
1	A	25	LEU	C-N-CA	-5.05	114.06	122.08
1	A	83	PHE	N-CA-C	-5.04	102.92	110.23
1	A	100	GLU	CB-CG-CD	-5.02	104.06	112.60
1	A	42	GLY	O-C-N	-5.02	118.14	122.91

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	27	0
2	A	258	0	0	6	1
All	All	2737	0	2379	27	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 6.

All (27) 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:HG3	1:A:112:ARG:HH11	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:125:TRP:CH2	1:A:225:MET:HE2	2.35	0.60
1:A:307:ALA:C	1:A:309:THR:H	2.10	0.59
1:A:112:ARG:HG3	1:A:112:ARG:NH1	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:154:ASP:OD1	1:A:157:THR:HG23	2.08	0.52
1:A:309:THR:O	1:A:309:THR:HG22	2.09	0.51
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:HB2	1:A:304:LYS:HE3	1.71	0.46
1:A:177:TYR:O	1:A:181:THR:HG23	2.15	0.46
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 [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	308/310 (99%)	291 (94%)	16 (5%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN

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	262/262 (100%)	247 (94%)	15 (6%)	18	11

All (15) 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	95	GLU
1	A	112	ARG
1	A	113	LEU
1	A	116	ARG
1	A	123	GLN
1	A	157	THR
1	A	180	VAL

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Mol	Chain	Res	Type
1	A	222	PHE
1	A	242	SER
1	A	271	MET
1	A	292	GLN
1	A	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	17	GLN
1	A	104	ASN
1	A	123	GLN
1	A	251	GLN
1	A	292	GLN

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 oligosaccharides 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 ⓘ

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.