

wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2024 – 10:03 AM EST

PDB ID	:	6UXU
Title	:	X-ray Crystal Structure of Chlorothalonil Dehalogenase: Analyzing the Cat-
		alytic Mechanism of Hydrolytic Dehalogenation
Authors	:	Catlin, D.S.; Liu, D.
Deposited on	:	2019-11-08
Resolution	:	1.96 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 (i) 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 (1)) were used in the production of this report:

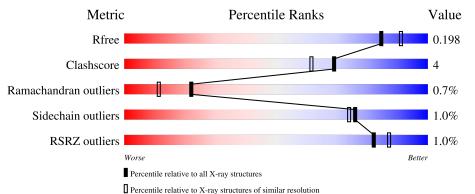
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.96 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	А	300	92%	8%
1	В	300	2% 88%	12%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5058 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	300	Total	С	Ν	Ο	S	0	2	0
	A	300	2315	1488	395	423	9	0	2	0
1	В	300	Total	С	Ν	0	S	0	5	0
	D	300	2338	1501	400	428	9	0	G	0

• Molecule 1 is a protein called Chlorothalonil hydrolytic dehalogenase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	310	PHE	TRP	conflict	UNP E2JB04
А	322	GLU	-	expression tag	UNP E2JB04
А	323	ASN	-	expression tag	UNP E2JB04
А	324	LEU	-	expression tag	UNP E2JB04
А	325	TYR	-	expression tag	UNP E2JB04
А	326	PHE	-	expression tag	UNP E2JB04
А	327	GLN	-	expression tag	UNP E2JB04
В	310	PHE	TRP	conflict	UNP E2JB04
В	322	GLU	-	expression tag	UNP E2JB04
В	323	ASN	-	expression tag	UNP E2JB04
В	324	LEU	-	expression tag	UNP E2JB04
В	325	TYR	-	expression tag	UNP E2JB04
В	326	PHE	-	expression tag	UNP E2JB04
В	327	GLN	-	expression tag	UNP E2JB04

There are 14 discrepancies between the modelled and reference sequences:

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mo	l Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0
2	В	1	Total Zn 1 1	0	0

• Molecule 3 is water.



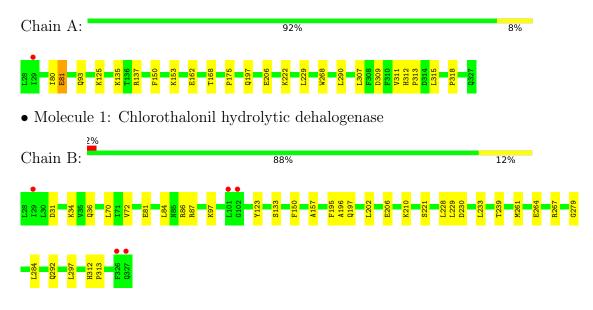
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	211	Total O 211 211	0	0
3	В	191	Total O 191 191	0	0



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 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: Chlorothalonil hydrolytic dehalogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	54.80Å 105.18Å 122.42Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.02 - 1.96	Depositor
Resolution (A)	50.02 - 1.96	EDS
% Data completeness	94.4 (50.02-1.96)	Depositor
(in resolution range)	94.4 (50.02-1.96)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.47 (at 1.97 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
D D.	0.162 , 0.198	Depositor
R, R_{free}	0.162 , 0.198	DCC
R_{free} test set	2399 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	19.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36, 62.8	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5058	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities 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: ZN

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 RMSZ	lengths	Bond angles	
	Moi Chain		# Z > 5	RMSZ	# Z > 5
1	А	0.37	0/2374	0.56	0/3225
1	В	0.38	0/2400	0.58	0/3259
All	All	0.38	0/4774	0.57	0/6484

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	А	2315	0	2332	17	0
1	В	2338	0	2354	22	0
2	А	2	0	0	0	0
2	В	1	0	0	0	0
3	А	211	0	0	2	1
3	В	191	0	0	4	1
All	All	5058	0	4686	35	1

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.

The worst 5 of 35 close contacts within the same asymmetric unit are listed below, sorted by their



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ARG:NH1	3:B:502:HOH:O	2.17	0.77
1:A:150:PHE:HD1	1:B:150:PHE:HD2	1.37	0.73
1:B:264:GLU:OE2	1:B:267:ARG:HD2	1.89	0.71
1:B:264:GLU:OE1	3:B:501:HOH:O	2.10	0.69
1:A:309:ASP:OD2	3:A:501:HOH:O	2.14	0.66

clash magnitude.

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
3:A:629:HOH:O	3:B:587:HOH:O[3_645]	2.18	0.02	

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	lysed Favoured Allowed		Outliers	Percentil	\mathbf{es}
1	А	300/300~(100%)	290~(97%)	8(3%)	2(1%)	22 11	
1	В	303/300 (101%)	293~(97%)	8 (3%)	2(1%)	22 11	
All	All	603/600~(100%)	583~(97%)	16 (3%)	4 (1%)	22 11	

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	197	GLN
1	А	81	GLU
1	В	81	GLU
1	В	197	GLN



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	А	242/240~(101%)	241 (100%)	1 (0%)	91 90		
1	В	245/240~(102%)	241 (98%)	4 (2%)	62 58		
All	All	487/480~(102%)	482 (99%)	5(1%)	76 74		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	206	GLU
1	В	84	LEU
1	В	202	LEU
1	В	206	GLU
1	В	284	LEU

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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. 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 (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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	300/300~(100%)	-0.08	1 (0%) 94 96	10, 21, 40, 52	0
1	В	300/300~(100%)	-0.08	5 (1%) 70 77	10, 20, 42, 73	0
All	All	600/600~(100%)	-0.08	6 (1%) 82 87	10, 20, 41, 73	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	326	PHE	3.7
1	В	101	LEU	2.9
1	В	327	GLN	2.7
1	В	29	ILE	2.6
1	В	102	GLY	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.

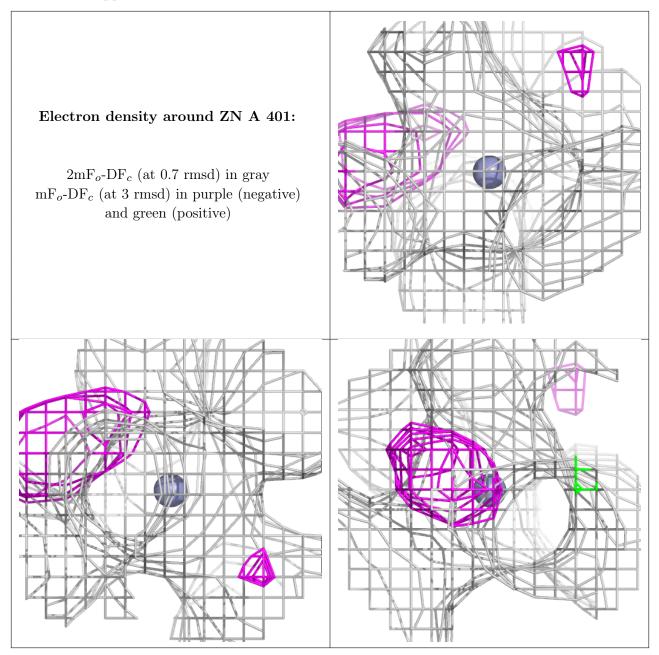
6.4 Ligands (i)

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^{th} 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.

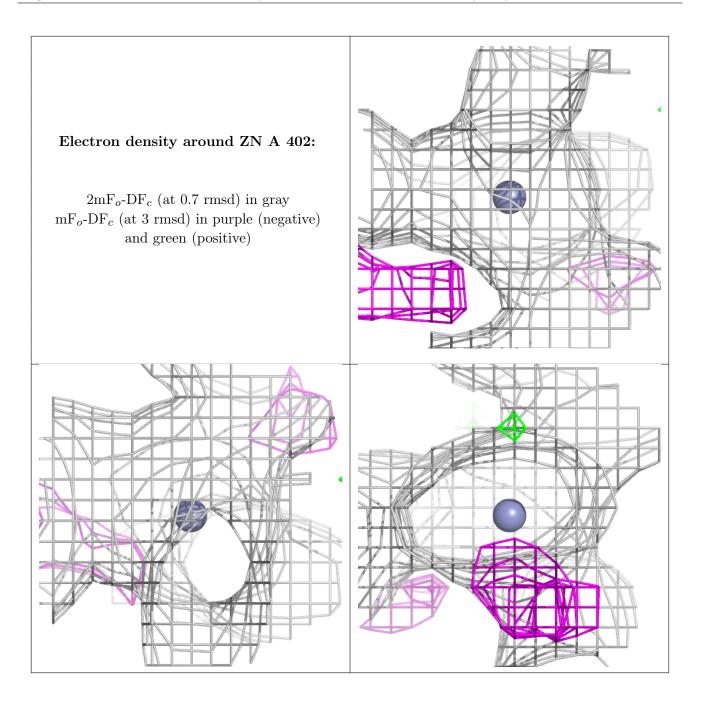


Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
2	ZN	А	401	1/1	0.99	0.07	16, 16, 16, 16	1
2	ZN	А	402	1/1	0.99	0.10	23,23,23,23	1
2	ZN	В	401	1/1	0.99	0.10	12,12,12,12	1

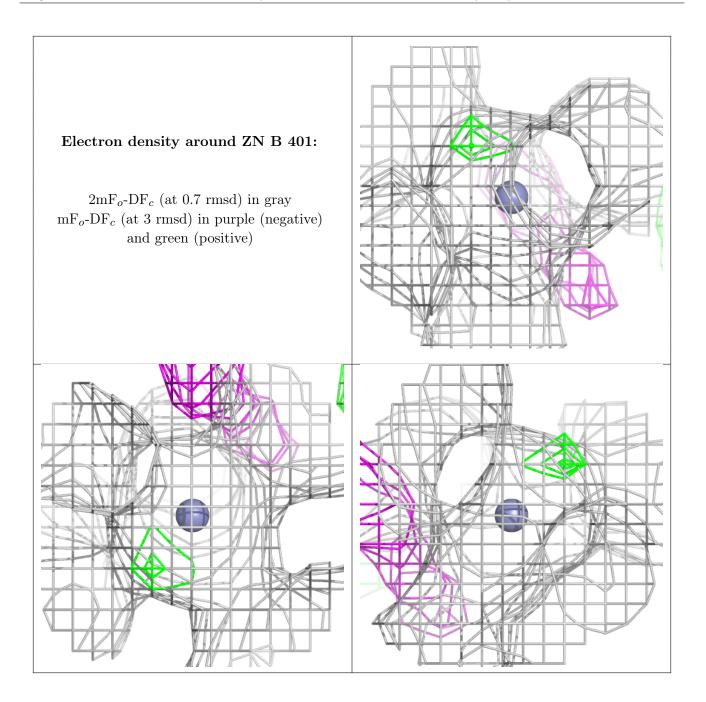
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











6.5 Other polymers (i)

There are no such residues in this entry.

