



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:13 AM UTC

PDB ID : 2EDA / pdb_00002eda
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 : 1993-08-30
Resolution : 2.19 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
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

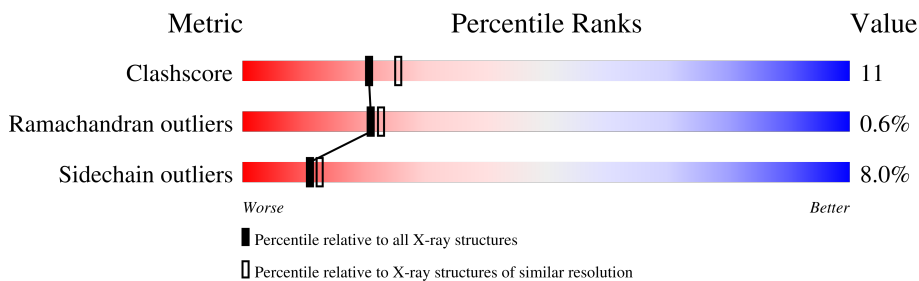
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 2694 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.

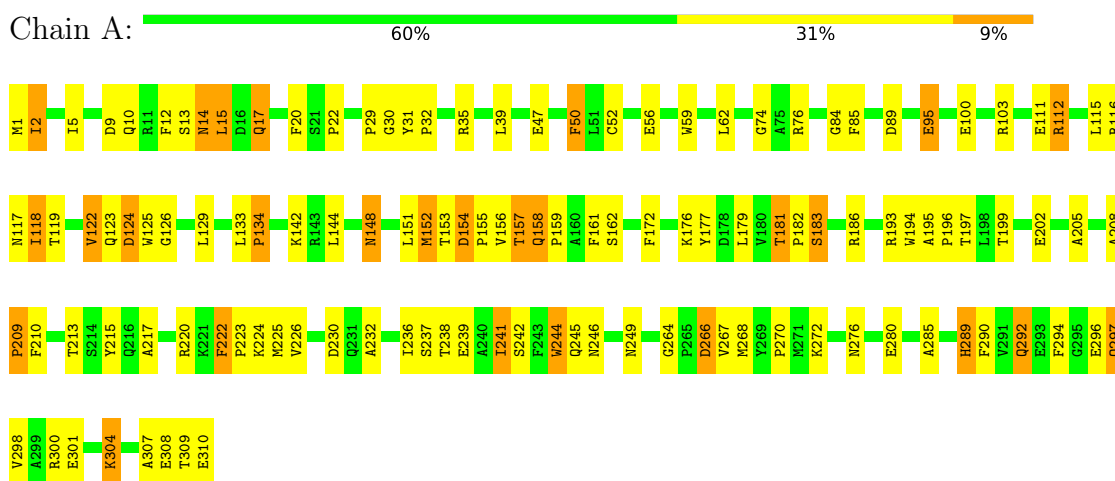
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		

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, α , β , γ	95.10Å 73.00Å 41.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.19	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.161 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2694	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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	0.95	1/2552 (0.0%)	2.03	92/3470 (2.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	TRP	NE1-CE2	-5.46	1.31	1.37

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	HIS	CA-CB-CG	10.30	124.11	113.80
1	A	222	PHE	CA-C-O	10.13	127.95	118.63
1	A	111	GLU	CA-C-O	-8.91	111.02	120.55
1	A	244	TRP	CA-C-O	8.88	129.96	120.55
1	A	199	THR	N-CA-C	-8.60	98.48	110.35
1	A	50	PHE	CA-CB-CG	-8.35	105.45	113.80
1	A	241	ILE	CA-C-O	8.13	129.50	121.05
1	A	129	LEU	CA-C-N	7.82	128.79	120.03
1	A	129	LEU	C-N-CA	7.82	128.79	120.03
1	A	264	GLY	CA-C-N	7.49	127.51	119.28
1	A	264	GLY	C-N-CA	7.49	127.51	119.28
1	A	111	GLU	N-CA-CB	7.47	121.18	110.13
1	A	95	GLU	CA-C-N	7.26	131.35	120.31
1	A	95	GLU	C-N-CA	7.26	131.35	120.31
1	A	172	PHE	CA-CB-CG	-7.18	106.61	113.80
1	A	222	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	245	GLN	N-CA-C	7.02	118.72	111.14
1	A	124	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	266	ASP	N-CA-CB	6.80	121.83	110.41
1	A	154	ASP	CA-CB-CG	-6.75	105.85	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	SER	N-CA-C	6.62	119.06	111.11
1	A	118	ILE	N-CA-C	6.55	117.49	109.30
1	A	156	VAL	N-CA-C	6.53	117.52	111.45
1	A	111	GLU	O-C-N	6.52	130.06	122.17
1	A	226	VAL	CA-C-O	6.49	127.48	120.47
1	A	290	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	298	VAL	CB-CA-C	-6.33	103.59	112.14
1	A	285	ALA	CA-C-O	-6.28	113.89	120.55
1	A	134	PRO	N-CA-CB	6.26	110.31	103.30
1	A	285	ALA	N-CA-C	6.25	118.10	111.28
1	A	159	PRO	N-CA-CB	6.22	110.11	103.52
1	A	152	MET	CA-C-O	6.22	129.40	120.51
1	A	276	ASN	O-C-N	-6.02	115.49	122.95
1	A	177	TYR	CB-CA-C	5.96	120.25	110.88
1	A	176	LYS	CA-C-O	5.95	127.06	120.82
1	A	179	LEU	N-CA-C	5.92	118.62	111.40
1	A	152	MET	O-C-N	-5.87	114.79	122.59
1	A	126	GLY	N-CA-C	-5.84	105.59	113.24
1	A	62	LEU	O-C-N	-5.83	114.81	122.39
1	A	22	PRO	CB-CA-C	-5.79	101.11	110.21
1	A	142	LYS	CB-CA-C	5.73	118.22	109.34
1	A	14	ASN	N-CA-C	5.67	119.51	112.59
1	A	59	TRP	CA-CB-CG	5.65	124.33	113.60
1	A	154	ASP	N-CA-CB	5.65	116.29	109.74
1	A	13	SER	CB-CA-C	-5.63	101.81	110.81
1	A	267	VAL	CA-C-O	-5.62	115.33	120.73
1	A	267	VAL	CA-C-N	5.61	128.36	120.28
1	A	267	VAL	C-N-CA	5.61	128.36	120.28
1	A	270	PRO	N-CA-C	-5.61	106.22	113.57
1	A	29	PRO	N-CA-CB	5.57	107.76	103.30
1	A	238	THR	CA-C-O	-5.56	114.53	120.42
1	A	239	GLU	CB-CG-CD	5.55	122.04	112.60
1	A	249	ASN	CA-C-N	5.48	128.29	121.83
1	A	249	ASN	C-N-CA	5.48	128.29	121.83
1	A	294	PHE	CA-C-N	5.46	126.01	119.94
1	A	294	PHE	C-N-CA	5.46	126.01	119.94
1	A	89	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	17	GLN	CB-CG-CD	5.45	121.87	112.60
1	A	161	PHE	CA-C-O	5.44	125.92	119.56
1	A	267	VAL	N-CA-C	-5.44	106.88	111.56
1	A	85	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	237	SER	CA-C-O	5.36	126.16	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	VAL	N-CA-C	5.35	117.78	108.95
1	A	209	PRO	N-CA-C	5.33	120.52	113.86
1	A	217	ALA	CA-C-N	5.32	125.88	119.98
1	A	217	ALA	C-N-CA	5.32	125.88	119.98
1	A	276	ASN	CA-C-O	5.28	126.94	120.92
1	A	157	THR	CA-C-N	5.26	127.68	122.00
1	A	157	THR	C-N-CA	5.26	127.68	122.00
1	A	210	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	193	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	89	ASP	CB-CG-OD2	-5.24	106.34	118.40
1	A	177	TYR	CA-C-N	5.24	127.31	120.28
1	A	177	TYR	C-N-CA	5.24	127.31	120.28
1	A	183	SER	N-CA-CB	5.24	118.68	110.46
1	A	144	LEU	CA-C-N	-5.21	116.14	123.13
1	A	144	LEU	C-N-CA	-5.21	116.14	123.13
1	A	84	GLY	CA-C-N	5.21	130.65	122.21
1	A	84	GLY	C-N-CA	5.21	130.65	122.21
1	A	290	PHE	CA-C-O	-5.21	116.38	122.37
1	A	245	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	52	CYS	N-CA-C	5.17	116.74	108.41
1	A	35	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	134	PRO	CA-C-N	-5.13	112.15	120.72
1	A	134	PRO	C-N-CA	-5.13	112.15	120.72
1	A	103	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	2	ILE	N-CA-CB	5.09	116.08	110.53
1	A	158	GLN	O-C-N	5.08	124.78	121.23
1	A	76	ARG	N-CA-C	-5.08	101.43	109.76
1	A	230	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	95	GLU	O-C-N	5.02	128.10	122.22
1	A	224	LYS	N-CA-C	-5.01	106.01	111.82

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	54	0
2	A	1	0	0	1	0
3	A	214	0	0	10	0
All	All	2694	0	2379	54	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 11.

All (54) 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:152:MET:HA	1:A:152:MET:HE2	1.48	0.96
1:A:292:GLN:HE21	1:A:292:GLN:H	1.19	0.90
1:A:153:THR:HG21	1:A:158:GLN:HB2	1.56	0.86
1:A:125:TRP:CH2	1:A:225:MET:HE2	2.16	0.79
1:A:220:ARG:HD3	3:A:445:HOH:O	1.82	0.77
1:A:186:ARG:HD3	3:A:584:HOH:O	1.88	0.74
1:A:151:LEU:HD13	1:A:241:ILE:HG13	1.71	0.70
1:A:309:THR:O	1:A:309:THR:HG22	1.91	0.70
1:A:309:THR:O	1:A:310:GLU:HG2	1.93	0.68
1:A:308:GLU:O	3:A:494:HOH:O	2.12	0.66
1:A:152:MET:HE2	1:A:152:MET:CA	2.25	0.66
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.62	0.64
1:A:301:GLU:O	1:A:304:LYS:HB3	1.98	0.62
1:A:307:ALA:C	1:A:309:THR:H	2.08	0.60
1:A:10:GLN:HG3	1:A:10:GLN:O	2.05	0.57
1:A:100:GLU:HG3	3:A:453:HOH:O	2.05	0.56
1:A:31:TYR:N	1:A:32:PRO:HD3	2.21	0.56
1:A:153:THR:CG2	1:A:158:GLN:HB2	2.32	0.55
1:A:31:TYR:N	1:A:32:PRO:CD	2.74	0.50
1:A:232:ALA:O	1:A:236:ILE:HG13	2.11	0.50
1:A:30:GLY:C	1:A:32:PRO:HD3	2.37	0.50
1:A:208:ALA:HB3	1:A:209:PRO:HD3	1.94	0.49
1:A:154:ASP:HB2	1:A:155:PRO:HD2	1.94	0.49
1:A:134:PRO:HG2	1:A:244:TRP:CZ2	2.47	0.49
1:A:12:PHE:HB3	1:A:15:LEU:HD22	1.94	0.48
1:A:50:PHE:CE2	1:A:119:THR:HG21	2.48	0.48
1:A:308:GLU:CB	3:A:566:HOH:O	2.63	0.47
1:A:74:GLY:HA2	3:A:518:HOH:O	2.13	0.47
1:A:280:GLU:HG3	3:A:537:HOH:O	2.14	0.46
1:A:152:MET:HA	1:A:152:MET:CE	2.32	0.45
1:A:297:GLN:HB3	3:A:491:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:OD2	1:A:289:HIS:NE2	2.34	0.44
1:A:296:GLU:O	1:A:300:ARG:HG3	2.18	0.44
1:A:133:LEU:HB2	1:A:134:PRO:HD3	1.99	0.43
1:A:181:THR:OG1	1:A:182:PRO:HD3	2.18	0.43
1:A:181:THR:N	1:A:182:PRO:CD	2.82	0.43
1:A:5:ILE:HD12	1:A:215:TYR:CE2	2.54	0.43
1:A:181:THR:H	1:A:182:PRO:CD	2.31	0.43
1:A:307:ALA:HB2	3:A:596:HOH:O	2.18	0.42
1:A:195:ALA:N	1:A:196:PRO:HD3	2.34	0.42
1:A:56:GLU:HG2	2:A:700:IOD:I	2.89	0.42
1:A:112:ARG:HH11	1:A:112:ARG:CG	2.32	0.42
1:A:307:ALA:C	1:A:309:THR:N	2.76	0.42
1:A:202:GLU:O	1:A:205:ALA:HB3	2.20	0.41
1:A:20:PHE:HB2	1:A:39:LEU:HD22	2.02	0.41
1:A:304:LYS:HE3	1:A:304:LYS:HB2	1.71	0.41
1:A:183:SER:O	1:A:213:THR:HG21	2.20	0.41
1:A:158:GLN:O	3:A:418:HOH:O	2.22	0.41
1:A:115:LEU:HB2	1:A:118:ILE:HD11	2.02	0.41
1:A:47:GLU:O	1:A:117:ASN:HB2	2.21	0.41
1:A:222:PHE:N	1:A:223:PRO:CD	2.85	0.40
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.86	0.40
1:A:148:ASN:HA	1:A:268:MET:SD	2.61	0.40
1:A:20:PHE:CB	1:A:39:LEU:HD22	2.52	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%)	290 (94%)	16 (5%)	2 (1%)	21 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	181	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%)	241 (92%)	21 (8%)	11 13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ILE
1	A	9	ASP
1	A	14	ASN
1	A	15	LEU
1	A	17	GLN
1	A	95	GLU
1	A	112	ARG
1	A	116	ARG
1	A	122	VAL
1	A	123	GLN
1	A	157	THR
1	A	162	SER
1	A	197	THR
1	A	242	SER
1	A	246	ASN
1	A	266	ASP
1	A	272	LYS
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	23	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.