Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 11:48 pm BST

PDB ID	:	6EQH
Title	:	Crystal structure of a polyethylene terephthalate degrading hydrolase from Ideonella sakaiensis in spacegroup C2221
Authors	:	Austin, H.P.; Allen, M.D.; Johnson, C.W.; Beckham, G.T.; McGeehan, J.E.
Deposited on	:	2017-10-12
Resolution	:	1.58 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 following versions of software and data (see references ⓘ) were used in the production of this report:

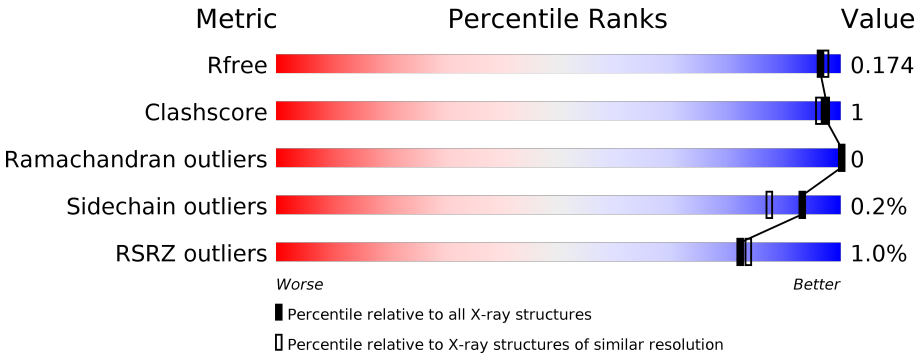
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.58 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}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 on 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	298	% 88% 12%
1	B	298	87% · 11%
1	C	298	% 86% · 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6833 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	263	Total	C	N	O	S	0	4	0
			1949	1207	345	384	13			
1	B	264	Total	C	N	O	S	0	4	0
			1958	1212	346	387	13			
1	C	262	Total	C	N	O	S	0	3	0
			1936	1196	345	384	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
B	291	LEU	-	expression tag	UNP A0A0K8P6T7
B	292	GLU	-	expression tag	UNP A0A0K8P6T7
B	293	HIS	-	expression tag	UNP A0A0K8P6T7
B	294	HIS	-	expression tag	UNP A0A0K8P6T7
B	295	HIS	-	expression tag	UNP A0A0K8P6T7
B	296	HIS	-	expression tag	UNP A0A0K8P6T7
B	297	HIS	-	expression tag	UNP A0A0K8P6T7
B	298	HIS	-	expression tag	UNP A0A0K8P6T7
C	291	LEU	-	expression tag	UNP A0A0K8P6T7
C	292	GLU	-	expression tag	UNP A0A0K8P6T7
C	293	HIS	-	expression tag	UNP A0A0K8P6T7
C	294	HIS	-	expression tag	UNP A0A0K8P6T7
C	295	HIS	-	expression tag	UNP A0A0K8P6T7
C	296	HIS	-	expression tag	UNP A0A0K8P6T7
C	297	HIS	-	expression tag	UNP A0A0K8P6T7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	298	HIS	-	expression tag	UNP A0A0K8P6T7

- Molecule 2 is water.

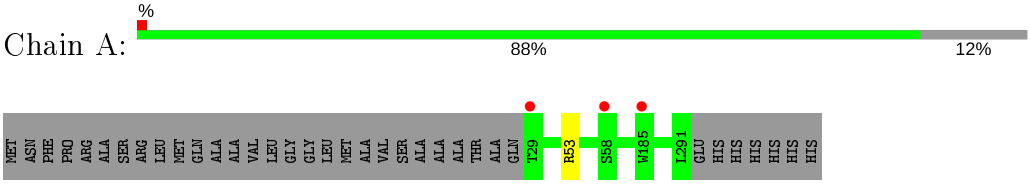
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	335	Total O 335 335	0	0
2	B	343	Total O 343 343	0	0
2	C	312	Total O 312 312	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

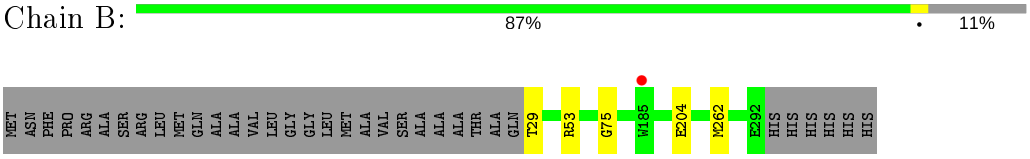
- Molecule 1: Poly(ethylene terephthalate) hydrolase

Chain A:



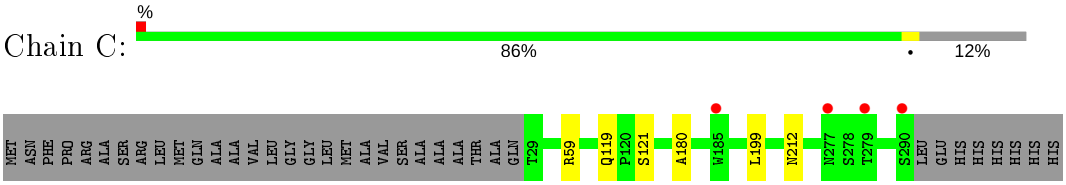
- Molecule 1: Poly(ethylene terephthalate) hydrolase

Chain B:



- Molecule 1: Poly(ethylene terephthalate) hydrolase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	52.70Å 234.13Å 165.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 1.58 49.81 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.68-1.58) 99.9 (49.81-1.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.58Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.169 , 0.184 0.172 , 0.174	Depositor DCC
R_{free} test set	6977 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6833	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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	0.36	0/2006	0.58	2/2731 (0.1%)
1	B	0.41	0/2015	0.57	1/2743 (0.0%)
1	C	0.36	0/1990	0.54	0/2711
All	All	0.38	0/6011	0.57	3/8185 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	NE-CZ-NH2	8.13	124.36	120.30
1	A	53	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	B	53	ARG	NE-CZ-NH2	-5.66	117.47	120.30

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	1949	0	1891	0	0
1	B	1958	0	1897	4	0
1	C	1936	0	1868	5	0
2	A	335	0	0	0	3
2	B	343	0	0	4	1
2	C	312	0	0	4	1
All	All	6833	0	5656	9	5

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 1.

All (9) 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:29:THR:N	2:B:302:HOH:O	2.18	0.76
1:B:204:GLU:OE2	2:B:301:HOH:O	2.08	0.70
1:C:119:GLN:OE1	2:C:302:HOH:O	2.14	0.65
1:C:121[A]:SER:OG	2:C:303:HOH:O	2.19	0.50
1:C:212[B]:ASN:OD1	2:C:304:HOH:O	2.21	0.44
1:C:180:ALA:HA	1:C:199:LEU:O	2.19	0.43
1:C:59:ARG:N	2:C:301:HOH:O	1.89	0.41
1:B:75:GLY:O	2:B:303:HOH:O	2.22	0.41
1:B:29:THR:CA	2:B:302:HOH:O	2.65	0.40

All (5) 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)
2:A:504:HOH:O	2:A:504:HOH:O[3_757]	2.02	0.18
2:A:608:HOH:O	2:A:627:HOH:O[3_757]	2.08	0.12
2:C:561:HOH:O	2:C:597:HOH:O[3_856]	2.09	0.11
2:B:304:HOH:O	2:B:346:HOH:O[8_477]	2.11	0.09
2:A:592:HOH:O	2:A:608:HOH:O[3_757]	2.16	0.04

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	265/298 (89%)	260 (98%)	5 (2%)	0	100	100
1	B	266/298 (89%)	263 (99%)	3 (1%)	0	100	100
1	C	263/298 (88%)	260 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	794/894 (89%)	783 (99%)	11 (1%)	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	213/234 (91%)	213 (100%)	0	100 100
1	B	214/234 (92%)	212 (99%)	2 (1%)	78 64
1	C	211/234 (90%)	211 (100%)	0	100 100
All	All	638/702 (91%)	636 (100%)	2 (0%)	93 86

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

Mol	Chain	Res	Type
1	B	262[A]	MET
1	B	262[B]	MET

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	263/298 (88%)	-0.29	3 (1%)	80	82	19, 24, 35, 55	0
1	B	264/298 (88%)	0.02	1 (0%)	92	93	17, 23, 36, 61	0
1	C	262/298 (87%)	-0.22	4 (1%)	73	75	18, 25, 36, 56	0
All	All	789/894 (88%)	-0.16	8 (1%)	82	83	17, 24, 36, 61	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	185	TRP	3.5
1	C	290	SER	3.0
1	A	58	SER	2.4
1	C	279	THR	2.3
1	A	185	TRP	2.3
1	A	29	THR	2.1
1	C	277	ASN	2.0
1	B	185	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.