



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:33 AM GMT

PDB ID : 4IY1  
Title : Structure of a 37-fold mutant of halohydrin dehalogenase (HheC) with chloride bound  
Authors : Floor, R.J.; Schallmeyer, M.; Hauer, B.; Breuer, M.; Jekel, P.A; Wijma, H.J.; Dijkstra, B.W.; Janssen, D.B.  
Deposited on : 2013-01-28  
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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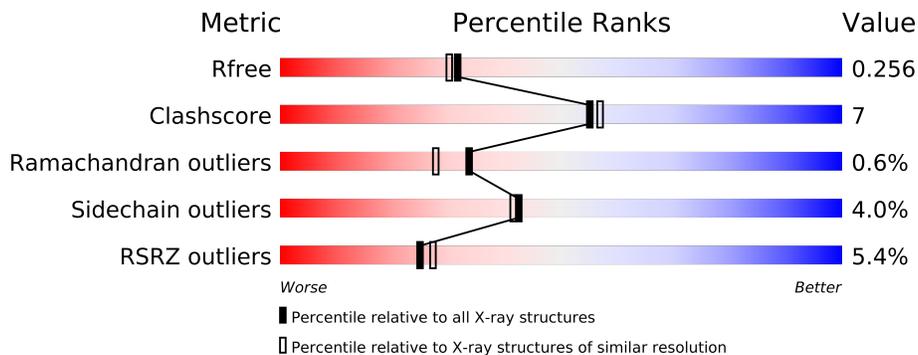
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	254	
1	B	254	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3949 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Halohydrin dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1926	1232	323	365	6	0	0	0
1	B	250	1930	1234	324	366	6	0	0	0

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	GLN	ENGINEERED MUTATION	UNP Q93D82
A	38	GLN	LYS	ENGINEERED MUTATION	UNP Q93D82
A	52	ILE	LYS	ENGINEERED MUTATION	UNP Q93D82
A	60	VAL	ALA	ENGINEERED MUTATION	UNP Q93D82
A	70	LEU	TYR	ENGINEERED MUTATION	UNP Q93D82
A	72	HIS	GLN	ENGINEERED MUTATION	UNP Q93D82
A	75	ILE	VAL	ENGINEERED MUTATION	UNP Q93D82
A	82	ALA	PHE	ENGINEERED MUTATION	UNP Q93D82
A	83	PRO	ALA	ENGINEERED MUTATION	UNP Q93D82
A	84	VAL	PRO	ENGINEERED MUTATION	UNP Q93D82
A	86	TRP	PHE	ENGINEERED MUTATION	UNP Q93D82
A	87	ARG	GLN	ENGINEERED MUTATION	UNP Q93D82
A	99	ASP	GLY	ENGINEERED MUTATION	UNP Q93D82
A	100	MET	ALA	ENGINEERED MUTATION	UNP Q93D82
A	107	LYS	ARG	ENGINEERED MUTATION	UNP Q93D82
A	112	ALA	VAL	ENGINEERED MUTATION	UNP Q93D82
A	121	ARG	LYS	ENGINEERED MUTATION	UNP Q93D82
A	134	ALA	THR	ENGINEERED MUTATION	UNP Q93D82
A	135	SER	PRO	ENGINEERED MUTATION	UNP Q93D82
A	146	ALA	THR	ENGINEERED MUTATION	UNP Q93D82
A	153	SER	CYS	ENGINEERED MUTATION	UNP Q93D82
A	154	ALA	THR	ENGINEERED MUTATION	UNP Q93D82
A	166	HIS	TYR	ENGINEERED MUTATION	UNP Q93D82
A	174	ALA	GLY	ENGINEERED MUTATION	UNP Q93D82
A	177	GLY	TYR	ENGINEERED MUTATION	UNP Q93D82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	178	VAL	LEU	ENGINEERED MUTATION	UNP Q93D82
A	179	ASP	HIS	ENGINEERED MUTATION	UNP Q93D82
A	181	GLY	GLU	ENGINEERED MUTATION	UNP Q93D82
A	186	TYR	PHE	ENGINEERED MUTATION	UNP Q93D82
A	189	SER	THR	ENGINEERED MUTATION	UNP Q93D82
A	195	SER	ASN	ENGINEERED MUTATION	UNP Q93D82
A	201	TRP	HIS	ENGINEERED MUTATION	UNP Q93D82
A	203	ARG	LYS	ENGINEERED MUTATION	UNP Q93D82
A	205	TYR	VAL	ENGINEERED MUTATION	UNP Q93D82
A	222	THR	ALA	ENGINEERED MUTATION	UNP Q93D82
A	245	VAL	MET	ENGINEERED MUTATION	UNP Q93D82
A	246	VAL	ILE	ENGINEERED MUTATION	UNP Q93D82
B	37	HIS	GLN	ENGINEERED MUTATION	UNP Q93D82
B	38	GLN	LYS	ENGINEERED MUTATION	UNP Q93D82
B	52	ILE	LYS	ENGINEERED MUTATION	UNP Q93D82
B	60	VAL	ALA	ENGINEERED MUTATION	UNP Q93D82
B	70	LEU	TYR	ENGINEERED MUTATION	UNP Q93D82
B	72	HIS	GLN	ENGINEERED MUTATION	UNP Q93D82
B	75	ILE	VAL	ENGINEERED MUTATION	UNP Q93D82
B	82	ALA	PHE	ENGINEERED MUTATION	UNP Q93D82
B	83	PRO	ALA	ENGINEERED MUTATION	UNP Q93D82
B	84	VAL	PRO	ENGINEERED MUTATION	UNP Q93D82
B	86	TRP	PHE	ENGINEERED MUTATION	UNP Q93D82
B	87	ARG	GLN	ENGINEERED MUTATION	UNP Q93D82
B	99	ASP	GLY	ENGINEERED MUTATION	UNP Q93D82
B	100	MET	ALA	ENGINEERED MUTATION	UNP Q93D82
B	107	LYS	ARG	ENGINEERED MUTATION	UNP Q93D82
B	112	ALA	VAL	ENGINEERED MUTATION	UNP Q93D82
B	121	ARG	LYS	ENGINEERED MUTATION	UNP Q93D82
B	134	ALA	THR	ENGINEERED MUTATION	UNP Q93D82
B	135	SER	PRO	ENGINEERED MUTATION	UNP Q93D82
B	146	ALA	THR	ENGINEERED MUTATION	UNP Q93D82
B	153	SER	CYS	ENGINEERED MUTATION	UNP Q93D82
B	154	ALA	THR	ENGINEERED MUTATION	UNP Q93D82
B	166	HIS	TYR	ENGINEERED MUTATION	UNP Q93D82
B	174	ALA	GLY	ENGINEERED MUTATION	UNP Q93D82
B	177	GLY	TYR	ENGINEERED MUTATION	UNP Q93D82
B	178	VAL	LEU	ENGINEERED MUTATION	UNP Q93D82
B	179	ASP	HIS	ENGINEERED MUTATION	UNP Q93D82
B	181	GLY	GLU	ENGINEERED MUTATION	UNP Q93D82
B	186	TYR	PHE	ENGINEERED MUTATION	UNP Q93D82
B	189	SER	THR	ENGINEERED MUTATION	UNP Q93D82

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	SER	ASN	ENGINEERED MUTATION	UNP Q93D82
B	201	TRP	HIS	ENGINEERED MUTATION	UNP Q93D82
B	203	ARG	LYS	ENGINEERED MUTATION	UNP Q93D82
B	205	TYR	VAL	ENGINEERED MUTATION	UNP Q93D82
B	222	THR	ALA	ENGINEERED MUTATION	UNP Q93D82
B	245	VAL	MET	ENGINEERED MUTATION	UNP Q93D82
B	246	VAL	ILE	ENGINEERED MUTATION	UNP Q93D82

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is water.

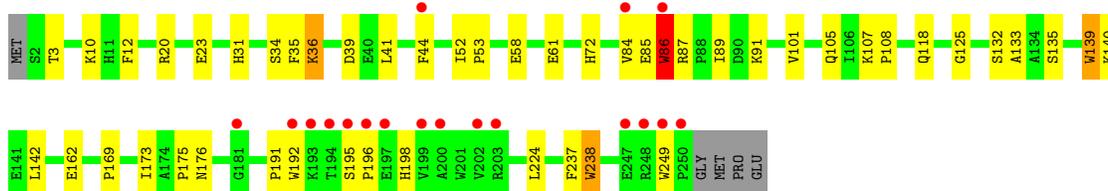
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	44	Total O 44 44	0	0
3	B	46	Total O 46 46	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

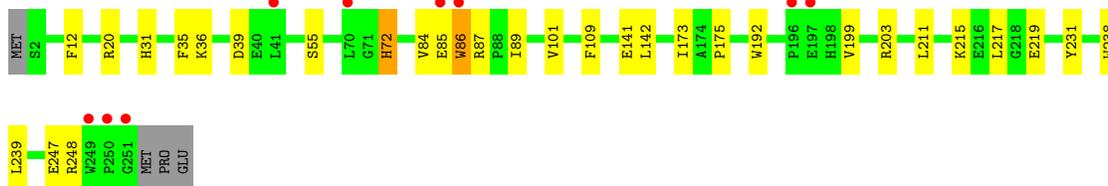
- Molecule 1: Halohydrin dehalogenase

Chain A: 



- Molecule 1: Halohydrin dehalogenase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.68Å 104.68Å 121.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.68 – 2.10 37.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.68-2.10) 98.2 (37.69-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.204 , 0.259 0.202 , 0.256	Depositor DCC
$R_{free}$ test set	1996 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.6	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 39422 reflections	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: 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	0.68	4/1979 (0.2%)	0.58	0/2697
1	B	0.66	2/1983 (0.1%)	0.58	0/2702
All	All	0.67	6/3962 (0.2%)	0.58	0/5399

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	TRP	CD2-CE2	6.62	1.49	1.41
1	A	139	TRP	CD2-CE2	5.62	1.48	1.41
1	A	238	TRP	CD2-CE2	5.56	1.48	1.41
1	A	86	TRP	CD2-CE2	5.32	1.47	1.41
1	B	86	TRP	CD2-CE2	5.30	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1926	0	1870	34	0
1	B	1930	0	1873	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	0	0	0
3	B	46	0	0	0	0
All	All	3949	0	3743	51	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 51 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:PHE:HD2	1:A:53:PRO:HG3	1.38	0.86
1:A:101:VAL:HG11	1:B:101:VAL:HG11	1.56	0.85
1:A:44:PHE:CD2	1:A:53:PRO:HG3	2.14	0.82
1:B:84:VAL:HG21	1:B:142:LEU:HD11	1.69	0.75
1:B:86:TRP:O	1:B:87:ARG:HG2	1.93	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	247/254 (97%)	232 (94%)	13 (5%)	2 (1%)	27	20
1	B	248/254 (98%)	236 (95%)	11 (4%)	1 (0%)	43	39
All	All	495/508 (97%)	468 (94%)	24 (5%)	3 (1%)	33	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	HIS
1	A	35	PHE
1	A	135	SER

### 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	202/206 (98%)	195 (96%)	7 (4%)	48	48
1	B	202/206 (98%)	193 (96%)	9 (4%)	38	35
All	All	404/412 (98%)	388 (96%)	16 (4%)	42	41

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	PHE
1	B	31	HIS
1	B	231	TYR
1	A	140	LYS
1	B	239	LEU

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

Mol	Chain	Res	Type
1	A	176	ASN
1	B	176	ASN

### 5.3.3 RNA [i](#)

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are 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.

## 5.7 Other polymers

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

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	249/254 (98%)	0.30	18 (7%) 15 17	19, 39, 68, 84	0
1	B	250/254 (98%)	0.08	9 (3%) 41 45	19, 35, 66, 97	0
All	All	499/508 (98%)	0.19	27 (5%) 25 27	19, 36, 68, 97	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	GLY	4.9
1	B	85	GLU	3.7
1	A	194	THR	3.5
1	A	196	PRO	3.3
1	B	86	TRP	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	B	302	1/1	0.08	-0.81	76,76,76,76	0
2	CL	A	301	1/1	0.06	-1.45	41,41,41,41	0
2	CL	B	301	1/1	0.07	-1.65	33,33,33,33	0

## 6.5 Other polymers

There are no such residues in this entry.