



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2025 – 01:01 AM JST

PDB ID : 9LDQ
Title : Crystal Structure of a triple-mutant(F12Y/P84T/F86W) of halohydrin dehalogenase HheC
Authors : Wan, N.W.; Hu, D.; Lu, Z.
Deposited on : 2025-01-06
Resolution : 2.24 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

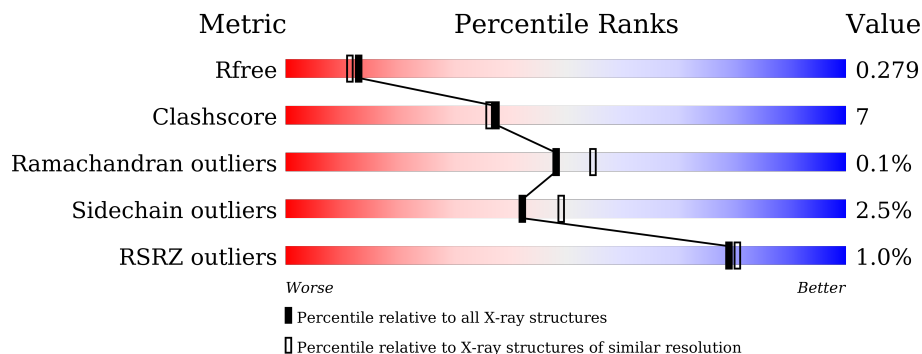
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	164625	3139 (2.26-2.22)
Clashscore	180529	3381 (2.26-2.22)
Ramachandran outliers	177936	3334 (2.26-2.22)
Sidechain outliers	177891	3335 (2.26-2.22)
RSRZ outliers	164620	3138 (2.26-2.22)

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 $\leq 5\%$. 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	261	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	B	261	<div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	C	261	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	D	261	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8267 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 Halohydrin dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1968	1261	324	375	8			
1	B	253	Total	C	N	O	S	0	0	0
			1968	1261	324	375	8			
1	C	253	Total	C	N	O	S	0	0	0
			1968	1261	324	375	8			
1	D	253	Total	C	N	O	S	0	0	0
			1968	1261	324	375	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q93D82
A	-5	ALA	-	expression tag	UNP Q93D82
A	-4	HIS	-	expression tag	UNP Q93D82
A	-3	HIS	-	expression tag	UNP Q93D82
A	-2	HIS	-	expression tag	UNP Q93D82
A	-1	HIS	-	expression tag	UNP Q93D82
A	0	HIS	-	expression tag	UNP Q93D82
A	1	HIS	-	expression tag	UNP Q93D82
A	12	TYR	PHE	engineered mutation	UNP Q93D82
A	84	THR	PRO	engineered mutation	UNP Q93D82
A	86	TRP	PHE	engineered mutation	UNP Q93D82
B	-6	MET	-	initiating methionine	UNP Q93D82
B	-5	ALA	-	expression tag	UNP Q93D82
B	-4	HIS	-	expression tag	UNP Q93D82
B	-3	HIS	-	expression tag	UNP Q93D82
B	-2	HIS	-	expression tag	UNP Q93D82
B	-1	HIS	-	expression tag	UNP Q93D82
B	0	HIS	-	expression tag	UNP Q93D82
B	1	HIS	-	expression tag	UNP Q93D82
B	12	TYR	PHE	engineered mutation	UNP Q93D82
B	84	THR	PRO	engineered mutation	UNP Q93D82

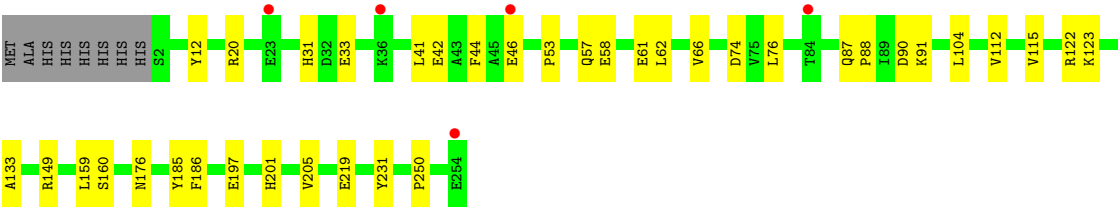
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Chain	Residue	Modelled	Actual	Comment	Reference
B	86	TRP	PHE	engineered mutation	UNP Q93D82
C	-6	MET	-	initiating methionine	UNP Q93D82
C	-5	ALA	-	expression tag	UNP Q93D82
C	-4	HIS	-	expression tag	UNP Q93D82
C	-3	HIS	-	expression tag	UNP Q93D82
C	-2	HIS	-	expression tag	UNP Q93D82
C	-1	HIS	-	expression tag	UNP Q93D82
C	0	HIS	-	expression tag	UNP Q93D82
C	1	HIS	-	expression tag	UNP Q93D82
C	12	TYR	PHE	engineered mutation	UNP Q93D82
C	84	THR	PRO	engineered mutation	UNP Q93D82
C	86	TRP	PHE	engineered mutation	UNP Q93D82
D	-6	MET	-	initiating methionine	UNP Q93D82
D	-5	ALA	-	expression tag	UNP Q93D82
D	-4	HIS	-	expression tag	UNP Q93D82
D	-3	HIS	-	expression tag	UNP Q93D82
D	-2	HIS	-	expression tag	UNP Q93D82
D	-1	HIS	-	expression tag	UNP Q93D82
D	0	HIS	-	expression tag	UNP Q93D82
D	1	HIS	-	expression tag	UNP Q93D82
D	12	TYR	PHE	engineered mutation	UNP Q93D82
D	84	THR	PRO	engineered mutation	UNP Q93D82
D	86	TRP	PHE	engineered mutation	UNP Q93D82

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	B	101	Total O 101 101	0	0
2	C	90	Total O 90 90	0	0
2	D	91	Total O 91 91	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.54Å 97.75Å 146.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.45 – 2.24 50.45 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.45-2.24) 99.1 (50.45-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.38 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.13_2998-000	Depositor
R, R_{free}	0.224 , 0.281 0.226 , 0.279	Depositor DCC
R_{free} test set	2438 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8267	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8381e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.44	0/2022	0.57	0/2751
1	B	0.42	0/2022	0.55	0/2751
1	C	0.42	0/2022	0.57	0/2751
1	D	0.41	0/2022	0.54	0/2751
All	All	0.42	0/8088	0.56	0/11004

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	1968	0	1912	39	0
1	B	1968	0	1912	20	0
1	C	1968	0	1912	35	0
1	D	1968	0	1912	23	0
2	A	113	0	0	5	0
2	B	101	0	0	3	0
2	C	90	0	0	0	0
2	D	91	0	0	0	0
All	All	8267	0	7648	107	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.

The worst 5 of 107 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:B:101:VAL:HG11	1:C:101:VAL:HG11	1.38	1.06
1:A:184:PRO:HA	1:A:188:PRO:HG3	1.60	0.83
1:A:84:THR:HG22	1:A:85:GLU:H	1.42	0.83
1:C:9:VAL:HG11	1:C:30:CYS:HB3	1.75	0.67
1:C:59:PRO:O	1:C:63:ILE:CD1	2.43	0.67

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	251/261 (96%)	239 (95%)	12 (5%)	0	100	100
1	B	251/261 (96%)	238 (95%)	12 (5%)	1 (0%)	30	31
1	C	251/261 (96%)	241 (96%)	10 (4%)	0	100	100
1	D	251/261 (96%)	234 (93%)	17 (7%)	0	100	100
All	All	1004/1044 (96%)	952 (95%)	51 (5%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	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	207/214 (97%)	201 (97%)	6 (3%)	37	43
1	B	207/214 (97%)	202 (98%)	5 (2%)	44	50
1	C	207/214 (97%)	202 (98%)	5 (2%)	44	50
1	D	207/214 (97%)	202 (98%)	5 (2%)	44	50
All	All	828/856 (97%)	807 (98%)	21 (2%)	42	49

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	124	SER
1	D	31	HIS
1	D	231	TYR
1	D	87	GLN
1	D	12	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [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, 95th 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 ²)	Q<0.9
1	A	253/261 (96%)	0.28	2 (0%) 82 84	18, 25, 39, 62	0
1	B	253/261 (96%)	0.29	1 (0%) 89 90	17, 25, 39, 71	0
1	C	253/261 (96%)	0.35	2 (0%) 82 84	16, 26, 41, 56	0
1	D	253/261 (96%)	0.58	5 (1%) 64 65	19, 28, 43, 60	0
All	All	1012/1044 (96%)	0.38	10 (0%) 79 80	16, 26, 41, 71	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	THR	3.5
1	D	36	LYS	2.8
1	B	254	GLU	2.7
1	C	46	GLU	2.5
1	D	23	GLU	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.