wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2024 – 12:57 PM JST

PDB ID	:	8Z0X
Title	:	Crystal structure of glyoxylate reductase from Acetobacter aceti in the apo form
Authors	:	Majumder, T.R.; Yoshizawa, T.; Inoue, M.; Aono, R.; Matsumura, H.; Mihara, H.
Deposited on	:	2024-04-10
Resolution	:	1.60 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:

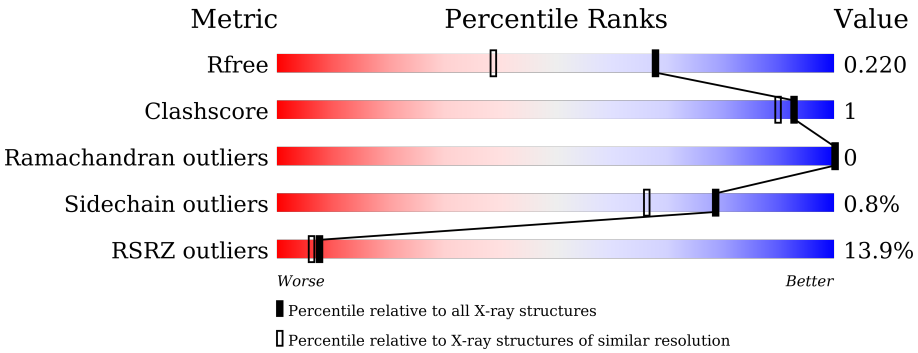
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.60 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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	313	19% 87% • 9%
1	B	313	14% 89% • 8%
1	C	313	16% 88% • 8%
1	D	313	7% 88% • 9%
1	E	313	3% 92% • 7%
1	F	313	2% 40% •• 57%

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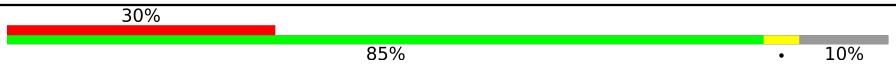
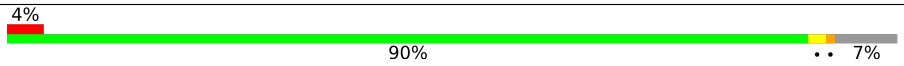
Mol	Chain	Length	Quality of chain
1	G	313	
1	H	313	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16816 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 3-hydroxyisobutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2075	1306	360	398	11			
1	B	289	Total	C	N	O	S	0	0	0
			2103	1321	366	405	11			
1	C	287	Total	C	N	O	S	0	0	0
			2085	1310	361	403	11			
1	D	286	Total	C	N	O	S	0	0	0
			2075	1306	359	399	11			
1	E	292	Total	C	N	O	S	0	0	0
			2118	1331	368	408	11			
1	F	135	Total	C	N	O	S	0	0	0
			1010	635	184	186	5			
1	G	282	Total	C	N	O	S	0	0	0
			2051	1291	355	394	11			
1	H	290	Total	C	N	O	S	0	0	0
			2103	1322	364	406	11			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
A	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
A	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
A	-12	LYS	-	expression tag	UNP A0A6S6PLJ6
A	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
A	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
A	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
A	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
A	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
A	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
A	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
A	-4	ILE	-	expression tag	UNP A0A6S6PLJ6
A	-3	GLU	-	expression tag	UNP A0A6S6PLJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
A	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
A	0	HIS	-	expression tag	UNP A0A6S6PLJ6
A	297	TYR	-	expression tag	UNP A0A6S6PLJ6
B	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
B	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
B	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
B	-12	LYS	-	expression tag	UNP A0A6S6PLJ6
B	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
B	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
B	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
B	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
B	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
B	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
B	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
B	-4	ILE	-	expression tag	UNP A0A6S6PLJ6
B	-3	GLU	-	expression tag	UNP A0A6S6PLJ6
B	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
B	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
B	0	HIS	-	expression tag	UNP A0A6S6PLJ6
B	297	TYR	-	expression tag	UNP A0A6S6PLJ6
C	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
C	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
C	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
C	-12	LYS	-	expression tag	UNP A0A6S6PLJ6
C	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
C	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
C	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
C	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
C	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
C	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
C	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
C	-4	ILE	-	expression tag	UNP A0A6S6PLJ6
C	-3	GLU	-	expression tag	UNP A0A6S6PLJ6
C	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
C	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
C	0	HIS	-	expression tag	UNP A0A6S6PLJ6
C	297	TYR	-	expression tag	UNP A0A6S6PLJ6
D	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
D	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
D	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
D	-12	LYS	-	expression tag	UNP A0A6S6PLJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
D	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
D	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
D	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
D	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
D	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
D	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
D	-4	ILE	-	expression tag	UNP A0A6S6PLJ6
D	-3	GLU	-	expression tag	UNP A0A6S6PLJ6
D	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
D	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
D	0	HIS	-	expression tag	UNP A0A6S6PLJ6
D	297	TYR	-	expression tag	UNP A0A6S6PLJ6
E	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
E	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
E	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
E	-12	LYS	-	expression tag	UNP A0A6S6PLJ6
E	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
E	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
E	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
E	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
E	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
E	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
E	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
E	-4	ILE	-	expression tag	UNP A0A6S6PLJ6
E	-3	GLU	-	expression tag	UNP A0A6S6PLJ6
E	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
E	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
E	0	HIS	-	expression tag	UNP A0A6S6PLJ6
E	297	TYR	-	expression tag	UNP A0A6S6PLJ6
F	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
F	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
F	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
F	-12	LYS	-	expression tag	UNP A0A6S6PLJ6
F	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
F	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
F	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
F	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
F	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
F	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
F	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
F	-4	ILE	-	expression tag	UNP A0A6S6PLJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLU	-	expression tag	UNP A0A6S6PLJ6
F	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
F	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
F	0	HIS	-	expression tag	UNP A0A6S6PLJ6
F	297	TYR	-	expression tag	UNP A0A6S6PLJ6
G	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
G	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
G	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
G	-12	LYS	-	expression tag	UNP A0A6S6PLJ6
G	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
G	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
G	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
G	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
G	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
G	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
G	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
G	-4	ILE	-	expression tag	UNP A0A6S6PLJ6
G	-3	GLU	-	expression tag	UNP A0A6S6PLJ6
G	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
G	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
G	0	HIS	-	expression tag	UNP A0A6S6PLJ6
G	297	TYR	-	expression tag	UNP A0A6S6PLJ6
H	-15	MET	-	initiating methionine	UNP A0A6S6PLJ6
H	-14	ASN	-	expression tag	UNP A0A6S6PLJ6
H	-13	HIS	-	expression tag	UNP A0A6S6PLJ6
H	-12	LYS	-	expression tag	UNP A0A6S6PLJ6
H	-11	VAL	-	expression tag	UNP A0A6S6PLJ6
H	-10	HIS	-	expression tag	UNP A0A6S6PLJ6
H	-9	HIS	-	expression tag	UNP A0A6S6PLJ6
H	-8	HIS	-	expression tag	UNP A0A6S6PLJ6
H	-7	HIS	-	expression tag	UNP A0A6S6PLJ6
H	-6	HIS	-	expression tag	UNP A0A6S6PLJ6
H	-5	HIS	-	expression tag	UNP A0A6S6PLJ6
H	-4	ILE	-	expression tag	UNP A0A6S6PLJ6
H	-3	GLU	-	expression tag	UNP A0A6S6PLJ6
H	-2	GLY	-	expression tag	UNP A0A6S6PLJ6
H	-1	ARG	-	expression tag	UNP A0A6S6PLJ6
H	0	HIS	-	expression tag	UNP A0A6S6PLJ6
H	297	TYR	-	expression tag	UNP A0A6S6PLJ6

- Molecule 2 is water.

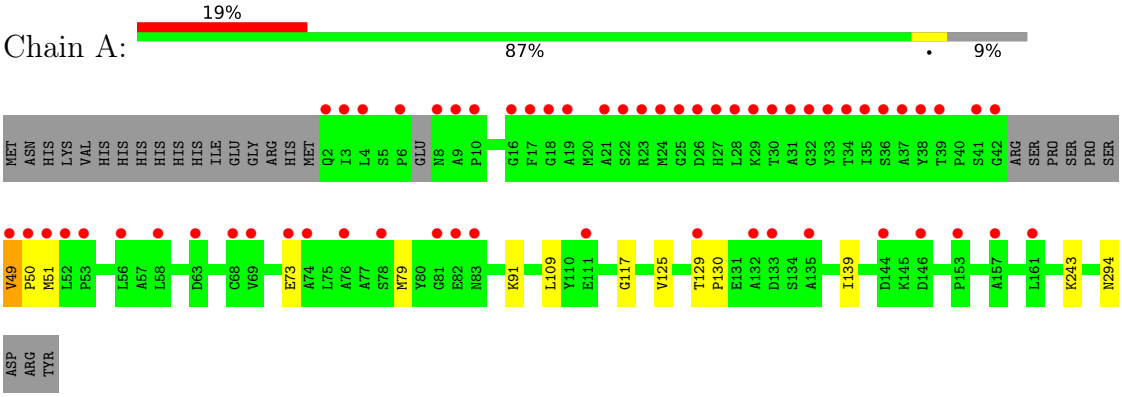
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	151	Total O 151 151	0	0
2	B	158	Total O 158 158	0	0
2	C	151	Total O 151 151	0	0
2	D	151	Total O 151 151	0	0
2	E	153	Total O 153 153	0	0
2	F	110	Total O 110 110	0	0
2	G	144	Total O 144 144	0	0
2	H	178	Total O 178 178	0	0

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.

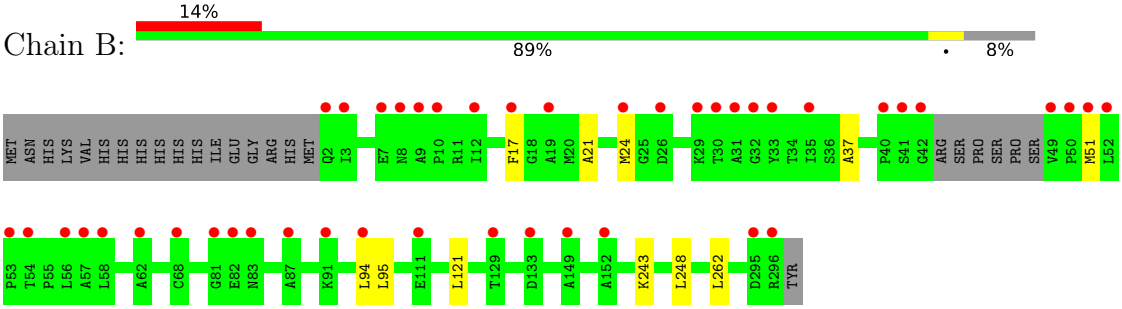
• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

Chain A:



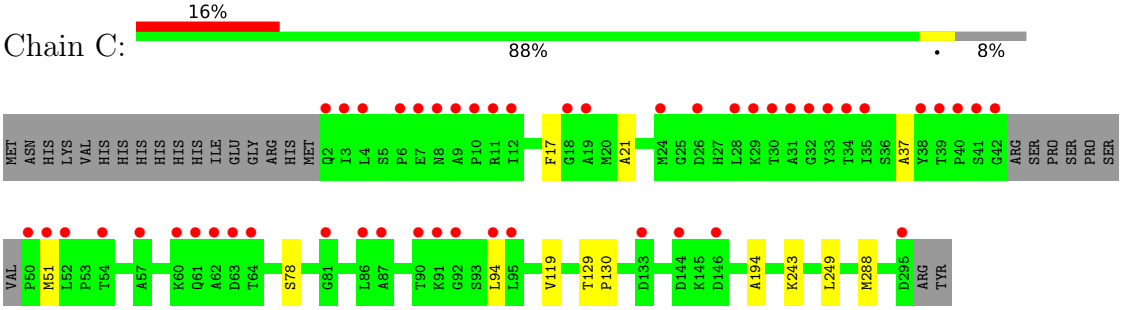
• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

Chain B:



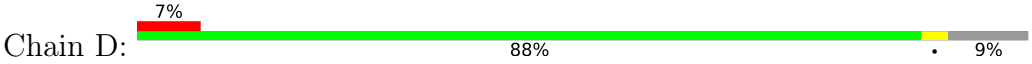
• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

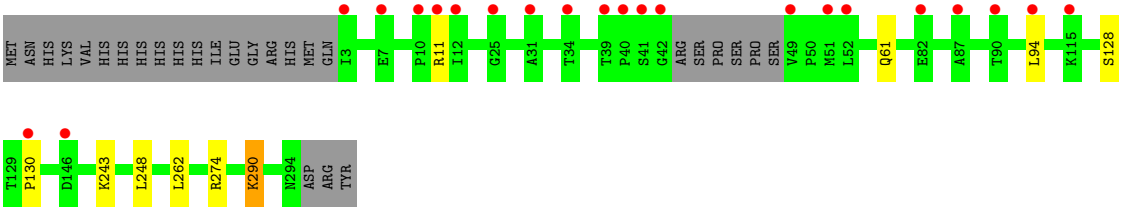
Chain C:



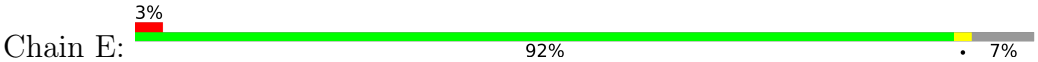
• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

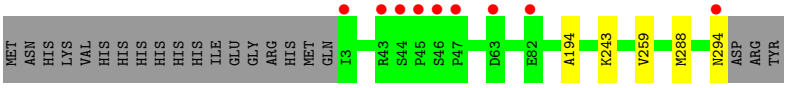
Chain D:



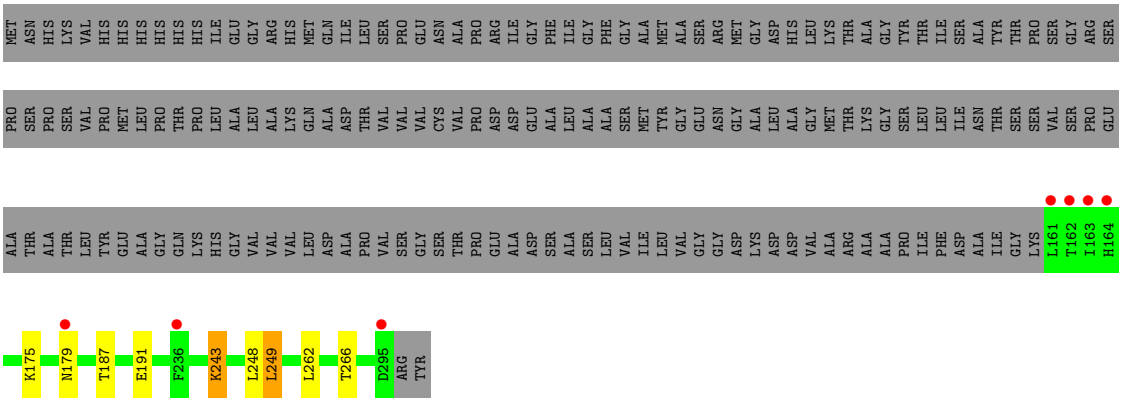


• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

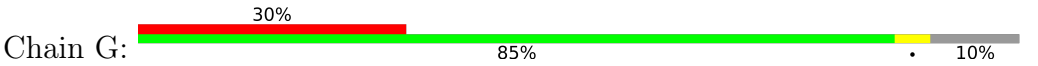


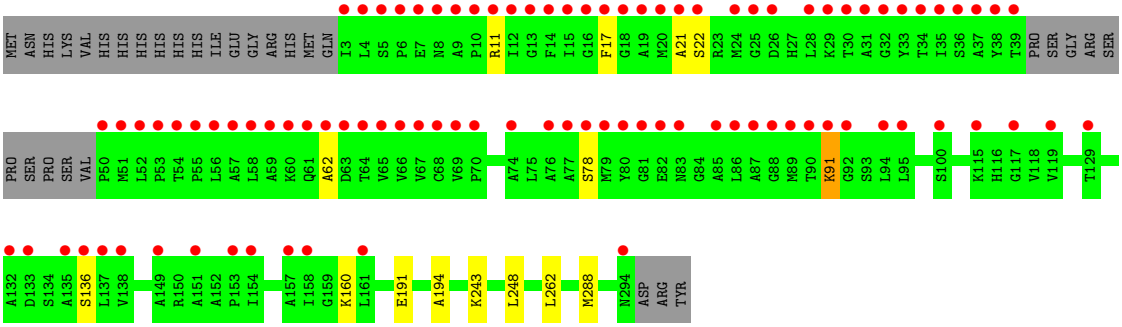


• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

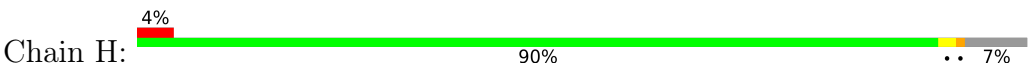


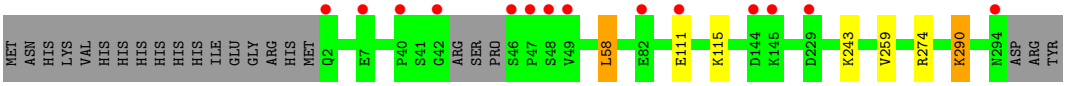
• Molecule 1: 3-hydroxyisobutyrate dehydrogenase





• Molecule 1: 3-hydroxyisobutyrate dehydrogenase




MET
ASN
HIS
LYS
VAL
HIS
HIS
HIS
HIS
HIS
ILE
GLU
GLY
ARG
HIS
MET
Q2
E7
P40
S41
G42
ARG
SER
PRO
S46
P47
S48
V49
L58
E82
E111
K115
D144
K145
D229
K243
V259
R274
K290
N294
ASP
ARG
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.45Å 191.88Å 117.85Å 90.00° 94.99° 90.00°	Depositor
Resolution (Å)	48.18 – 1.60 48.18 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.18-1.60) 99.4 (48.18-1.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.17 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.202 , 0.221 0.200 , 0.220	Depositor DCC
R_{free} test set	18463 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16816	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.65% 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	0.37	0/2107	0.62	0/2861
1	B	0.35	0/2136	0.60	0/2901
1	C	0.35	0/2118	0.60	1/2876 (0.0%)
1	D	0.36	0/2108	0.61	0/2864
1	E	0.37	0/2154	0.63	0/2929
1	F	0.38	0/1024	0.69	1/1385 (0.1%)
1	G	0.35	0/2083	0.59	0/2828
1	H	0.38	0/2137	0.65	2/2904 (0.1%)
All	All	0.36	0/15867	0.62	4/21548 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	58	LEU	CA-CB-CG	-6.82	99.61	115.30
1	H	290	LYS	CD-CE-NZ	6.79	127.32	111.70
1	F	249	LEU	CB-CG-CD1	-6.58	99.82	111.00
1	C	249	LEU	CB-CG-CD1	-5.40	101.82	111.00

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	2075	0	2128	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2103	0	2152	6	0
1	C	2085	0	2131	5	0
1	D	2075	0	2127	6	0
1	E	2118	0	2170	3	0
1	F	1010	0	1055	6	0
1	G	2051	0	2104	8	0
1	H	2103	0	2152	5	0
2	A	151	0	0	0	0
2	B	158	0	0	0	0
2	C	151	0	0	0	0
2	D	151	0	0	1	0
2	E	153	0	0	0	0
2	F	110	0	0	0	0
2	G	144	0	0	0	0
2	H	178	0	0	1	0
All	All	16816	0	16019	43	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 1.

The worst 5 of 43 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:21:ALA:HA	1:B:24:MET:HE2	1.77	0.65
1:F:191:GLU:HB3	1:H:259:VAL:HG12	1.80	0.62
1:H:290:LYS:HE3	2:H:432:HOH:O	2.04	0.57
1:B:94:LEU:HD21	1:B:121:LEU:HG	1.86	0.56
1:G:91:LYS:HE3	1:G:91:LYS:H	1.71	0.55

There are no symmetry-related clashes.

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	280/313 (90%)	277 (99%)	3 (1%)	0	100	100
1	B	285/313 (91%)	281 (99%)	4 (1%)	0	100	100
1	C	283/313 (90%)	280 (99%)	3 (1%)	0	100	100
1	D	282/313 (90%)	278 (99%)	4 (1%)	0	100	100
1	E	290/313 (93%)	286 (99%)	4 (1%)	0	100	100
1	F	133/313 (42%)	133 (100%)	0	0	100	100
1	G	278/313 (89%)	272 (98%)	6 (2%)	0	100	100
1	H	286/313 (91%)	283 (99%)	3 (1%)	0	100	100
All	All	2117/2504 (84%)	2090 (99%)	27 (1%)	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	218/244 (89%)	216 (99%)	2 (1%)	75	62
1	B	221/244 (91%)	220 (100%)	1 (0%)	86	78
1	C	219/244 (90%)	217 (99%)	2 (1%)	75	62
1	D	218/244 (89%)	216 (99%)	2 (1%)	75	62
1	E	224/244 (92%)	223 (100%)	1 (0%)	89	82
1	F	106/244 (43%)	105 (99%)	1 (1%)	75	62
1	G	215/244 (88%)	212 (99%)	3 (1%)	62	43
1	H	222/244 (91%)	221 (100%)	1 (0%)	86	78
All	All	1643/1952 (84%)	1630 (99%)	13 (1%)	79	66

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	243	LYS
1	F	243	LYS

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Mol	Chain	Res	Type
1	H	243	LYS
1	G	91	LYS
1	G	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	268	GLN
1	F	235	GLN
1	H	212	GLN
1	B	8	ASN
1	A	8	ASN

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, 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	286/313 (91%)	0.71	59 (20%) 3 2	7, 18, 36, 45	1 (0%)
1	B	289/313 (92%)	0.61	44 (15%) 6 5	7, 18, 35, 44	0
1	C	287/313 (91%)	0.66	49 (17%) 5 4	7, 18, 39, 49	0
1	D	286/313 (91%)	0.36	22 (7%) 21 20	7, 17, 34, 42	0
1	E	292/313 (93%)	-0.00	9 (3%) 51 52	7, 15, 27, 43	2 (0%)
1	F	135/313 (43%)	-0.09	7 (5%) 34 33	8, 12, 25, 47	0
1	G	282/313 (90%)	1.06	94 (33%) 1 1	7, 20, 45, 50	0
1	H	290/313 (92%)	0.10	14 (4%) 36 36	7, 15, 27, 44	1 (0%)
All	All	2147/2504 (85%)	0.46	298 (13%) 7 6	7, 16, 37, 50	4 (0%)

The worst 5 of 298 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	VAL	8.7
1	F	161	LEU	8.4
1	G	50	PRO	5.6
1	D	3	ILE	5.4
1	G	57	ALA	5.4

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.