



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:26 PM GMT

PDB ID : 1EAA
Title : ATOMIC STRUCTURE OF THE CUBIC CORE OF THE PYRUVATE DE-
HYDROGENASE MULTIENZYME COMPLEX
Authors : Mattevi, A.; Hol, W.G.J.
Deposited on : 1992-12-16
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

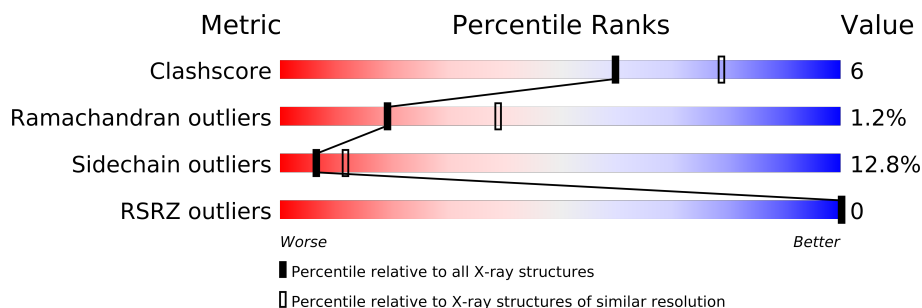
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.60 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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	243	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1849 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DIHYDROLIPOYL-TRANSACETYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1812	1168	310	327	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	LYS	GLU	CONFLICT	UNP P10802

^ Molecule 2 is water.

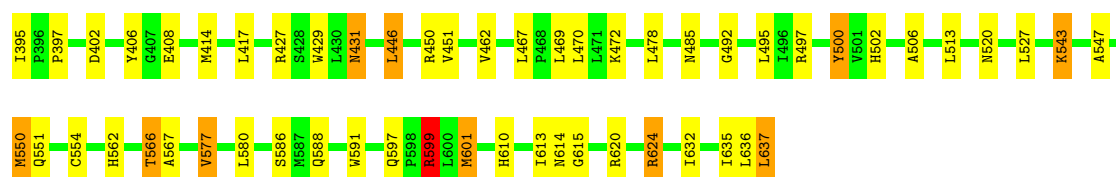
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DIHYDROLIPOYL-TRANSACETYLASE

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.77 Å 224.77 Å 224.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 11.02 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 71.8 (11.02-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.01 (at 2.65 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 10391 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1849	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.94	0/1849	1.58	19/2519 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	620	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	A	624	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	591	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	637	LEU	CA-CB-CG	8.47	134.78	115.30
1	A	497	ARG	CA-CB-CG	-7.66	96.56	113.40
1	A	599	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	A	429	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	591	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	A	601	MET	CG-SD-CE	-6.98	89.03	100.20
1	A	500	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	A	495	LEU	CB-CG-CD2	-6.47	100.01	111.00
1	A	577	VAL	N-CA-CB	-6.38	97.46	111.50
1	A	406	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	A	591	TRP	CG-CD1-NE1	-6.00	104.09	110.10
1	A	429	TRP	CE2-CD2-CG	-5.92	102.56	107.30
1	A	566	THR	N-CA-CB	-5.58	99.70	110.30
1	A	637	LEU	CB-CG-CD1	-5.54	101.57	111.00
1	A	446	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	429	TRP	CG-CD1-NE1	-5.25	104.85	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	500	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1812	0	1855	22	2
2	A	37	0	0	2	0
All	All	1849	0	1855	22	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (22) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:586:SER:HB2	1:A:588:GLN:HE21	1.59	0.66
1:A:506:ALA:HB1	1:A:513:LEU:HD11	1.86	0.57
1:A:450:ARG:HG3	1:A:469:LEU:HD11	1.88	0.56
1:A:502:HIS:HD2	1:A:520:ASN:H	1.53	0.55
1:A:599:ARG:HB2	1:A:601:MET:HE3	1.90	0.54
1:A:462:VAL:HG21	1:A:527:LEU:HD22	1.93	0.51
1:A:502:HIS:CD2	1:A:520:ASN:H	2.30	0.48
1:A:562:HIS:CD2	1:A:562:HIS:H	2.32	0.47
1:A:547:ALA:HA	1:A:550:MET:HE2	1.98	0.46
1:A:614:ASN:HB3	2:A:650:HOH:O	2.16	0.45
1:A:599:ARG:CB	1:A:601:MET:HE3	2.47	0.45
1:A:462:VAL:CG2	1:A:527:LEU:HD22	2.47	0.44
1:A:632:ILE:O	1:A:635:ILE:HB	2.19	0.43
1:A:485:ASN:OD1	1:A:554:CYS:HB3	2.19	0.42
1:A:624:ARG:HD2	1:A:624:ARG:HA	1.81	0.42
1:A:599:ARG:HA	1:A:599:ARG:HD2	1.94	0.42
1:A:450:ARG:HG3	1:A:469:LEU:CD1	2.49	0.41
1:A:427:ARG:O	1:A:431:ASN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:550:MET:HE2	1:A:550:MET:HB2	1.89	0.40
1:A:635:ILE:HG21	1:A:635:ILE:HD13	1.79	0.40
1:A:632:ILE:CD1	1:A:635:ILE:HD12	2.51	0.40
1:A:615:GLY:HA3	2:A:663:HOH:O	2.20	0.40

All (2) 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	Distance(Å)	Clash(Å)
1:A:402:ASP:OD1	1:A:402:ASP:OD1[28_555]	0.50	1.70
1:A:402:ASP:CG	1:A:402:ASP:OD1[28_555]	1.65	0.55

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	241/243 (99%)	228 (95%)	10 (4%)	3 (1%)	19	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	LYS
1	A	567	ALA
1	A	492	GLY

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	187/195 (96%)	163 (87%)	24 (13%)	6	12

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	ILE
1	A	397	PRO
1	A	408	GLU
1	A	414	MET
1	A	417	LEU
1	A	431	ASN
1	A	446	LEU
1	A	451	VAL
1	A	467	LEU
1	A	470	LEU
1	A	472	LYS
1	A	478	LEU
1	A	543	LYS
1	A	550	MET
1	A	551	GLN
1	A	566	THR
1	A	577	VAL
1	A	580	LEU
1	A	597	GLN
1	A	599	ARG
1	A	610	HIS
1	A	613	ILE
1	A	636	LEU
1	A	637	LEU

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

Mol	Chain	Res	Type
1	A	502	HIS
1	A	588	GLN

5.3.3 RNA

There are no RNA chains 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, 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	243/243 (100%)	-1.18	0 100 100	2, 17, 52, 67	0

There are no RSRZ outliers to report.

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

There are no such residues in this entry.