



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:59 PM UTC

PDB ID : 2EDC / pdb\_00002edc  
Title : CRYSTALLOGRAPHIC AND FLUORESCENCE STUDIES OF THE INTERACTION OF HALOALKANE DEHALOGENASE WITH HALIDE IONS: STUDIES WITH HALIDE COMPOUNDS REVEAL A HALIDE BINDING SITE IN THE ACTIVE SITE  
Authors : Verschueren, K.H.G.; Dijkstra, B.W.  
Deposited on : 1993-08-31  
Resolution : 2.30 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

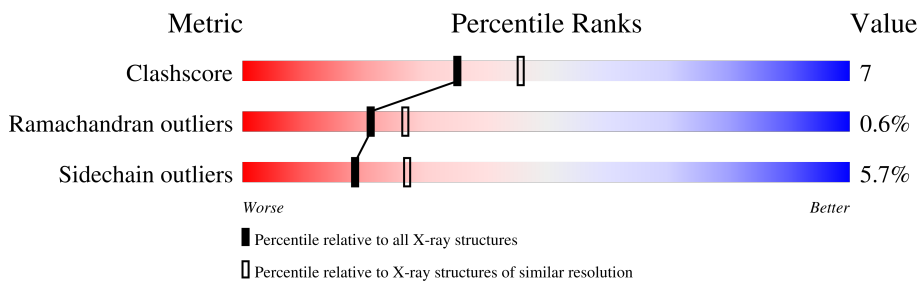
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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  $\geq 3$ , 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 [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2605 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
			Total	C	N	O	S			
1	A	310	2479	1596	406	462	15	0	0	0

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

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

- Molecule 3 is water.

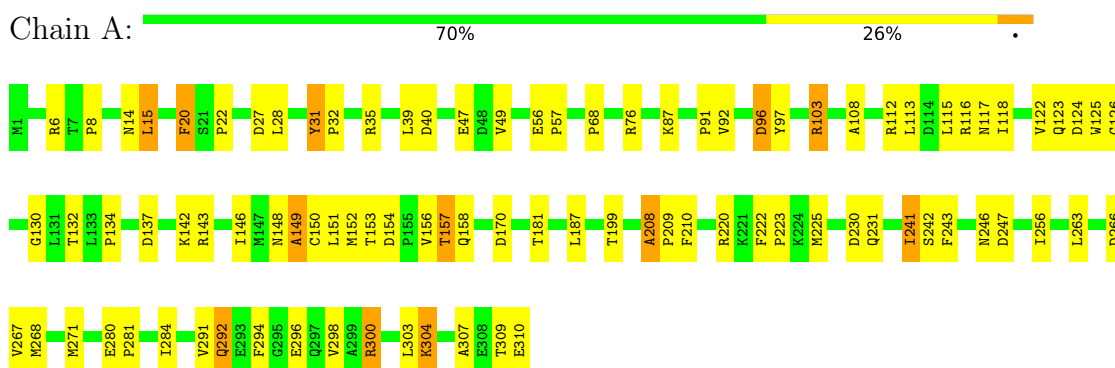
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	0
			125	125		

### 3 Residue-property plots

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



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	94.90Å 73.10Å 41.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/2552	1.89	57/3470 (1.6%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASP	CA-CB-CG	11.48	124.08	112.60
1	A	124	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	231	GLN	N-CA-C	7.96	119.59	111.07
1	A	223	PRO	N-CA-CB	7.19	111.24	103.33
1	A	281	PRO	CB-CA-C	-6.73	101.00	110.63
1	A	230	ASP	CA-C-O	-6.72	114.08	121.87
1	A	22	PRO	O-C-N	6.71	131.58	123.13
1	A	103	ARG	CD-NE-CZ	-6.68	115.05	124.40
1	A	31	TYR	CA-C-N	6.63	127.67	119.98
1	A	31	TYR	C-N-CA	6.63	127.67	119.98
1	A	118	ILE	N-CA-C	6.33	117.25	108.89
1	A	122	VAL	N-CA-C	6.19	118.65	108.99
1	A	96	ASP	CA-CB-CG	-5.95	106.65	112.60
1	A	156	VAL	N-CA-C	5.93	116.57	110.82
1	A	132	THR	CB-CA-C	-5.87	100.64	110.56
1	A	242	SER	CA-C-N	5.85	128.05	120.44
1	A	242	SER	C-N-CA	5.85	128.05	120.44
1	A	22	PRO	CA-C-O	-5.78	114.81	121.86
1	A	35	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	A	267	VAL	CA-C-N	5.72	128.41	120.29
1	A	267	VAL	C-N-CA	5.72	128.41	120.29
1	A	210	PHE	N-CA-CB	-5.66	101.01	110.12
1	A	241	ILE	CA-C-N	5.62	127.81	120.28
1	A	241	ILE	C-N-CA	5.62	127.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	LYS	N-CA-CB	5.54	118.69	110.49
1	A	300	ARG	CD-NE-CZ	5.50	132.10	124.40
1	A	132	THR	N-CA-CB	5.49	118.58	110.56
1	A	126	GLY	N-CA-C	-5.48	106.03	113.37
1	A	230	ASP	N-CA-C	-5.47	103.30	110.53
1	A	20	PHE	CA-C-O	-5.42	114.69	120.92
1	A	199	THR	N-CA-C	-5.41	101.97	110.36
1	A	268	MET	N-CA-C	5.41	117.25	111.36
1	A	294	PHE	N-CA-C	-5.39	103.98	110.88
1	A	130	GLY	N-CA-C	5.38	120.28	113.24
1	A	146	ILE	N-CA-C	5.33	115.52	107.80
1	A	181	THR	CA-C-N	-5.33	114.44	119.76
1	A	181	THR	C-N-CA	-5.33	114.44	119.76
1	A	149	ALA	CA-C-O	-5.30	115.47	121.25
1	A	300	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	A	118	ILE	O-C-N	5.23	128.62	122.81
1	A	15	LEU	CA-C-N	5.23	129.36	122.30
1	A	15	LEU	C-N-CA	5.23	129.36	122.30
1	A	108	ALA	CA-C-N	5.22	127.23	120.44
1	A	108	ALA	C-N-CA	5.22	127.23	120.44
1	A	68	PRO	CB-CA-C	-5.22	104.49	112.11
1	A	28	LEU	CB-CA-C	5.19	116.89	109.11
1	A	208	ALA	CA-C-O	5.17	123.08	118.33
1	A	303	LEU	N-CA-CB	5.16	118.28	110.28
1	A	170	ASP	N-CA-CB	-5.11	103.51	110.56
1	A	247	ASP	N-CA-C	5.08	119.56	112.90
1	A	6	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	A	256	ILE	CB-CA-C	-5.08	103.27	110.83
1	A	150	CYS	CA-C-N	-5.06	115.59	122.93
1	A	150	CYS	C-N-CA	-5.06	115.59	122.93
1	A	76	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	A	40	ASP	O-C-N	5.03	129.57	123.14
1	A	92	VAL	N-CA-C	5.00	119.45	112.50

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	36	0
2	A	1	0	0	0	0
3	A	125	0	0	3	0
All	All	2605	0	2379	36	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 7.

All (36) 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	1.19	0.85
1:A:307:ALA:C	1:A:309:THR:H	1.95	0.72
1:A:220:ARG:HD3	3:A:472:HOH:O	1.89	0.72
1:A:309:THR:O	1:A:309:THR:HG22	1.91	0.70
1:A:142:LYS:HG2	1:A:143:ARG:HG3	1.77	0.67
1:A:125:TRP:CH2	1:A:225:MET:HE2	2.33	0.64
1:A:309:THR:O	1:A:310:GLU:HG2	2.01	0.60
1:A:96:ASP:OD2	3:A:406:HOH:O	2.17	0.58
1:A:307:ALA:C	1:A:309:THR:N	2.64	0.56
1:A:149:ALA:HA	1:A:263:LEU:HD13	1.87	0.56
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.71	0.54
1:A:153:THR:HG21	1:A:158:GLN:HB2	1.91	0.53
1:A:151:LEU:HD13	1:A:241:ILE:HG13	1.92	0.51
1:A:103:ARG:HD3	3:A:420:HOH:O	2.09	0.51
1:A:152:MET:HA	1:A:152:MET:HE2	1.95	0.48
1:A:296:GLU:O	1:A:300:ARG:HG3	2.13	0.48
1:A:31:TYR:N	1:A:32:PRO:CD	2.77	0.48
1:A:157:THR:C	1:A:158:GLN:HG2	2.38	0.47
1:A:304:LYS:HE3	1:A:304:LYS:HB2	1.60	0.46
1:A:91:PRO:HD2	1:A:97:TYR:OH	2.15	0.46
1:A:284:ILE:HD12	1:A:291:VAL:HG13	1.99	0.45
1:A:112:ARG:HG3	1:A:112:ARG:NH1	2.32	0.44
1:A:134:PRO:HB2	1:A:243:PHE:CE2	2.53	0.44
1:A:284:ILE:HD11	1:A:298:VAL:HG22	2.00	0.43
1:A:47:GLU:O	1:A:117:ASN:HB2	2.19	0.42
1:A:154:ASP:OD1	1:A:157:THR:CG2	2.67	0.42
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.84	0.42
1:A:20:PHE:HB2	1:A:39:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HG11	1:A:115:LEU:HD22	2.03	0.41
1:A:103:ARG:HD3	1:A:103:ARG:HH11	1.41	0.41
1:A:208:ALA:N	1:A:209:PRO:CD	2.84	0.41
1:A:307:ALA:O	1:A:309:THR:N	2.50	0.41
1:A:157:THR:O	1:A:158:GLN:HG2	2.21	0.41
1:A:153:THR:CG2	1:A:158:GLN:HB2	2.51	0.40
1:A:208:ALA:HB3	1:A:209:PRO:HD3	2.03	0.40
1:A:56:GLU:HA	1:A:57:PRO:HA	1.96	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	308/310 (99%)	289 (94%)	17 (6%)	2 (1%)	21 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	137	ASP

### 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 27

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	14	ASN
1	A	15	LEU
1	A	27	ASP
1	A	113	LEU
1	A	116	ARG
1	A	123	GLN
1	A	157	THR
1	A	222	PHE
1	A	246	ASN
1	A	266	ASP
1	A	271	MET
1	A	280	GLU
1	A	292	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	10	GLN
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](#)

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.