



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8J5N / pdb_00008j5n
Title : Crystal structure of a PETase variant V20 from Ideonella sakaiensis
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Deposited on : 2023-04-23
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

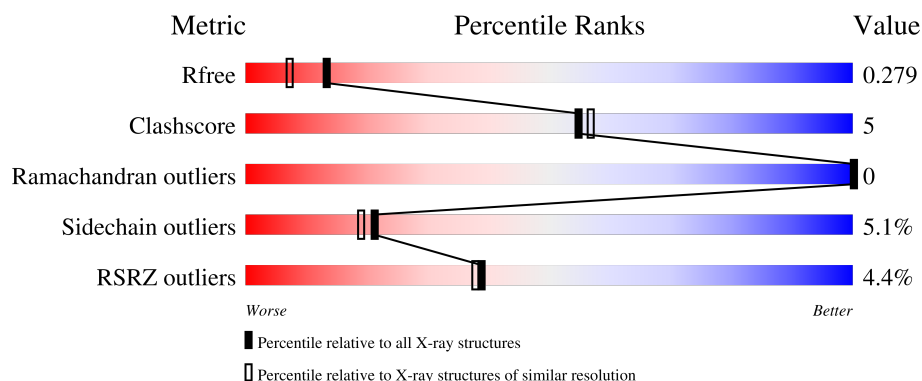
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	298	4% 76% 11% • 12%
1	D	298	4% 77% 10% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4043 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 Poly(ethylene terephthalate) hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1917	1185	343	378	11			
1	D	261	Total	C	N	O	S	0	0	0
			1917	1185	343	378	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLU	VAL	engineered mutation	UNP A0A0K8P6T7
A	18	PRO	LEU	engineered mutation	UNP A0A0K8P6T7
A	53	GLN	ARG	engineered mutation	UNP A0A0K8P6T7
A	84	LEU	VAL	engineered mutation	UNP A0A0K8P6T7
A	186	HIS	ASP	engineered mutation	UNP A0A0K8P6T7
A	201	ILE	PHE	engineered mutation	UNP A0A0K8P6T7
A	229	TYR	PHE	engineered mutation	UNP A0A0K8P6T7
A	233	LYS	ASN	engineered mutation	UNP A0A0K8P6T7
A	280	GLU	ARG	engineered mutation	UNP A0A0K8P6T7
A	283	ARG	ASP	engineered mutation	UNP A0A0K8P6T7
A	291	LEU	-	expression tag	UNP A0A0K8P6T7
A	292	GLU	-	expression tag	UNP A0A0K8P6T7
A	293	HIS	-	expression tag	UNP A0A0K8P6T7
A	294	HIS	-	expression tag	UNP A0A0K8P6T7
A	295	HIS	-	expression tag	UNP A0A0K8P6T7
A	296	HIS	-	expression tag	UNP A0A0K8P6T7
A	297	HIS	-	expression tag	UNP A0A0K8P6T7
A	298	HIS	-	expression tag	UNP A0A0K8P6T7
D	14	GLU	VAL	engineered mutation	UNP A0A0K8P6T7
D	18	PRO	LEU	engineered mutation	UNP A0A0K8P6T7
D	53	GLN	ARG	engineered mutation	UNP A0A0K8P6T7
D	84	LEU	VAL	engineered mutation	UNP A0A0K8P6T7
D	186	HIS	ASP	engineered mutation	UNP A0A0K8P6T7
D	201	ILE	PHE	engineered mutation	UNP A0A0K8P6T7
D	229	TYR	PHE	engineered mutation	UNP A0A0K8P6T7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	233	LYS	ASN	engineered mutation	UNP A0A0K8P6T7
D	280	GLU	ARG	engineered mutation	UNP A0A0K8P6T7
D	283	ARG	ASP	engineered mutation	UNP A0A0K8P6T7
D	291	LEU	-	expression tag	UNP A0A0K8P6T7
D	292	GLU	-	expression tag	UNP A0A0K8P6T7
D	293	HIS	-	expression tag	UNP A0A0K8P6T7
D	294	HIS	-	expression tag	UNP A0A0K8P6T7
D	295	HIS	-	expression tag	UNP A0A0K8P6T7
D	296	HIS	-	expression tag	UNP A0A0K8P6T7
D	297	HIS	-	expression tag	UNP A0A0K8P6T7
D	298	HIS	-	expression tag	UNP A0A0K8P6T7

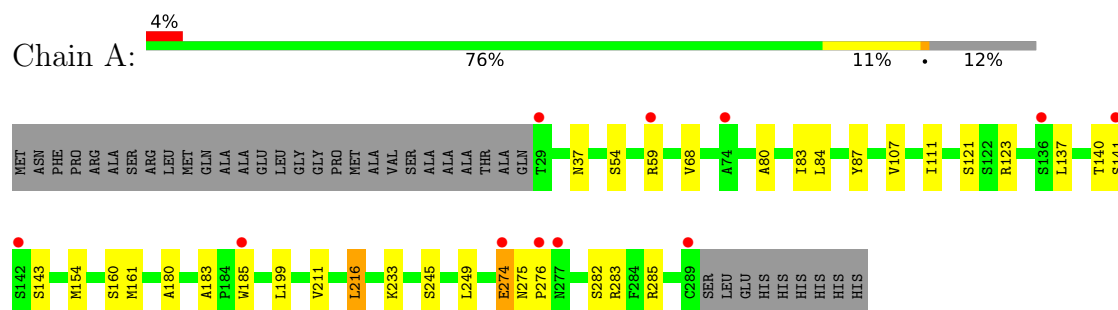
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	101	Total O 101 101	0	0
2	D	108	Total O 108 108	0	0

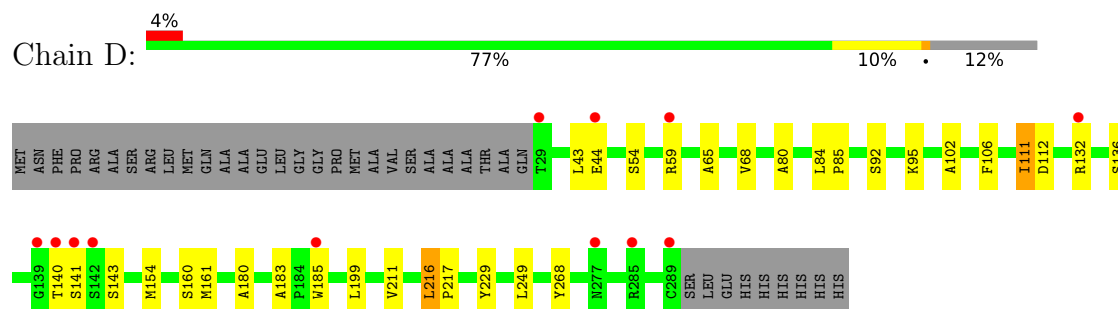
3 Residue-property plots [i](#)

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: Poly(ethylene terephthalate) hydrolase



- Molecule 1: Poly(ethylene terephthalate) hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	50.28Å 77.92Å 125.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.00 48.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.81-2.00) 97.5 (48.81-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.226 , 0.278 0.234 , 0.279	Depositor DCC
R_{free} test set	1585 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4043	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 51.96 % 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 5.2044e-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

5.1 Standard geometry

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	1.05	0/1962	1.38	2/2673 (0.1%)
1	D	1.11	0/1962	1.37	0/2673
All	All	1.08	0/3924	1.38	2/5346 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	MET	CA-C-N	7.36	127.27	121.61
1	A	154	MET	C-N-CA	7.36	127.27	121.61

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1917	0	1849	19	0
1	D	1917	0	1849	24	0
2	A	101	0	0	1	0
2	D	108	0	0	0	0
All	All	4043	0	3698	36	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 5.

All (36) 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:A:161:MET:HE2	1:A:185:TRP:CZ3	2.30	0.66
1:A:161:MET:HE3	1:D:132:ARG:HG3	1.86	0.58
1:D:161:MET:HE2	1:D:185:TRP:CZ3	2.40	0.56
1:A:185:TRP:CH2	1:D:136:SER:HB2	2.40	0.56
1:A:180:ALA:HA	1:A:199:LEU:O	2.11	0.51
1:A:245:SER:N	2:A:307:HOH:O	2.44	0.51
1:D:85:PRO:HD3	1:D:111:ILE:O	2.12	0.49
1:D:211:VAL:O	1:D:216:LEU:HB2	2.14	0.48
1:A:87:TYR:CD2	1:D:132:ARG:HB2	2.49	0.48
1:D:80:ALA:O	1:D:154:MET:HA	2.13	0.48
1:A:249:LEU:CD2	1:A:276:PRO:HB3	2.44	0.47
1:A:185:TRP:HH2	1:D:136:SER:HB2	1.80	0.47
1:A:160:SER:HA	1:A:183:ALA:O	2.15	0.46
1:A:80:ALA:HA	1:A:107:VAL:O	2.16	0.46
1:D:54:SER:HA	1:D:68:VAL:O	2.15	0.45
1:A:54:SER:HA	1:A:68:VAL:O	2.16	0.45
1:D:216:LEU:N	1:D:217:PRO:HD2	2.31	0.45
1:A:84:LEU:HD13	1:A:123:ARG:HB3	1.98	0.45
1:D:160:SER:HA	1:D:183:ALA:O	2.17	0.45
1:D:140:THR:O	1:D:143:SER:HB3	2.16	0.45
1:A:87:TYR:CE2	1:D:132:ARG:HB2	2.54	0.43
1:A:185:TRP:CZ2	1:D:136:SER:HB2	2.53	0.43
1:D:161:MET:CE	1:D:185:TRP:CZ3	3.02	0.43
1:A:274:GLU:HG3	1:A:275:ASN:O	2.19	0.43
1:A:185:TRP:CH2	1:D:136:SER:CB	3.02	0.42
1:A:137:LEU:HA	1:A:140:THR:HB	2.01	0.42
1:D:216:LEU:HD13	1:D:229:TYR:CZ	2.54	0.42
1:A:211:VAL:O	1:A:216:LEU:HB2	2.20	0.42
1:D:65:ALA:HB3	1:D:112:ASP:HB2	2.02	0.42
1:A:249:LEU:HD21	1:A:276:PRO:HB3	2.02	0.42
1:D:43:LEU:HD21	1:D:268:TYR:HE2	1.85	0.41
1:D:84:LEU:CD2	1:D:111:ILE:HD11	2.50	0.41
1:D:180:ALA:HA	1:D:199:LEU:O	2.21	0.41
1:D:84:LEU:HD23	1:D:111:ILE:CD1	2.51	0.40
1:D:102:ALA:HA	1:D:106:PHE:O	2.22	0.40
1:D:216:LEU:HD13	1:D:229:TYR:CE1	2.57	0.40

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	259/298 (87%)	252 (97%)	7 (3%)	0	100	100
1	D	259/298 (87%)	253 (98%)	6 (2%)	0	100	100
All	All	518/596 (87%)	505 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	206/234 (88%)	193 (94%)	13 (6%)	16	13
1	D	206/234 (88%)	198 (96%)	8 (4%)	28	28
All	All	412/468 (88%)	391 (95%)	21 (5%)	21	19

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	59	ARG
1	A	83	ILE
1	A	111	ILE
1	A	121	SER
1	A	141	SER
1	A	143	SER
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	233	LYS
1	A	274	GLU
1	A	282	SER
1	A	283	ARG
1	A	285	ARG
1	D	44	GLU
1	D	59	ARG
1	D	92	SER
1	D	95	LYS
1	D	111	ILE
1	D	141	SER
1	D	216	LEU
1	D	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	247	GLN
1	D	119	GLN

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 [i](#)

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, 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	261/298 (87%)	0.29	11 (4%) 40 39	11, 19, 32, 51	0
1	D	261/298 (87%)	0.35	12 (4%) 37 36	11, 20, 33, 51	0
All	All	522/596 (87%)	0.32	23 (4%) 39 38	11, 19, 33, 51	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ARG	4.2
1	A	276	PRO	4.1
1	A	274	GLU	4.1
1	A	29	THR	4.1
1	D	185	TRP	4.0
1	D	277	ASN	4.0
1	D	142	SER	3.8
1	D	44	GLU	3.5
1	D	29	THR	3.4
1	D	59	ARG	3.1
1	D	139	GLY	3.0
1	A	142	SER	2.7
1	D	285	ARG	2.6
1	A	289	CYS	2.5
1	A	141	SER	2.5
1	D	141	SER	2.5
1	A	74	ALA	2.4
1	A	185	TRP	2.4
1	A	277	ASN	2.2
1	A	136	SER	2.2
1	D	289	CYS	2.1
1	D	132	ARG	2.1
1	D	140	THR	2.0

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 oligosaccharides 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.