



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 10:57 PM EDT

PDB ID : 3EJ9
Title : Structural and mechanistic analysis of trans-3-chloroacrylic acid dehalogenase activity
Authors : Pegan, S.; Serrano, H.; Whitman, C.P.; Mesecar, A.D.
Deposited on : 2008-09-17
Resolution : 1.50 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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

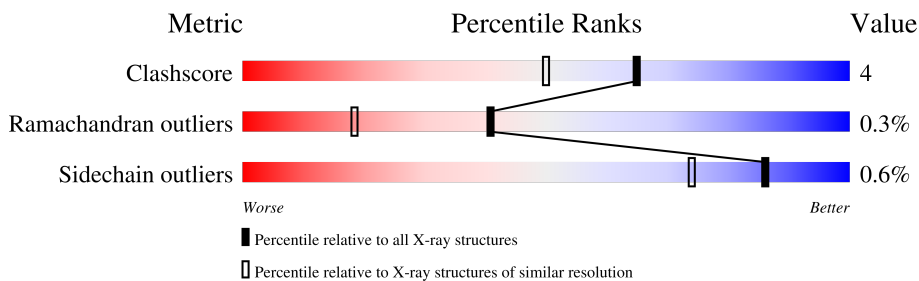
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	76	
1	C	76	
1	E	76	
2	B	70	
2	D	70	
2	F	70	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3280 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 Alpha-subunit of trans-3-chloroacrylic acid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	62	499	312	92	92	3	0	1	0
1	C	63	511	321	93	94	3	8	3	0
1	E	64	516	326	92	95	3	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLN	GLU	engineered mutation	UNP Q9EV85
C	52	GLN	GLU	engineered mutation	UNP Q9EV85
E	52	GLN	GLU	engineered mutation	UNP Q9EV85

- Molecule 2 is a protein called Beta-subunit of trans-3-chloroacrylic acid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	59	465	293	82	87	3	0	4	0
2	D	58	457	290	81	84	2	0	4	0
2	F	58	454	289	81	82	2	0	3	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total O 77 77	0	0
3	B	59	Total O 59 59	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	68	Total O 68 68	0	0
3	D	56	Total O 56 56	0	0
3	E	71	Total O 71 71	0	0
3	F	47	Total O 47 47	0	0

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. 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.

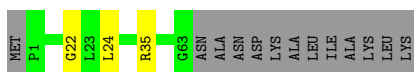
- Molecule 1: Alpha-subunit of trans-3-chloroacrylic acid dehalogenase

Chain A:  75% 7% 18%




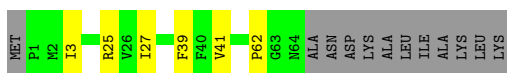
- Molecule 1: Alpha-subunit of trans-3-chloroacrylic acid dehalogenase

Chain C:  79% 0% 17%




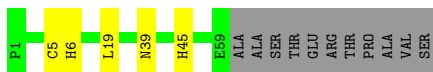
- Molecule 1: Alpha-subunit of trans-3-chloroacrylic acid dehalogenase

Chain E:  76% 8% 16%




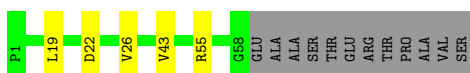
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase

Chain B:  77% 7% 16%



- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase

Chain D:  76% 7% 17%



- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase

Chain F:  70% 11% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.28Å 69.67Å 89.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.05 – 1.50 37.77 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (55.05-1.50) 97.3 (37.77-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.247 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3280	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.38	0/512	0.56	0/688
1	C	0.39	0/530	0.53	0/712
1	E	0.39	0/535	0.54	0/722
2	B	0.35	0/482	0.50	0/650
2	D	0.39	0/474	0.58	0/640
2	F	0.78	3/468 (0.6%)	0.64	0/632
All	All	0.47	3/3001 (0.1%)	0.56	0/4044

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	14	ALA	CA-CB	-5.28	1.41	1.52
2	F	16	LYS	C-O	5.13	1.33	1.23
2	F	13	VAL	C-N	5.11	1.45	1.34

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	499	0	494	6	0
1	C	511	0	513	4	0
1	E	516	0	519	8	0
2	B	465	0	495	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	457	0	493	3	0
2	F	454	0	490	6	0
3	A	77	0	0	1	0
3	B	59	0	0	0	0
3	C	68	0	0	0	0
3	D	56	0	0	0	0
3	E	71	0	0	1	0
3	F	47	0	0	0	0
All	All	3280	0	3004	24	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 (24) 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)
2:F:16:LYS:HG2	2:F:42[B]:LEU:HD21	1.61	0.82
1:E:39:PHE:CZ	1:E:41[B]:VAL:HG13	2.16	0.81
1:A:1:PRO:HD2	1:A:33:GLU:HG2	1.71	0.72
1:A:37:ASN:HD22	2:D:55:ARG:HH11	1.45	0.65
1:A:27:ILE:HD13	2:D:19:LEU:HD11	1.79	0.64
2:B:6:HIS:HD2	2:B:45:HIS:NE2	2.02	0.57
1:A:33:GLU:HG3	1:A:37:ASN:HB3	1.88	0.54
2:B:5[B]:CYS:SG	1:E:27:ILE:HD11	2.48	0.53
2:B:5[B]:CYS:SG	1:E:27:ILE:CD1	2.98	0.52
1:C:22:GLY:HA3	2:F:26[A]:VAL:HG21	1.92	0.52
2:D:22:ASP:O	2:D:26[B]:VAL:HG22	2.10	0.51
1:A:33:GLU:CG	1:A:37:ASN:HB3	2.45	0.46
2:B:39:ASN:HD22	2:F:52:ILE:HA	1.81	0.46
2:B:19:LEU:HD11	1:E:27:ILE:HD13	1.97	0.45
2:B:6:HIS:CD2	2:B:45:HIS:NE2	2.83	0.44
1:E:3:ILE:HD11	1:E:27:ILE:HG13	2.01	0.43
1:A:29:GLU:HB3	3:A:125:HOH:O	2.18	0.43
1:E:39:PHE:HZ	1:E:41[B]:VAL:HG13	1.75	0.42
1:C:22:GLY:CA	2:F:26[A]:VAL:HG21	2.49	0.42
2:B:5[B]:CYS:SG	1:E:27:ILE:HD12	2.60	0.41
1:C:22:GLY:HA3	2:F:26[A]:VAL:CG2	2.50	0.41
1:E:25:ARG:NH1	3:E:134:HOH:O	2.54	0.41
2:F:12:SER:OG	2:F:15:ARG:HB2	2.21	0.40
1:C:24:LEU:HD23	1:C:35[B]:ARG:HG2	2.02	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	61/76 (80%)	60 (98%)	1 (2%)	0	100	100
1	C	64/76 (84%)	64 (100%)	0	0	100	100
1	E	65/76 (86%)	63 (97%)	1 (2%)	1 (2%)	10	1
2	B	61/70 (87%)	61 (100%)	0	0	100	100
2	D	60/70 (86%)	60 (100%)	0	0	100	100
2	F	59/70 (84%)	59 (100%)	0	0	100	100
All	All	370/438 (84%)	367 (99%)	2 (0%)	1 (0%)	41	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	62	PRO

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	54/63 (86%)	54 (100%)	0	100	100
1	C	56/63 (89%)	56 (100%)	0	100	100
1	E	57/63 (90%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	55/59 (93%)	55 (100%)	0	100	100
2	D	54/59 (92%)	53 (98%)	1 (2%)	57	27
2	F	53/59 (90%)	52 (98%)	1 (2%)	57	27
All	All	329/366 (90%)	327 (99%)	2 (1%)	86	74

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

Mol	Chain	Res	Type
2	D	43	VAL
2	F	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
2	B	6	HIS
2	B	28	ASN
2	B	39	ASN
1	E	52	GLN
1	E	64	ASN

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](#)

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.