wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 05:07 PM EDT

PDB ID	:	3CKY
Title	:	Structural and Kinetic Properties of a beta-hydroxyacid dehydrogenase involved in nicotinate fermentation
Authors	:	Reitz, S.; Alhapel, A.; Pierik, A.J.; Essen, L.-O.
Deposited on	:	2008-03-18
Resolution	:	2.30 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:

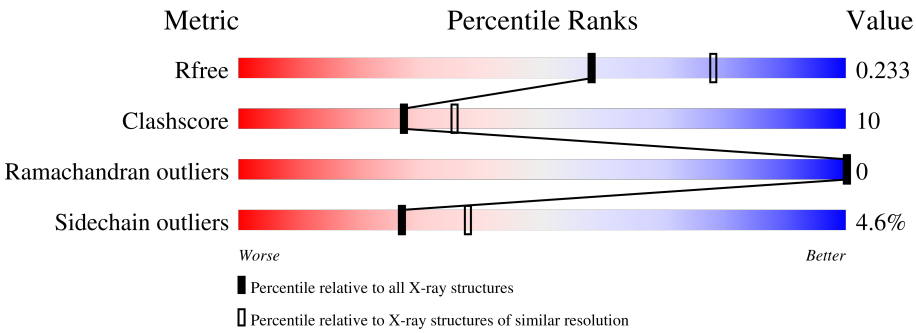
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Mol	Chain	Length	Quality of chain
1	A	301	82% 14% • •
1	B	301	85% 12% • •
1	C	301	82% 15% • •
1	D	301	67% 11% • 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8515 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 2-hydroxymethyl glutarate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2117	1333	349	412	23	3	1	0
1	B	296	2113	1331	348	411	23	6	1	0
1	C	296	2111	1330	348	410	23	14	1	0
1	D	240	1727	1089	282	338	18	0	2	0

- Molecule 2 is water.

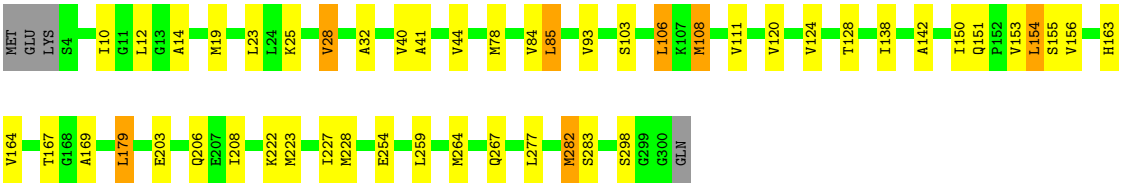
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	123	123	123	0	0
2	B	158	158	158	0	0
2	C	96	96	96	0	0
2	D	70	70	70	0	0

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. 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. 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.

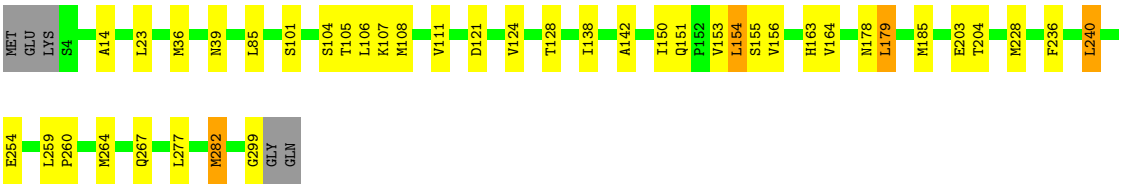
• Molecule 1: 2-hydroxymethyl glutarate dehydrogenase

Chain A:



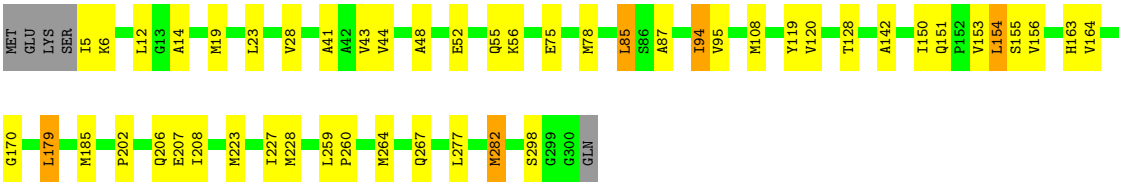
• Molecule 1: 2-hydroxymethyl glutarate dehydrogenase

Chain B:



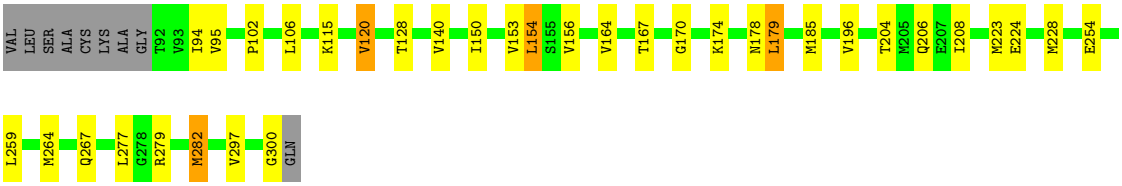
• Molecule 1: 2-hydroxymethyl glutarate dehydrogenase

Chain C:



• Molecule 1: 2-hydroxymethyl glutarate dehydrogenase

Chain D:


VAL
LEU
SER
ALA
CYS
LYS
ALA
GLY
T92
V93
I94
V95
P102
L106
K115
V120
T128
V140
I150
V153
L154
S155
V156
V164
T167
G170
K174
N178
L179
M185
V196
T204
M205
Q206
E207
I208
M223
E224
M228
E254
L259
M264
Q267
L277
G278
R279
M282
V297
G300
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.98Å 175.78Å 83.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.47 – 2.30 24.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (24.47-2.30) 95.2 (24.47-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.222 0.203 , 0.233	Depositor DCC
R_{free} test set	2674 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8515	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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)

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	0.45	0/2144	0.53	1/2888 (0.0%)
1	B	0.51	0/2140	0.57	1/2883 (0.0%)
1	C	0.45	0/2138	0.54	1/2880 (0.0%)
1	D	0.45	0/1751	0.54	1/2354 (0.0%)
All	All	0.47	0/8173	0.54	4/11005 (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	B	179	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	179	LEU	CA-CB-CG	5.76	128.56	115.30
1	D	179	LEU	CA-CB-CG	5.67	128.35	115.30
1	C	179	LEU	CA-CB-CG	5.33	127.56	115.30

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	2117	0	2174	60	0
1	B	2113	0	2171	46	0
1	C	2111	0	2169	55	0
1	D	1727	0	1772	43	0
2	A	123	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	158	0	0	3	0
2	C	96	0	0	0	0
2	D	70	0	0	2	0
All	All	8515	0	8286	165	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 10.

The worst 5 of 165 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:264[A]:MET:CE	1:B:264[A]:MET:HE3	1.45	1.46
1:C:264[B]:MET:HE1	1:D:264[B]:MET:SD	1.83	1.16
1:C:264[B]:MET:CE	1:D:264[B]:MET:HE1	1.76	1.14
1:A:264[A]:MET:SD	1:B:264[A]:MET:HE3	1.89	1.13
1:C:264[B]:MET:HE2	1:D:264[B]:MET:CE	1.81	1.10

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	296/301 (98%)	294 (99%)	2 (1%)	0	100	100
1	B	295/301 (98%)	293 (99%)	2 (1%)	0	100	100
1	C	295/301 (98%)	290 (98%)	5 (2%)	0	100	100
1	D	236/301 (78%)	230 (98%)	6 (2%)	0	100	100
All	All	1122/1204 (93%)	1107 (99%)	15 (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	221/224 (99%)	212 (96%)	9 (4%)	30	43
1	B	221/224 (99%)	212 (96%)	9 (4%)	30	43
1	C	220/224 (98%)	206 (94%)	14 (6%)	17	23
1	D	183/224 (82%)	176 (96%)	7 (4%)	33	47
All	All	845/896 (94%)	806 (95%)	39 (5%)	27	38

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	179	LEU
1	D	179	LEU
1	C	207	GLU
1	D	115	LYS
1	D	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	79	ASN
1	C	256	ASN
1	C	163	HIS
1	C	267	GLN
1	A	267	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.