



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 2DHE / pdb_00002dhe
Title : CRYSTALLOGRAPHIC ANALYSIS OF THE CATALYTIC MECHANISM
OF HALOALKANE DEHALOGENASE
Authors : Verschueren, K.H.G.; Dijkstra, B.W.
Deposited on : 1993-06-24
Resolution : 2.13 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

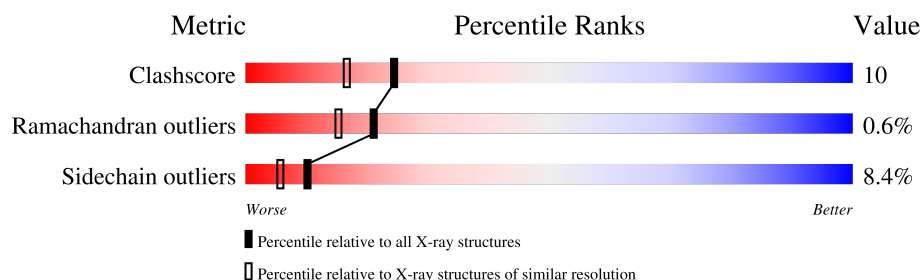
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)

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	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2665 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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

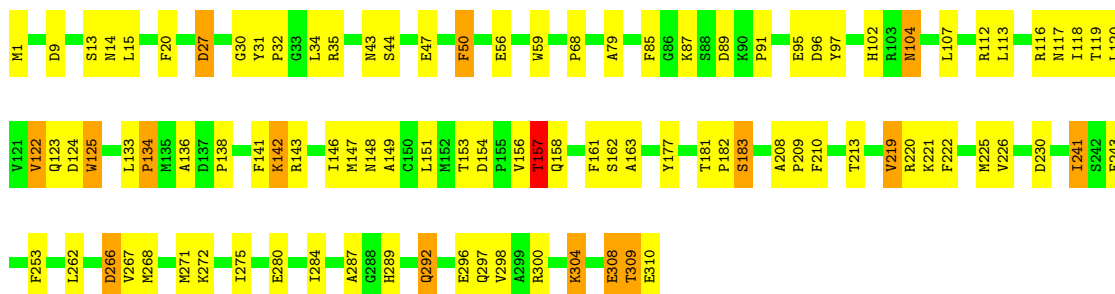
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	0
			185	185		

Note EDS was not executed.

Chain A: 68% 27% 5%



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	95.00Å 72.60Å 41.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.13	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.13)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2665	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.94	2/2552 (0.1%)	1.77	43/3470 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	TRP	NE1-CE2	-5.52	1.31	1.37
1	A	59	TRP	NE1-CE2	-5.09	1.31	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	GLU	CB-CA-C	7.59	121.69	111.14
1	A	243	PHE	CA-CB-CG	-6.95	106.85	113.80
1	A	163	ALA	N-CA-C	6.45	119.13	111.33
1	A	134	PRO	N-CA-CB	6.41	110.56	103.26
1	A	226	VAL	CA-C-N	6.38	129.12	120.44
1	A	226	VAL	C-N-CA	6.38	129.12	120.44
1	A	147	MET	CA-C-O	-6.37	113.85	121.56
1	A	35	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	A	50	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	79	ALA	O-C-N	6.20	126.23	121.27
1	A	271	MET	N-CA-C	-6.19	104.62	111.36
1	A	141	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	183	SER	N-CA-C	-6.13	105.81	113.28
1	A	287	ALA	CA-C-O	-6.11	113.89	120.92
1	A	138	PRO	N-CA-CB	6.09	110.03	103.33
1	A	68	PRO	N-CA-CB	5.92	109.84	103.33
1	A	221	LYS	N-CA-C	5.88	118.64	111.82
1	A	142	LYS	N-CA-CB	-5.74	102.31	110.81
1	A	230	ASP	N-CA-CB	5.72	118.54	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ALA	CA-C-O	5.61	126.41	119.79
1	A	149	ALA	CB-CA-C	-5.53	100.99	110.95
1	A	43	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	104	ASN	O-C-N	-5.46	115.55	122.27
1	A	68	PRO	N-CD-CG	5.46	111.39	103.20
1	A	156	VAL	CA-C-O	5.35	126.99	121.05
1	A	267	VAL	CA-C-N	5.33	128.42	120.31
1	A	267	VAL	C-N-CA	5.33	128.42	120.31
1	A	241	ILE	CA-C-O	5.31	126.80	121.17
1	A	85	PHE	N-CA-C	5.28	117.21	109.24
1	A	287	ALA	O-C-N	5.26	129.27	123.16
1	A	122	VAL	N-CA-CB	-5.21	105.22	112.52
1	A	182	PRO	N-CA-CB	5.20	107.94	103.31
1	A	253	PHE	CA-C-O	-5.20	113.89	120.28
1	A	219	VAL	O-C-N	5.20	126.91	121.87
1	A	118	ILE	O-C-N	5.17	128.55	122.81
1	A	266	ASP	N-CA-CB	5.16	119.43	110.39
1	A	87	LYS	O-C-N	-5.13	115.92	122.34
1	A	89	ASP	CA-C-O	-5.09	116.01	121.56
1	A	20	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	157	THR	CB-CA-C	5.04	119.16	110.79
1	A	210	PHE	CA-C-N	5.03	124.81	119.28
1	A	210	PHE	C-N-CA	5.03	124.81	119.28
1	A	102	HIS	N-CA-C	-5.00	105.93	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	48	0
2	A	1	0	0	0	0
3	A	185	0	0	7	0
All	All	2665	0	2379	48	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 10.

All (48) 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:308:GLU:HB2	3:A:541:HOH:O	1.55	1.03
1:A:308:GLU:OE1	3:A:541:HOH:O	1.80	0.99
1:A:292:GLN:HE21	1:A:292:GLN:H	1.01	0.96
1:A:142:LYS:HG2	1:A:143:ARG:HG3	1.69	0.75
1:A:292:GLN:H	1:A:292:GLN:NE2	1.83	0.70
1:A:292:GLN:HE21	1:A:292:GLN:N	1.84	0.69
1:A:220:ARG:HD3	3:A:450:HOH:O	1.93	0.68
1:A:308:GLU:CB	3:A:541:HOH:O	2.27	0.62
1:A:296:GLU:O	1:A:300:ARG:HG3	2.01	0.60
1:A:262:LEU:HD23	3:A:442:HOH:O	2.03	0.58
1:A:284:ILE:HD11	1:A:298:VAL:HG22	1.86	0.58
1:A:153:THR:HG21	1:A:158:GLN:HB2	1.87	0.57
1:A:56:GLU:OE2	1:A:219:VAL:O	2.23	0.56
1:A:272:LYS:O	1:A:272:LYS:HG2	2.05	0.56
1:A:96:ASP:OD2	3:A:423:HOH:O	2.17	0.56
1:A:309:THR:O	1:A:309:THR:HG22	2.05	0.55
1:A:14:ASN:O	1:A:14:ASN:ND2	2.39	0.55
1:A:124:ASP:OD1	1:A:289:HIS:NE2	2.34	0.55
1:A:208:ALA:HB3	1:A:209:PRO:HD3	1.90	0.54
1:A:146:ILE:HG12	1:A:268:MET:HE1	1.91	0.53
1:A:50:PHE:CE2	1:A:119:THR:HG21	2.44	0.53
1:A:183:SER:O	1:A:213:THR:HG21	2.10	0.51
1:A:125:TRP:CH2	1:A:225:MET:HE2	2.46	0.51
1:A:154:ASP:OD1	1:A:157:THR:CG2	2.60	0.49
1:A:30:GLY:C	1:A:32:PRO:HD3	2.37	0.49
1:A:310:GLU:O	1:A:310:GLU:HG2	2.13	0.49
1:A:133:LEU:HB2	1:A:134:PRO:HD3	1.95	0.48
1:A:142:LYS:HG2	1:A:143:ARG:CG	2.43	0.47
1:A:177:TYR:CD1	1:A:181:THR:HG21	2.50	0.47
1:A:151:LEU:HD13	1:A:241:ILE:HG13	1.97	0.47
1:A:31:TYR:N	1:A:32:PRO:HD3	2.31	0.46
1:A:153:THR:CG2	1:A:158:GLN:HB2	2.46	0.46
1:A:154:ASP:CG	1:A:157:THR:HG23	2.41	0.45
1:A:304:LYS:HE3	1:A:304:LYS:HB2	1.64	0.45
1:A:31:TYR:N	1:A:32:PRO:CD	2.79	0.45
1:A:309:THR:O	1:A:310:GLU:HB2	2.18	0.44
1:A:104:ASN:ND2	3:A:432:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD13	1:A:275:ILE:HG21	1.68	0.42
1:A:125:TRP:CH2	1:A:225:MET:CE	3.03	0.42
1:A:161:PHE:CD1	1:A:161:PHE:N	2.88	0.42
1:A:30:GLY:C	1:A:32:PRO:CD	2.93	0.41
1:A:142:LYS:O	1:A:143:ARG:HG2	2.20	0.41
1:A:154:ASP:CG	1:A:157:THR:CG2	2.93	0.41
1:A:27:ASP:OD1	1:A:27:ASP:N	2.53	0.41
1:A:91:PRO:HD2	1:A:97:TYR:OH	2.20	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.84	0.41
1:A:120:LEU:HG	1:A:122:VAL:HG13	2.03	0.41
1:A:14:ASN:HD22	1:A:14:ASN:C	2.29	0.41

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	308/310 (99%)	293 (95%)	13 (4%)	2 (1%)	21	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	309	THR

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%)	240 (92%)	22 (8%)	10 6

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ASP
1	A	13	SER
1	A	15	LEU
1	A	27	ASP
1	A	34	LEU
1	A	44	SER
1	A	47	GLU
1	A	95	GLU
1	A	112	ARG
1	A	113	LEU
1	A	116	ARG
1	A	117	ASN
1	A	123	GLN
1	A	157	THR
1	A	162	SER
1	A	222	PHE
1	A	266	ASP
1	A	280	GLU
1	A	292	GLN
1	A	297	GLN
1	A	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	123	GLN
1	A	228	GLN
1	A	245	GLN
1	A	246	ASN
1	A	292	GLN
1	A	305	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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.