wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:49 PM GMT

PDB ID	:	1QS0
Title	:	Crystal Structure of Pseudomonas Putida 2-oxoisovalerate Dehydrogenase (Branched-Chain Alpha-Keto Acid Dehydrogenase, E1B)
Authors	:	Aevarsson, A.; Seger, K.; Turley, S.; Sokatch, J.R.; Hol, W.G.J.
Deposited on	:	1999-06-24
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

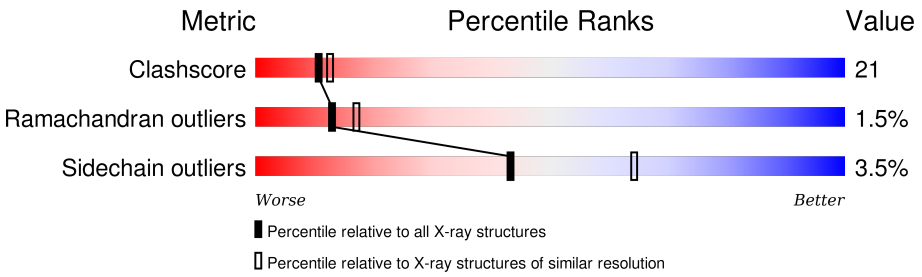
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	407	71% 27% •
2	B	338	56% 42% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5999 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-OXOISOVALERATE DEHYDROGENASE ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	407	3165	1983	568	598	4	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	84	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	94	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	103	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	107	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	128	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	140	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	149	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	169	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	196	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	389	MSE	MET	MODIFIED RESIDUE	UNP P09060
A	397	MSE	MET	MODIFIED RESIDUE	UNP P09060

- Molecule 2 is a protein called 2-OXOISOVALERATE DEHYDROGENASE BETA-SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	338	2602	1652	441	492	7	10	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	8	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	16	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	19	MSE	MET	MODIFIED RESIDUE	UNP P09061

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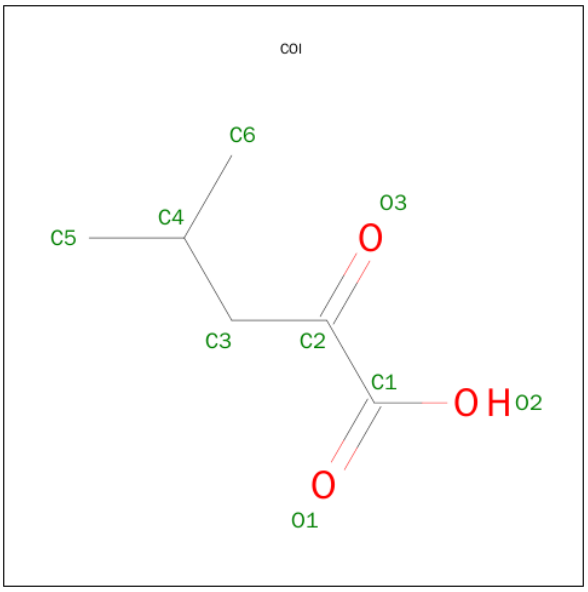
Chain	Residue	Modelled	Actual	Comment	Reference
B	72	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	100	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	119	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	138	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	149	MSE	MET	MODIFIED RESIDUE	UNP P09061
B	337	MSE	MET	MODIFIED RESIDUE	UNP P09061

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

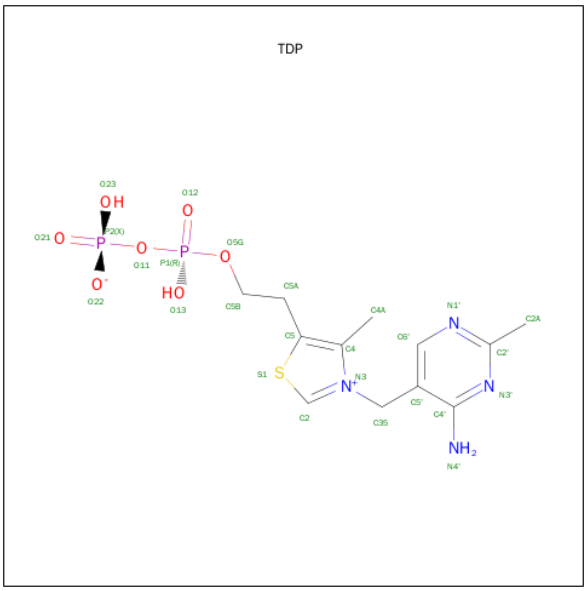
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is 2-OXO-4-METHYLPENTANOIC ACID (three-letter code: COI) (formula: $C_6H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 8 6 2	0	0

- Molecule 5 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: $C_{12}H_{18}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	26	12	4	7	2	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	129	129	129	0	0
			Total	O		
6	B	68	68	68	0	0

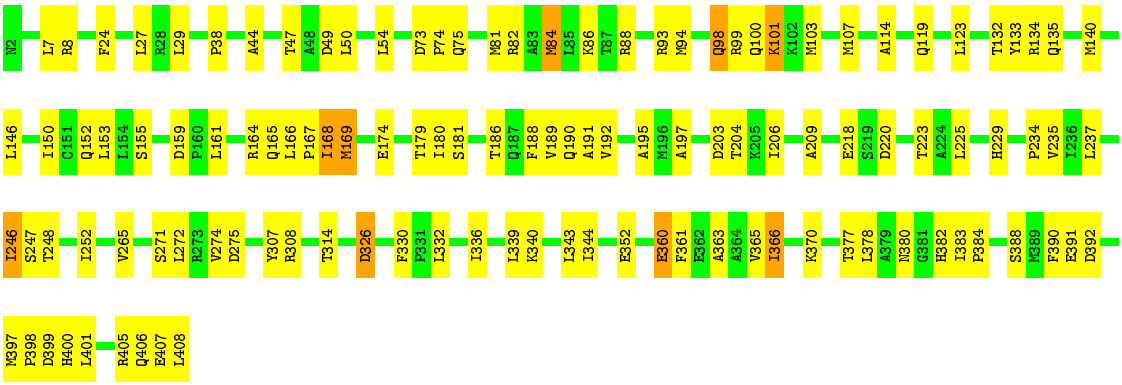
3 Residue-property plots (i)

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

Note EDS was not executed.

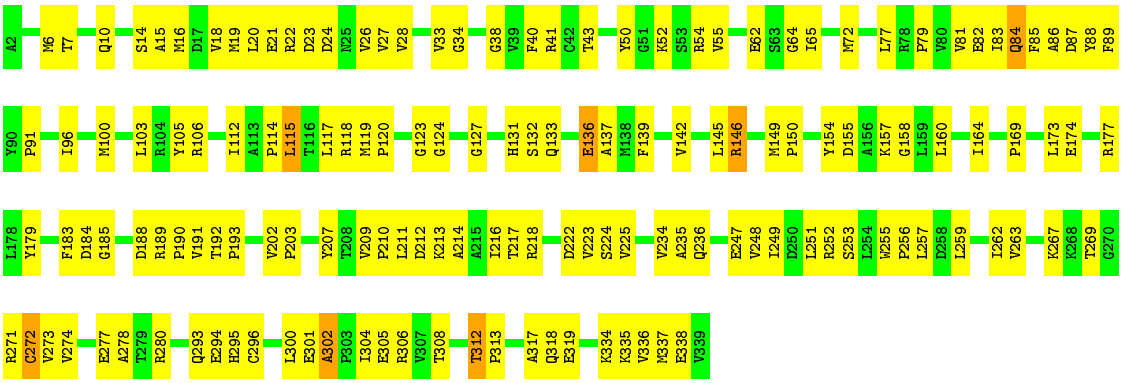
- Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA-SUBUNIT

Chain A:



- Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA-SUBUNIT

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	101.34Å 101.34Å 381.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.9 (40.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.218 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5999	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

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: COI, MG, TDP

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	0.42	1/3225 (0.0%)	0.60	0/4355
2	B	0.42	0/2660	0.59	0/3608
All	All	0.42	1/5885 (0.0%)	0.59	0/7963

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	MSE	CG-SE	-5.56	1.76	1.95

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	3165	0	3075	103	1
2	B	2602	0	2532	141	0
3	A	1	0	0	0	0
4	B	8	0	9	2	0
5	A	26	0	16	1	0
6	A	129	0	0	10	0
6	B	68	0	0	12	0
All	All	5999	0	5632	242	1

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 21.

The worst 5 of 242 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)
5:A:500:TDP:C2	5:A:500:TDP:H2	0.97	1.47
1:A:377:THR:HG22	1:A:378:LEU:H	1.24	1.01
2:B:280:ARG:HG2	2:B:308:THR:OG1	1.66	0.96
1:A:165:GLN:HG2	1:A:169:MSE:HB3	1.55	0.88
1:A:47:THR:HG21	1:A:271:SER:H	1.36	0.88

All (1) 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)
1:A:360:GLU:OE2	1:A:360:GLU:OE2[7_545]	1.68	0.52

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	405/407 (100%)	371 (92%)	29 (7%)	5 (1%)	16 23
2	B	336/338 (99%)	297 (88%)	33 (10%)	6 (2%)	11 13
All	All	741/745 (100%)	668 (90%)	62 (8%)	11 (2%)	13 17

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ILE
1	A	101	LYS
1	A	246	ILE
2	B	84	GLN

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Mol	Chain	Res	Type
2	B	214	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	326/314 (104%)	314 (96%)	12 (4%)	41	62
2	B	279/269 (104%)	270 (97%)	9 (3%)	46	68
All	All	605/583 (104%)	584 (96%)	21 (4%)	43	64

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	ASP
1	A	366	ILE
2	B	257	LEU
1	A	272	LEU
2	B	272	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	229	HIS
2	B	293	GLN
1	A	165	GLN
2	B	236	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TDP	A	500	3	21,27,27	1.39	3 (14%)	31,40,40	1.45	6 (19%)
4	COI	B	502	2	4,7,8	0.19	0	5,8,10	1.85	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TDP	A	500	3	-	0/16/17/17	0/2/2/2
4	COI	B	502	2	-	0/3/5/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	TDP	C2'-N1'	2.89	1.39	1.34
5	A	500	TDP	C35-N3	2.91	1.54	1.48
5	A	500	TDP	C4'-N3'	3.00	1.39	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	500	TDP	N1'-C2'-N3'	-2.37	121.21	125.60
5	A	500	TDP	C4A-C4-C5	-2.15	124.07	128.90
5	A	500	TDP	C5'-C35-N3	-2.12	109.78	113.33
5	A	500	TDP	P1-O5G-C5B	2.33	134.78	121.50
4	B	502	COI	C3-C2-C1	2.58	123.53	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	TDP	1	0
4	B	502	COI	2	0

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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.