



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 10:09 pm BST

PDB ID : 8B6N  
Title : X-ray structure of the haloalkane dehalogenase HaloTag7 circular permuted at positions 141-156 (cpHaloTagDelta)  
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Deposited on : 2022-09-27  
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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

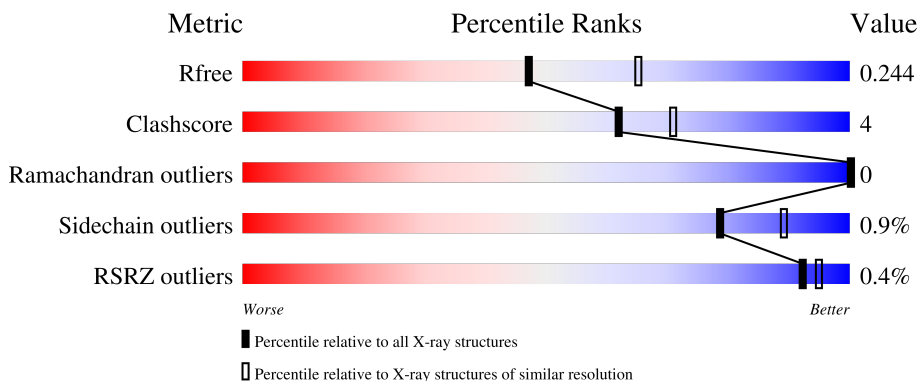
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	 81% 12% 7%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2189 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	272	2163	1407	365	382	9	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

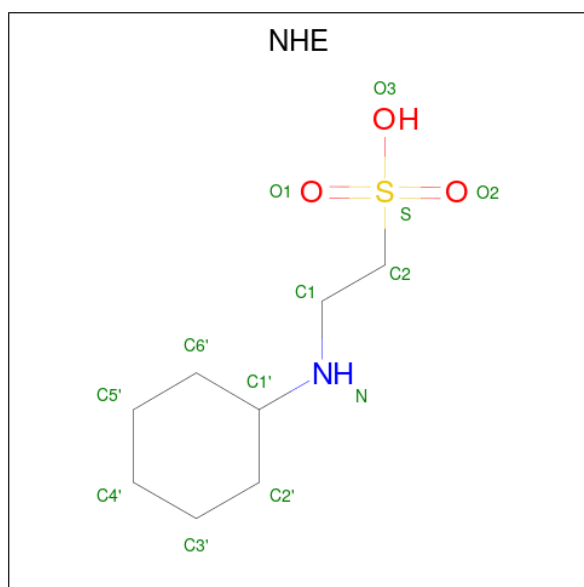
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0A3G3
A	6	LYS	GLU	conflict	UNP P0A3G3
A	13	VAL	ALA	conflict	UNP P0A3G3
A	18	THR	ALA	conflict	UNP P0A3G3
A	21	MET	LYS	conflict	UNP P0A3G3
A	22	GLY	CYS	conflict	UNP P0A3G3
A	41	ASN	LYS	conflict	UNP P0A3G3
A	70	GLU	ALA	conflict	UNP P0A3G3
A	73	ASP	ASN	conflict	UNP P0A3G3
A	103	LYS	GLU	conflict	UNP P0A3G3
A	110	ALA	THR	conflict	UNP P0A3G3
A	118	ASN	HIS	conflict	UNP P0A3G3
A	119	LEU	TYR	conflict	UNP P0A3G3
A	137	SER	PRO	conflict	UNP P0A3G3
A	138	THR	ALA	conflict	UNP P0A3G3
A	140	GLU	-	linker	UNP P0A3G3
A	141	ILE	-	linker	UNP P0A3G3
A	142	GLY	-	linker	UNP P0A3G3
A	143	GLY	-	linker	UNP P0A3G3
A	144	THR	-	linker	UNP P0A3G3
A	145	GLY	-	linker	UNP P0A3G3
A	146	GLY	-	linker	UNP P0A3G3
A	147	SER	-	linker	UNP P0A3G3
A	148	GLY	-	linker	UNP P0A3G3
A	149	GLY	-	linker	UNP P0A3G3
A	150	THR	-	linker	UNP P0A3G3
A	151	GLY	-	linker	UNP P0A3G3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLY	-	linker	UNP P0A3G3
A	153	SER	-	linker	UNP P0A3G3
A	154	GLY	-	linker	UNP P0A3G3
A	155	GLY	-	linker	UNP P0A3G3
A	156	SER	-	linker	UNP P0A3G3
A	200	VAL	LEU	conflict	UNP P0A3G3
A	211	THR	SER	conflict	UNP P0A3G3
A	231	GLY	ASP	conflict	UNP P0A3G3
A	240	PHE	TYR	conflict	UNP P0A3G3
A	241	MET	LEU	conflict	UNP P0A3G3
A	281	PHE	CYS	conflict	UNP P0A3G3

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	13	8	1	3	1	0	0


- Molecule 3 is water.

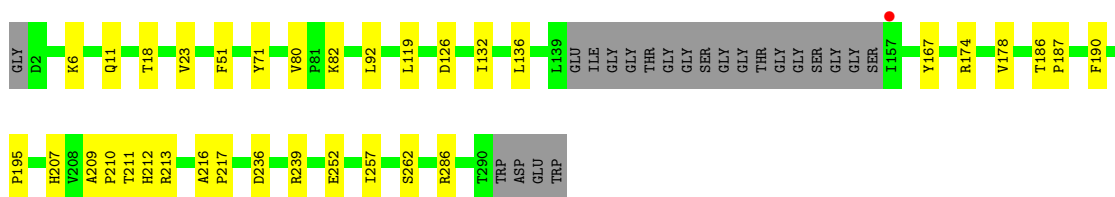
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		

### 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Haloalkane dehalogenase

Chain A:  81% 12% 7%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.85Å 79.32Å 154.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.30 39.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.70-2.30) 99.1 (39.70-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.215 , 0.250 0.209 , 0.244	Depositor DCC
$R_{free}$ test set	640 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtrriage
Anisotropy	0.502	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.045 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: NHE

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	0.27	0/2233	0.51	0/3052

There are no bond length outliers.

There are no bond angle outliers.

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	2163	0	2129	19	0
2	A	13	0	16	2	0
3	A	13	0	0	0	0
All	All	2189	0	2145	19	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 4.

All (19) 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:92:LEU:O	1:A:286:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:THR:HG23	1:A:252:GLU:HG2	1.81	0.61
1:A:80:VAL:O	1:A:82:LYS:NZ	2.34	0.60
1:A:18:THR:HG22	2:A:301:NHE:H4'2	1.84	0.59
1:A:6:LYS:HD2	1:A:11:GLN:HE22	1.74	0.52
1:A:187:PRO:HB3	1:A:213:ARG:HD3	1.93	0.51
1:A:132:ILE:O	1:A:136:LEU:HG	2.11	0.49
1:A:257:ILE:HD12	1:A:262:SER:HA	1.94	0.49
1:A:23:VAL:HG22	1:A:119:LEU:HB2	1.95	0.49
1:A:211:THR:OG1	1:A:212:HIS:ND1	2.46	0.48
1:A:178:VAL:HB	1:A:216:ALA:HB3	1.96	0.48
1:A:167:TYR:CD1	1:A:174:ARG:HD3	2.51	0.46
1:A:126:ASP:HA	1:A:207:HIS:HE1	1.82	0.45
1:A:6:LYS:HD2	1:A:11:GLN:NE2	2.32	0.44
1:A:257:ILE:HB	1:A:262:SER:HA	1.99	0.44
1:A:195:PRO:HD3	2:A:301:NHE:H6'2	2.01	0.43
1:A:190:PHE:O	1:A:217:PRO:HD2	2.20	0.42
1:A:236:ASP:OD1	1:A:239:ARG:NH1	2.49	0.42
1:A:209:ALA:N	1:A:210:PRO:HD2	2.34	0.42

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	268/294 (91%)	259 (97%)	9 (3%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

#### 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	234/245 (96%)	232 (99%)	2 (1%)	78 89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	71	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	207	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NHE	A	301	-	13,13,13	0.46	0	16,17,17	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NHE	A	301	-	-	1/7/15/15	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NHE	C2-C1-N-C1'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NHE	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	272/294 (92%)	-0.07	1 (0%) <b>92</b> <b>95</b>	39, 55, 81, 97	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ILE	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NHE	A	301	13/13	0.98	0.17	39,41,43,44	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.