

Full wwPDB X-ray Structure Validation Report (i)

Mar 25, 2024 – 10:48 AM JST

PDB ID : 8XHO

Title : Deep sea bacterial PET plastic hydrolase MtCut with mutation S178C

Authors : Yang, J. Deposited on : 2023-12-18

Resolution : 2.50 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 (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:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$

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)

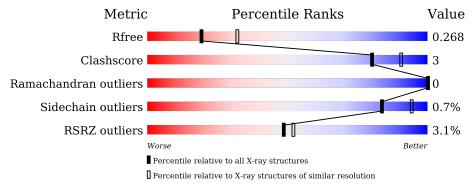
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	270	91%	6%	-
1	В	270	89%	8%	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4272 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 PET plastic hydrolase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	262	Total 2022	C 1264	N 339	O 411	S 8	0	0	0
1	В	262	Total 2022	_	N 339	O 411	S 8	0	0	0

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

M	[ol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	2	A	1	Total Ca 1 1	0	0
2	2	В	2	Total Ca 2 2	0	0

• Molecule 3 is water.

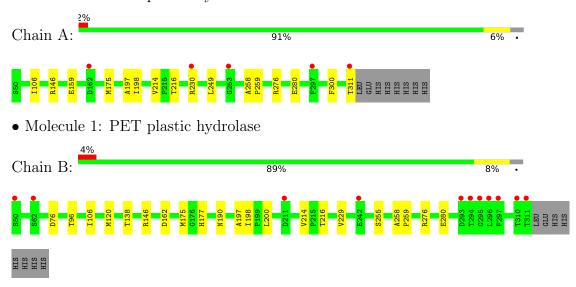
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	В	118	Total O 118 118	0	0



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: PET plastic hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	88.15Å 85.56Å 69.52Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.64 - 2.50	Depositor
Resolution (A)	19.63 - 2.50	EDS
% Data completeness	99.1 (19.64-2.50)	Depositor
(in resolution range)	91.7 (19.63-2.50)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.88 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
D.D.	0.222 , 0.256	Depositor
R, R_{free}	0.236 , 0.268	DCC
R_{free} test set	1873 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.959	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 23.2	EDS
L-test for twinning ²	$< L > = 0.46, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4272	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.21% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ 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: CA

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		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.28	0/2074	0.52	0/2831	
1	В	0.27	0/2074	0.53	0/2831	
All	All	0.27	0/4148	0.53	0/5662	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	${ m Chain} \mid \# { m Chirality \ outliers} \mid \# { m Planarity \ out} \mid$	
1	A	0	2
1	В	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ARG	Sidechain
1	A	230	ARG	Sidechain
1	В	146	ARG	Sidechain

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



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the asymmetr	ne unit	whereas S	vmm-Clashes	lists svr	${ m mmetry}$ -related	clashes
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2022	0	1887	7	0
1	В	2022	0	1887	12	1
2	A	1	0	0	0	0
2	В	2	0	0	0	0
3	A	107	0	0	0	0
3	В	118	0	0	3	0
All	All	4272	0	3774	19	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 3.

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:B:214:VAL:O	1:B:216:THR:HG23	2.00	$\frac{0.60}{0.60}$
1:A:214:VAL:O	1:A:216:THR:HG23	2.01	0.60
1:B:197:ALA:HB3	1:B:216:THR:HG22	1.90	0.53
1:A:175:MET:HG2	1:A:198:ILE:HB	1.93	0.50
1:A:197:ALA:HB3	1:A:216:THR:HG22	1.93	0.49
1:B:175:MET:HG2	1:B:198:ILE:HB	1.95	0.48
1:B:96:THR:HG22	3:B:608:HOH:O	2.12	0.48
1:A:258:ALA:N	1:A:259:PRO:CD	2.78	0.46
1:B:258:ALA:N	1:B:259:PRO:CD	2.77	0.46
1:B:106:ILE:HG12	1:B:175:MET:HB2	1.98	0.44
1:B:76:ASP:OD2	1:B:162:ASP:HB2	2.17	0.43
1:A:276:ARG:O	1:A:280:GLU:HA	2.18	0.43
1:A:106:ILE:HG12	1:A:175:MET:HB2	2.00	0.43
1:B:276:ARG:O	1:B:280:GLU:HA	2.19	0.43
1:B:120:MET:HE1	1:B:200:LEU:HD11	2.02	0.41
1:B:229:VAL:HG22	3:B:576:HOH:O	2.20	0.41
1:B:177:HIS:HD2	3:B:573:HOH:O	2.03	0.41
1:A:249:LEU:HD21	1:A:300:PHE:CE2	2.56	0.41
1:B:190:ASN:HD22	1:B:190:ASN:HA	1.67	0.40

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-1 Atom-2		$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:B:255:SER:OG	1:B:255:SER:OG[2_565]	1.88	0.32	



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	Perce	entiles
1	A	260/270~(96%)	250 (96%)	10 (4%)	0	100	100
1	В	260/270~(96%)	251 (96%)	9 (4%)	0	100	100
All	All	520/540 (96%)	501 (96%)	19 (4%)	0	100	100

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	$219/227 \ (96\%)$	217 (99%)	2 (1%)	78	92	
1	В	219/227 (96%)	218 (100%)	1 (0%)	88	96	
All	All	438/454 (96%)	435 (99%)	3 (1%)	84	94	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	GLU
1	A	311	THR
1	В	138	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	204	HIS
1	A	260	ASN
1	A	309	HIS
1	В	177	HIS
1	В	190	ASN
1	В	260	ASN
1	В	309	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)

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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	$262/270 \ (97\%)$	0.21	5 (1%) 66 69	14, 14, 14, 14	0
1	В	$262/270 \ (97\%)$	0.28	11 (4%) 36 39	14, 14, 14, 14	0
All	All	524/540 (97%)	0.24	16 (3%) 49 52	14, 14, 14, 14	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	297	PHE	5.0
1	В	295	GLY	4.5
1	В	50	SER	4.2
1	В	294	THR	3.9
1	В	296	LEU	3.7
1	В	311	THR	3.4
1	A	297	PHE	3.3
1	В	310	THR	3.3
1	A	311	THR	2.9
1	В	293	ASP	2.7
1	В	242	GLU	2.5
1	A	162	ASP	2.4
1	A	230	ARG	2.2
1	В	211	ASP	2.1
1	В	62	SER	2.1
1	A	253	GLY	2.1

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.

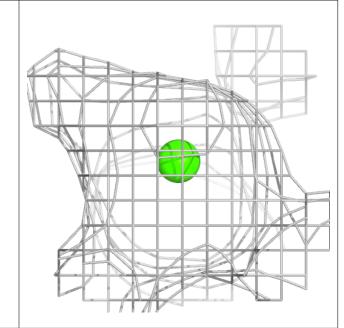
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
2	CA	A	401	1/1	0.89	0.07	22,22,22,22	0
2	CA	В	401	1/1	0.96	0.08	22,22,22,22	0
2	CA	В	402	1/1	0.98	0.12	22,22,22,22	0

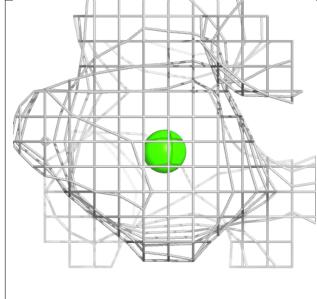
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

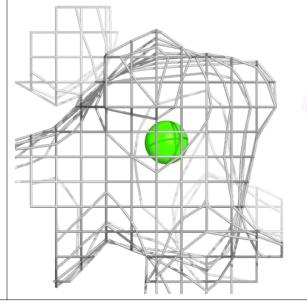


Electron density around CA A 401:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

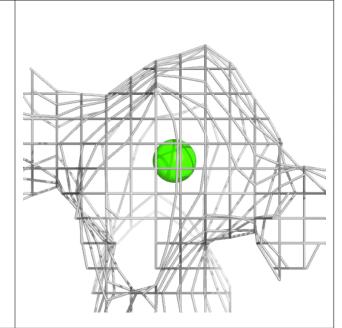


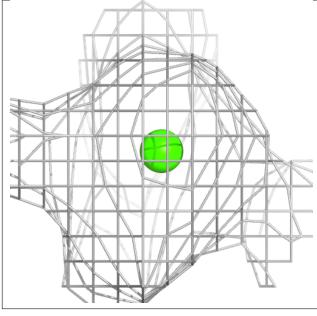


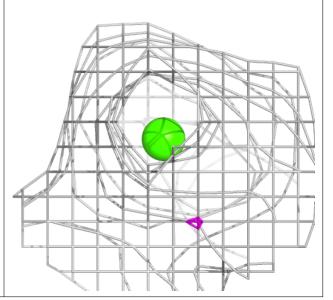


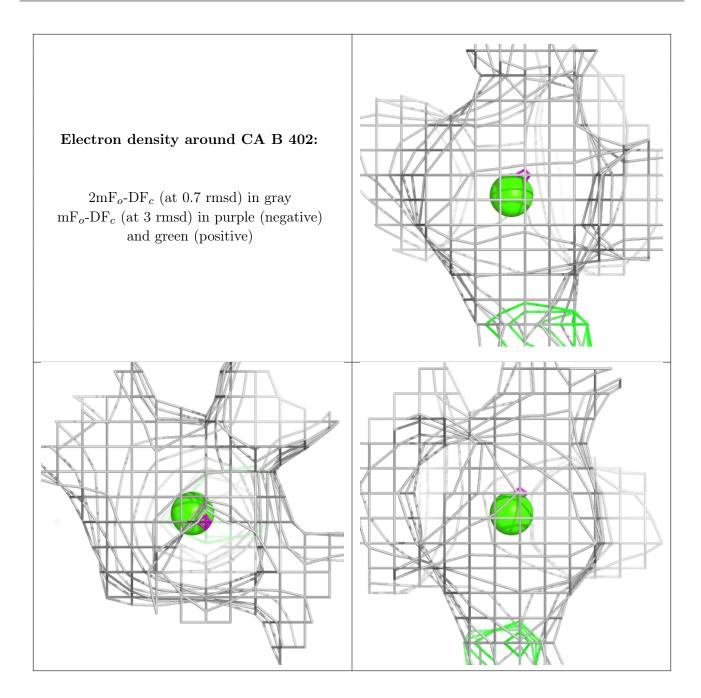
Electron density around CA B 401:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

