wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 01:58 PM EDT

PDB ID	:	6QZ2
Title	:	Structure of MHETase from Ideonella sakaiensis
Authors	:	Allen, M.D.; Johnson, C.W.; Knott, B.C.; Beckham, G.T.; McGeehan, J.E.
Deposited on	:	2019-03-10
Resolution	:	1.90 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:

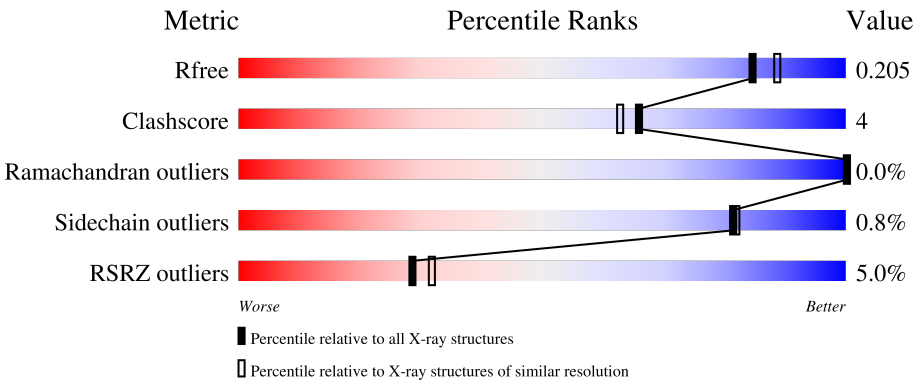
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	611	.% 87% 5% 8%
1	B	611	.% 88% • 8%
1	C	611	.% 86% 5% 8%
1	D	611	.% 88% • 8%
1	E	611	85% 7% 8%

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Mol	Chain	Length	Quality of chain
1	F	611	%, 87%, 5%, 8%
1	G	611	%, 85%, 7%, 8%
1	H	611	4%, 84%, 8%, 8%
1	I	611	16%, 82%, 9%, 8%
1	J	611	22%, 73%, 18%, 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47549 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	562	4147	2597	729	793	28	0	0	0
1	B	561	4140	2592	728	792	28	0	0	0
1	C	561	4140	2592	728	792	28	0	0	0
1	D	561	4140	2592	728	792	28	0	0	0
1	E	561	4140	2592	728	792	28	0	0	0
1	F	561	4140	2592	728	792	28	0	0	0
1	G	562	4147	2597	729	793	28	0	0	0
1	H	562	4147	2597	729	793	28	0	0	0
1	I	561	4140	2592	728	792	28	0	0	0
1	J	560	4133	2587	727	791	28	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	LEU	-	expression tag	UNP A0A0K8P8E7
A	605	GLU	-	expression tag	UNP A0A0K8P8E7
A	606	HIS	-	expression tag	UNP A0A0K8P8E7
A	607	HIS	-	expression tag	UNP A0A0K8P8E7
A	608	HIS	-	expression tag	UNP A0A0K8P8E7
A	609	HIS	-	expression tag	UNP A0A0K8P8E7
A	610	HIS	-	expression tag	UNP A0A0K8P8E7
A	611	HIS	-	expression tag	UNP A0A0K8P8E7
B	604	LEU	-	expression tag	UNP A0A0K8P8E7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	605	GLU	-	expression tag	UNP A0A0K8P8E7
B	606	HIS	-	expression tag	UNP A0A0K8P8E7
B	607	HIS	-	expression tag	UNP A0A0K8P8E7
B	608	HIS	-	expression tag	UNP A0A0K8P8E7
B	609	HIS	-	expression tag	UNP A0A0K8P8E7
B	610	HIS	-	expression tag	UNP A0A0K8P8E7
B	611	HIS	-	expression tag	UNP A0A0K8P8E7
C	604	LEU	-	expression tag	UNP A0A0K8P8E7
C	605	GLU	-	expression tag	UNP A0A0K8P8E7
C	606	HIS	-	expression tag	UNP A0A0K8P8E7
C	607	HIS	-	expression tag	UNP A0A0K8P8E7
C	608	HIS	-	expression tag	UNP A0A0K8P8E7
C	609	HIS	-	expression tag	UNP A0A0K8P8E7
C	610	HIS	-	expression tag	UNP A0A0K8P8E7
C	611	HIS	-	expression tag	UNP A0A0K8P8E7
D	604	LEU	-	expression tag	UNP A0A0K8P8E7
D	605	GLU	-	expression tag	UNP A0A0K8P8E7
D	606	HIS	-	expression tag	UNP A0A0K8P8E7
D	607	HIS	-	expression tag	UNP A0A0K8P8E7
D	608	HIS	-	expression tag	UNP A0A0K8P8E7
D	609	HIS	-	expression tag	UNP A0A0K8P8E7
D	610	HIS	-	expression tag	UNP A0A0K8P8E7
D	611	HIS	-	expression tag	UNP A0A0K8P8E7
E	604	LEU	-	expression tag	UNP A0A0K8P8E7
E	605	GLU	-	expression tag	UNP A0A0K8P8E7
E	606	HIS	-	expression tag	UNP A0A0K8P8E7
E	607	HIS	-	expression tag	UNP A0A0K8P8E7
E	608	HIS	-	expression tag	UNP A0A0K8P8E7
E	609	HIS	-	expression tag	UNP A0A0K8P8E7
E	610	HIS	-	expression tag	UNP A0A0K8P8E7
E	611	HIS	-	expression tag	UNP A0A0K8P8E7
F	604	LEU	-	expression tag	UNP A0A0K8P8E7
F	605	GLU	-	expression tag	UNP A0A0K8P8E7
F	606	HIS	-	expression tag	UNP A0A0K8P8E7
F	607	HIS	-	expression tag	UNP A0A0K8P8E7
F	608	HIS	-	expression tag	UNP A0A0K8P8E7
F	609	HIS	-	expression tag	UNP A0A0K8P8E7
F	610	HIS	-	expression tag	UNP A0A0K8P8E7
F	611	HIS	-	expression tag	UNP A0A0K8P8E7
G	604	LEU	-	expression tag	UNP A0A0K8P8E7
G	605	GLU	-	expression tag	UNP A0A0K8P8E7
G	606	HIS	-	expression tag	UNP A0A0K8P8E7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	607	HIS	-	expression tag	UNP A0A0K8P8E7
G	608	HIS	-	expression tag	UNP A0A0K8P8E7
G	609	HIS	-	expression tag	UNP A0A0K8P8E7
G	610	HIS	-	expression tag	UNP A0A0K8P8E7
G	611	HIS	-	expression tag	UNP A0A0K8P8E7
H	604	LEU	-	expression tag	UNP A0A0K8P8E7
H	605	GLU	-	expression tag	UNP A0A0K8P8E7
H	606	HIS	-	expression tag	UNP A0A0K8P8E7
H	607	HIS	-	expression tag	UNP A0A0K8P8E7
H	608	HIS	-	expression tag	UNP A0A0K8P8E7
H	609	HIS	-	expression tag	UNP A0A0K8P8E7
H	610	HIS	-	expression tag	UNP A0A0K8P8E7
H	611	HIS	-	expression tag	UNP A0A0K8P8E7
I	604	LEU	-	expression tag	UNP A0A0K8P8E7
I	605	GLU	-	expression tag	UNP A0A0K8P8E7
I	606	HIS	-	expression tag	UNP A0A0K8P8E7
I	607	HIS	-	expression tag	UNP A0A0K8P8E7
I	608	HIS	-	expression tag	UNP A0A0K8P8E7
I	609	HIS	-	expression tag	UNP A0A0K8P8E7
I	610	HIS	-	expression tag	UNP A0A0K8P8E7
I	611	HIS	-	expression tag	UNP A0A0K8P8E7
J	604	LEU	-	expression tag	UNP A0A0K8P8E7
J	605	GLU	-	expression tag	UNP A0A0K8P8E7
J	606	HIS	-	expression tag	UNP A0A0K8P8E7
J	607	HIS	-	expression tag	UNP A0A0K8P8E7
J	608	HIS	-	expression tag	UNP A0A0K8P8E7
J	609	HIS	-	expression tag	UNP A0A0K8P8E7
J	610	HIS	-	expression tag	UNP A0A0K8P8E7
J	611	HIS	-	expression tag	UNP A0A0K8P8E7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0
2	I	1	1	1	0	0
2	J	1	1	1	0	0

- Molecule 3 is water.

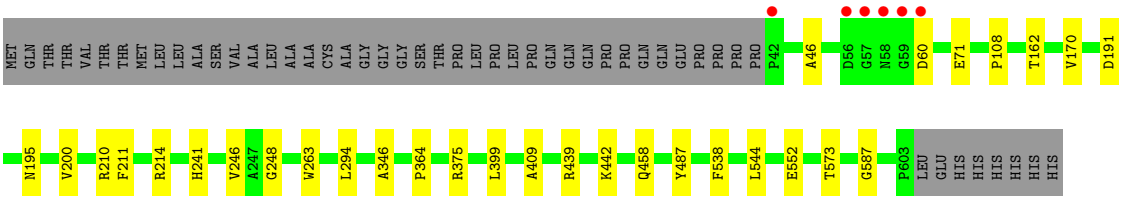
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	777	777	777	0	0
3	B	759	759	759	0	0
3	C	785	785	785	0	0
3	D	706	706	706	0	0
3	E	724	724	724	0	0
3	F	773	773	773	0	0
3	G	567	567	567	0	0
3	H	461	461	461	0	0
3	I	341	341	341	0	0
3	J	232	232	232	0	0

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.

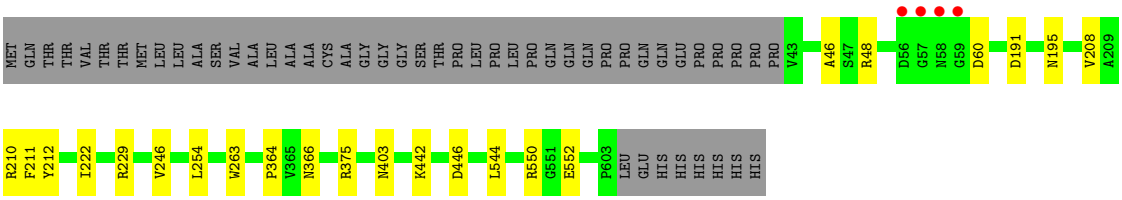
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain A:



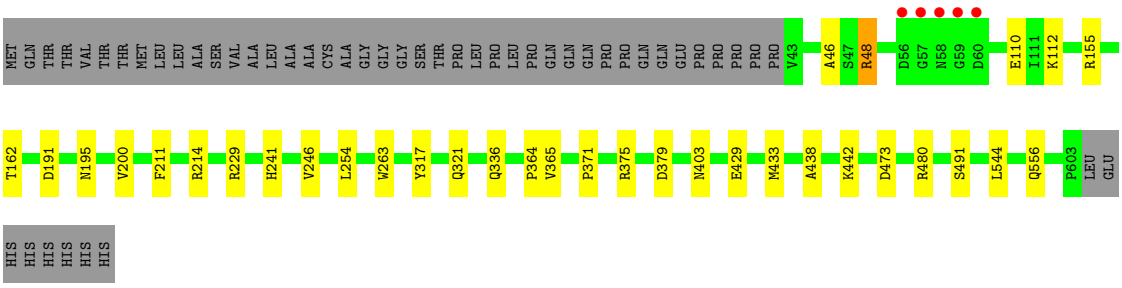
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain B:



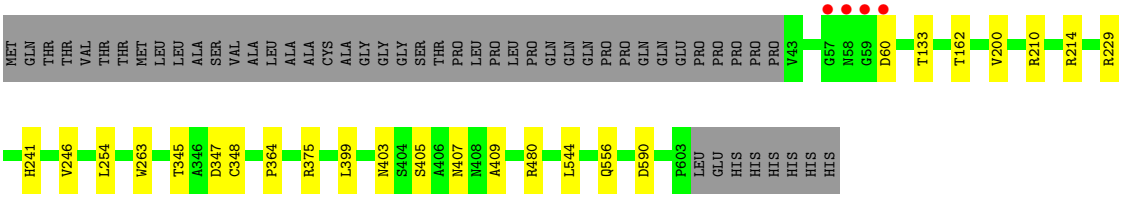
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain C:



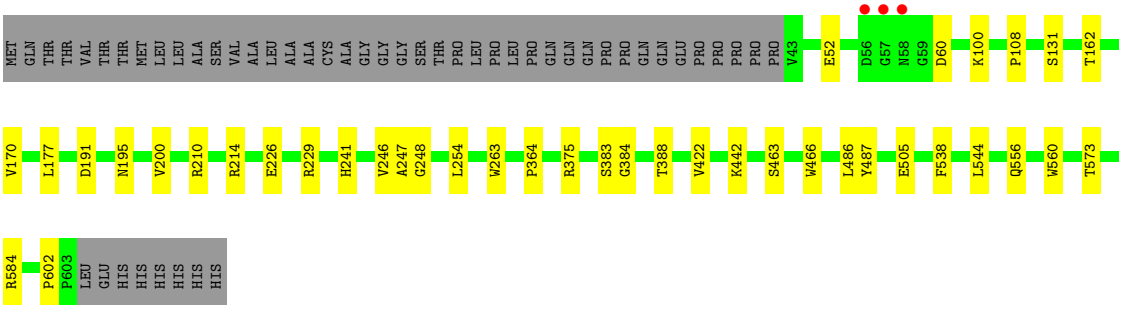
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain D:



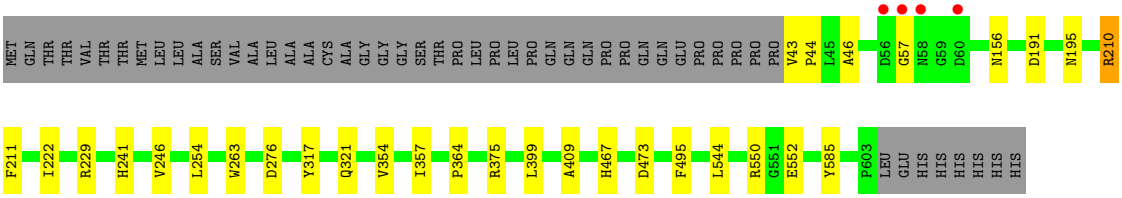
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain E:



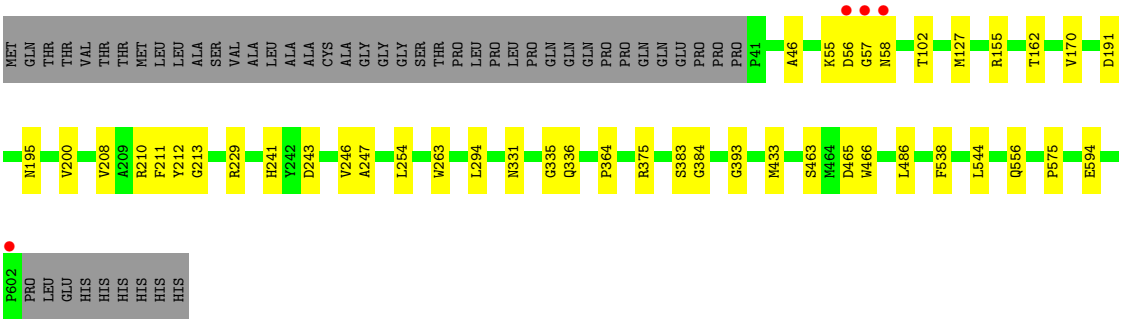
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain F:



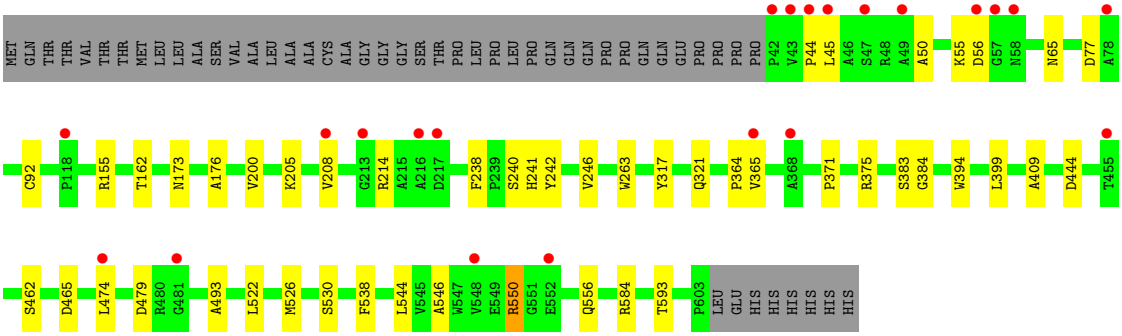
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain G:



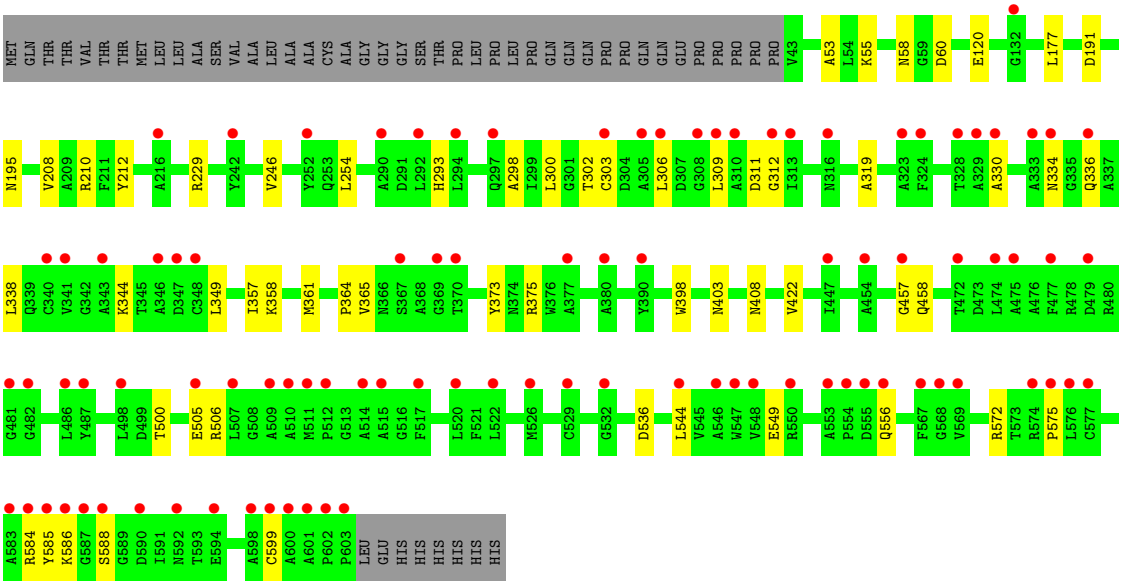
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain H:



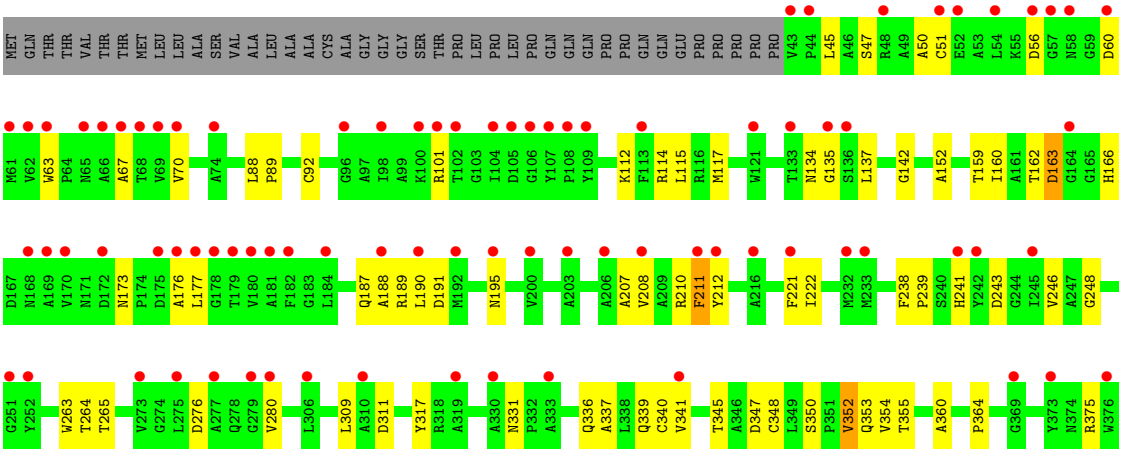
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

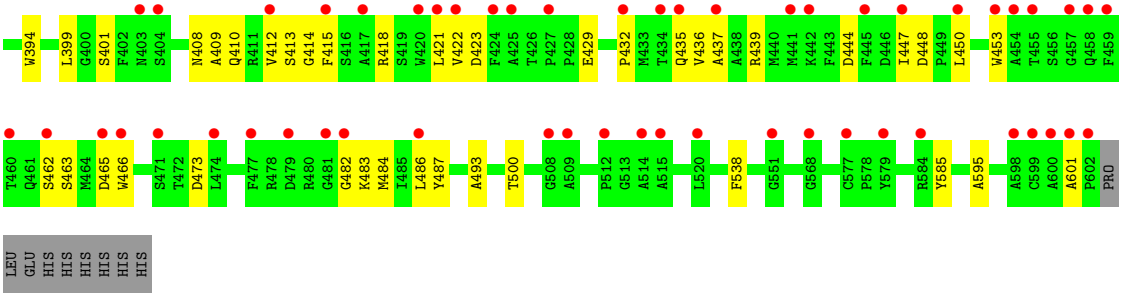
Chain I:



• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain J:




W394
L399
G400
S401
F402
N403
S404
N408
A409
Q410
R411
V412
S413
G414
F415
S416
A417
R418
S419
W420
L421
V422
D423
F424
A425
T426
P427
P428
E429
P432
M433
T434
Q435
V436
A437
A438
R439
M440
M441
K442
F443
D444
F445
D446
I447
D448
P449
L450
W453
A454
T455
S456
G457
Q458
F459
T460
Q461
S462
S463
M464
D465
W466
S471
T472
D473
L474
F477
R478
D479
R480
G481
G482
K483
M484
I485
L486
Y487
A493
T500
G508
A509
P512
G513
A514
A515
L520
F538
G551
G568
C577
P578
Y579
R584
Y585
A596
A598
C599
A600
A601
P602
PRO
LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	110.49Å 135.63Å 138.15Å 83.09° 67.91° 67.57°	Depositor
Resolution (Å)	57.62 – 1.90 88.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (57.62-1.90) 93.7 (88.35-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.185 , 0.205 0.185 , 0.205	Depositor DCC
R_{free} test set	24892 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h,l,h-k 0.016 for h,h-l,k 0.023 for h,h-k,h-l 0.017 for -h,-h+k,-l 0.017 for -h,-k,-h+l 0.023 for -h,-l,-k 0.055 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	47549	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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 (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	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.26	0/4256	0.46	0/5796
1	B	0.27	0/4248	0.47	0/5785
1	C	0.27	0/4248	0.47	0/5785
1	D	0.26	0/4248	0.47	0/5785
1	E	0.26	0/4248	0.46	0/5785
1	F	0.26	0/4248	0.47	0/5785
1	G	0.26	0/4256	0.45	0/5796
1	H	0.26	0/4256	0.46	0/5796
1	I	0.28	0/4248	0.47	0/5785
1	J	0.28	0/4240	0.49	0/5773
All	All	0.27	0/42496	0.47	0/57871

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	A	4147	0	3937	19	0
1	B	4140	0	3929	16	0
1	C	4140	0	3929	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4140	0	3929	24	0
1	E	4140	0	3929	27	0
1	F	4140	0	3929	22	0
1	G	4147	0	3937	31	0
1	H	4147	0	3937	32	0
1	I	4140	0	3929	50	0
1	J	4133	0	3922	85	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	777	0	0	7	4
3	B	759	0	0	7	1
3	C	785	0	0	11	3
3	D	706	0	0	14	3
3	E	724	0	0	14	8
3	F	773	0	0	8	1
3	G	567	0	0	16	4
3	H	461	0	0	14	3
3	I	341	0	0	25	0
3	J	232	0	0	29	1
All	All	47549	0	39307	326	14

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 326 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:H:92:CYS:SG	3:H:1295:HOH:O	2.21	0.98
1:J:345:THR:HG23	1:J:347:ASP:H	1.26	0.98
1:E:602:PRO:O	3:E:901:HOH:O	1.87	0.91
1:G:58:ASN:N	3:G:901:HOH:O	2.02	0.90
1:F:57:GLY:N	3:F:902:HOH:O	2.05	0.89

The worst 5 of 14 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:E:1449:HOH:O	3:H:1218:HOH:O[1_655]	1.83	0.37
3:D:1450:HOH:O	3:E:1566:HOH:O[1_455]	1.92	0.28
3:A:1307:HOH:O	3:G:1262:HOH:O[1_655]	1.93	0.27
3:A:1530:HOH:O	3:G:1310:HOH:O[1_655]	2.01	0.19
3:D:1176:HOH:O	3:E:1039:HOH:O[1_455]	2.02	0.18

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	560/611 (92%)	544 (97%)	16 (3%)	0	100	100
1	B	559/611 (92%)	543 (97%)	16 (3%)	0	100	100
1	C	559/611 (92%)	544 (97%)	15 (3%)	0	100	100
1	D	559/611 (92%)	541 (97%)	18 (3%)	0	100	100
1	E	559/611 (92%)	545 (98%)	14 (2%)	0	100	100
1	F	559/611 (92%)	544 (97%)	15 (3%)	0	100	100
1	G	560/611 (92%)	547 (98%)	13 (2%)	0	100	100
1	H	560/611 (92%)	544 (97%)	16 (3%)	0	100	100
1	I	559/611 (92%)	540 (97%)	19 (3%)	0	100	100
1	J	558/611 (91%)	536 (96%)	21 (4%)	1 (0%)	47	38
All	All	5592/6110 (92%)	5428 (97%)	163 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	50	ALA

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	408/449 (91%)	405 (99%)	3 (1%)	84	84
1	B	407/449 (91%)	406 (100%)	1 (0%)	93	94
1	C	407/449 (91%)	403 (99%)	4 (1%)	76	76
1	D	407/449 (91%)	405 (100%)	2 (0%)	88	89
1	E	407/449 (91%)	404 (99%)	3 (1%)	84	84
1	F	407/449 (91%)	404 (99%)	3 (1%)	84	84
1	G	408/449 (91%)	405 (99%)	3 (1%)	84	84
1	H	408/449 (91%)	404 (99%)	4 (1%)	76	76
1	I	407/449 (91%)	405 (100%)	2 (0%)	88	89
1	J	406/449 (90%)	398 (98%)	8 (2%)	55	51
All	All	4072/4490 (91%)	4039 (99%)	33 (1%)	81	82

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	210	ARG
1	J	211	PHE
1	J	538	PHE
1	E	538	PHE
1	E	375	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	403	ASN
1	J	241	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 10 ligands modelled in this entry, 10 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, 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	562/611 (91%)	-0.09	6 (1%)	80	82	13, 20, 33, 63	0
1	B	561/611 (91%)	0.00	4 (0%)	87	88	12, 19, 31, 57	0
1	C	561/611 (91%)	-0.11	5 (0%)	84	85	11, 19, 31, 53	0
1	D	561/611 (91%)	-0.03	4 (0%)	87	88	14, 21, 33, 61	0
1	E	561/611 (91%)	0.04	3 (0%)	91	92	14, 21, 33, 59	0
1	F	561/611 (91%)	-0.16	4 (0%)	87	88	11, 20, 33, 57	0
1	G	562/611 (91%)	-0.11	4 (0%)	87	88	18, 27, 38, 66	0
1	H	562/611 (91%)	0.35	22 (3%)	39	42	21, 31, 50, 70	0
1	I	561/611 (91%)	0.98	95 (16%)	1	1	26, 41, 59, 72	0
1	J	560/611 (91%)	1.25	136 (24%)	0	0	28, 49, 64, 80	0
All	All	5612/6110 (91%)	0.21	283 (5%)	28	32	11, 24, 54, 80	0

The worst 5 of 283 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	43	VAL	7.3
1	E	57	GLY	6.9
1	I	603	PRO	6.8
1	J	63	TRP	6.3
1	I	602	PRO	6.2

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, 95th 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	B-factors(Å^2)	Q<0.9
2	CA	I	801	1/1	0.91	0.07	47,47,47,47	0
2	CA	B	801	1/1	0.97	0.37	51,51,51,51	0
2	CA	J	801	1/1	0.98	0.05	44,44,44,44	0
2	CA	F	801	1/1	0.99	0.11	23,23,23,23	0
2	CA	G	801	1/1	0.99	0.08	25,25,25,25	0
2	CA	H	801	1/1	0.99	0.09	26,26,26,26	0
2	CA	A	801	1/1	0.99	0.12	21,21,21,21	0
2	CA	C	801	1/1	0.99	0.08	19,19,19,19	0
2	CA	E	801	1/1	1.00	0.10	21,21,21,21	0
2	CA	D	801	1/1	1.00	0.15	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.