



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 09:54 AM UTC

PDB ID : 2BP7 / pdb_00002bp7
Title : New crystal form of the Pseudomonas putida branched-chain dehydrogenase (E1)
Authors : Frank, R.A.W.; Pratap, J.V.; Pei, X.Y.; Perham, R.N.; Luisi, B.F.
Deposited on : 2005-04-18
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

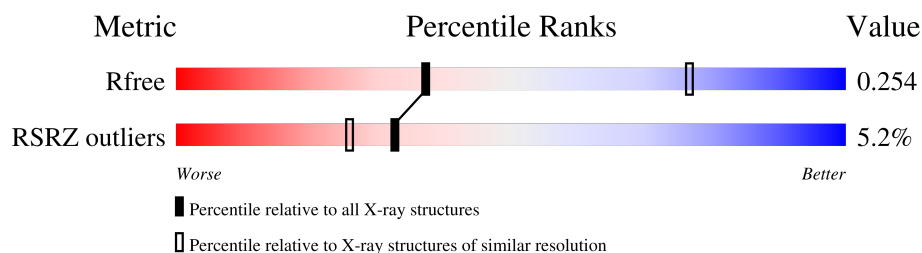
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23118 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 SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3153	1983	568	598	4			
1	C	407	Total	C	N	O	S	0	0	0
			3153	1983	568	598	4			
1	E	407	Total	C	N	O	S	0	0	0
			3153	1983	568	598	4			
1	G	407	Total	C	N	O	S	0	0	0
			3153	1983	568	598	4			

- Molecule 2 is a protein called 2-OXOISOVALERATE DEHYDROGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	338	Total	C	N	O	S	0	0	0
			2592	1652	441	492	7			
2	D	338	Total	C	N	O	S	0	0	0
			2592	1652	441	492	7			
2	F	338	Total	C	N	O	S	0	0	0
			2592	1652	441	492	7			
2	H	338	Total	C	N	O	S	0	0	0
			2592	1652	441	492	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	13	Total	O	0	0
			13	13		
3	C	25	Total	O	0	0
			25	25		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	15	Total 15	O 15	0	0
3	E	16	Total 16	O 16	0	0
3	F	13	Total 13	O 13	0	0
3	G	22	Total 22	O 22	0	0
3	H	16	Total 16	O 16	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.87Å 156.87Å 619.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	76.5 (20.00-2.90) 76.2 (20.00-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.254 0.227 , 0.254	Depositor DCC
R_{free} test set	3870 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23118	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	407/410 (99%)	0.12	26 (6%)	25	20	15, 28, 54, 87	0
1	C	407/410 (99%)	0.09	14 (3%)	48	39	15, 28, 54, 87	0
1	E	407/410 (99%)	0.10	7 (1%)	69	61	15, 28, 54, 87	0
1	G	407/410 (99%)	0.06	20 (4%)	35	27	15, 28, 54, 87	0
2	B	338/339 (99%)	0.31	20 (5%)	28	22	19, 36, 70, 107	0
2	D	338/339 (99%)	0.20	14 (4%)	41	33	19, 36, 70, 107	0
2	F	338/339 (99%)	0.51	31 (9%)	14	12	19, 36, 70, 107	0
2	H	338/339 (99%)	0.41	22 (6%)	25	20	19, 36, 70, 107	0
All	All	2980/2996 (99%)	0.21	154 (5%)	33	26	15, 32, 64, 107	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	9.0
2	F	198	PRO	8.7
2	F	242	SER	5.8
2	F	19	MET	4.4
1	A	371	GLU	4.3
2	F	301	GLU	4.3
2	D	337	MET	4.2
1	E	378	LEU	4.2
2	H	198	PRO	4.1
1	G	377	THR	4.1
1	C	103	MET	4.1
2	F	188	ASP	4.0
2	F	243	GLY	3.9
1	C	379	ALA	3.9
2	F	41	ARG	3.8
2	B	337	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	402	ARG	3.7
2	H	242	SER	3.7
2	F	218	ARG	3.7
1	C	378	LEU	3.7
1	G	371	GLU	3.7
2	B	267	LYS	3.6
1	E	371	GLU	3.6
2	H	189	ARG	3.6
2	B	339	VAL	3.5
2	B	41	ARG	3.5
2	H	267	LYS	3.5
2	B	198	PRO	3.5
1	E	103	MET	3.4
2	F	190	PRO	3.4
1	A	377	THR	3.4
2	F	337	MET	3.4
1	G	103	MET	3.4
2	H	41	ARG	3.4
2	D	41	ARG	3.3
1	A	158	ARG	3.3
2	B	301	GLU	3.3
1	A	406	GLN	3.3
1	A	70	GLU	3.2
2	F	267	LYS	3.2
1	G	329	HIS	3.2
2	H	213	LYS	3.2
2	H	337	MET	3.2
1	C	399	ASP	3.2
1	G	158	ARG	3.2
2	F	240	GLU	3.2
1	A	381	GLY	3.1
1	A	3	GLU	3.1
2	H	19	MET	3.0
2	D	190	PRO	3.0
2	F	197	HIS	3.0
2	H	270	GLY	2.9
1	A	84	MET	2.9
2	F	338	GLU	2.9
2	F	72	MET	2.9
1	A	103	MET	2.9
1	A	389	MET	2.9
2	F	6	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	72	MET	2.9
2	B	8	MET	2.8
1	A	28	ARG	2.8
1	C	397	MET	2.8
1	A	397	MET	2.8
2	F	119	MET	2.7
1	G	406	GLN	2.7
1	G	128	MET	2.7
2	B	218	ARG	2.7
1	G	380	ASN	2.7
2	F	189	ARG	2.7
2	H	190	PRO	2.7
2	H	301	GLU	2.7
1	G	379	ALA	2.7
1	G	378	LEU	2.6
2	F	339	VAL	2.6
1	C	128	MET	2.6
2	D	6	MET	2.6
1	G	2	ASN	2.6
2	F	196	LYS	2.6
2	F	300	LEU	2.6
2	D	149	MET	2.6
1	E	397	MET	2.6
1	A	378	LEU	2.6
2	F	8	MET	2.6
1	C	8	ARG	2.5
1	G	389	MET	2.5
1	G	140	MET	2.5
2	H	218	ARG	2.5
2	H	119	MET	2.5
2	H	243	GLY	2.5
2	B	191	VAL	2.5
1	G	397	MET	2.5
2	F	2	ALA	2.5
1	A	156	ASN	2.5
2	H	6	MET	2.4
2	B	240	GLU	2.4
1	A	379	ALA	2.4
1	E	379	ALA	2.4
2	D	188	ASP	2.4
2	B	196	LYS	2.4
1	A	94	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	84	MET	2.4
2	F	149	MET	2.4
1	A	380	ASN	2.4
1	G	20	CYS	2.4
2	H	280	ARG	2.3
2	H	339	VAL	2.3
1	C	156	ASN	2.3
1	C	81	MET	2.3
2	B	213	LYS	2.3
2	B	6	MET	2.3
1	C	319	SER	2.3
2	F	327	SER	2.3
2	F	223	VAL	2.3
1	C	295	ARG	2.3
2	D	189	ARG	2.3
2	D	339	VAL	2.3
1	A	140	MET	2.2
1	G	156	ASN	2.2
1	E	21	GLN	2.2
2	F	213	LYS	2.2
1	A	366	ILE	2.2
2	D	299	HIS	2.2
2	B	265	SER	2.2
1	G	402	ARG	2.2
1	A	149	MET	2.2
2	F	138	MET	2.2
1	A	374	GLN	2.2
2	D	198	PRO	2.2
2	B	100	MET	2.2
2	D	327	SER	2.2
1	C	149	MET	2.1
2	B	119	MET	2.1
2	D	8	MET	2.1
1	E	156	ASN	2.1
1	A	128	MET	2.1
2	H	272	CYS	2.1
2	D	72	MET	2.1
2	F	221	ASN	2.1
2	H	191	VAL	2.1
2	H	188	ASP	2.1
1	C	232	ARG	2.1
1	G	169	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	72	MET	2.1
1	G	99	ARG	2.1
1	G	84	MET	2.0
2	B	197	HIS	2.0
2	H	244	VAL	2.0
2	F	305	GLU	2.0
1	A	169	MET	2.0
2	B	242	SER	2.0
1	A	99	ARG	2.0
2	D	218	ARG	2.0
2	B	215	ALA	2.0
2	F	302	ALA	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.