



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 02:08 PM UTC

PDB ID : 2V7B / pdb_00002v7b
Title : Crystal structures of a benzoate CoA ligase from Burkholderia xenovorans LB400
Authors : J Boulanger, M.; Bains, J.
Deposited on : 2007-07-27
Resolution : 1.84 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

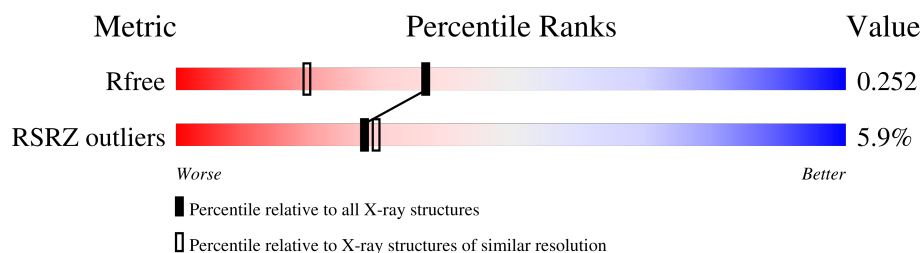
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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

2 Entry composition [i](#)

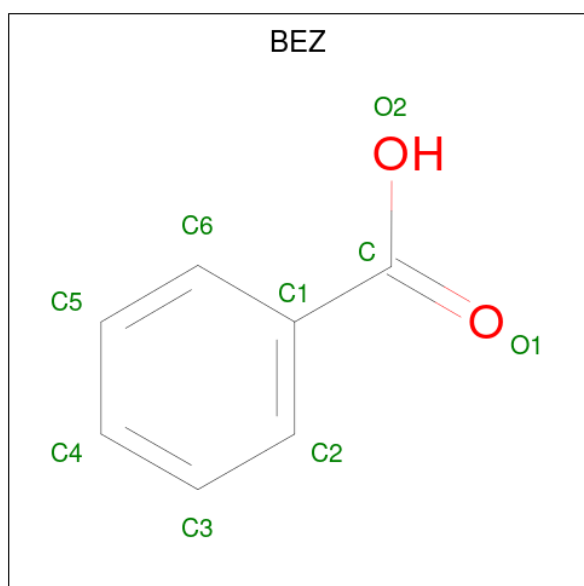
There are 3 unique types of molecules in this entry. The entry contains 8600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BENZOATE-COENZYME A LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3760	2416	641	689	14			
1	B	489	Total	C	N	O	S	0	0	0
			3760	2416	641	689	14			

- Molecule 2 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	547	Total 547	O 547	0	0
3	B	515	Total 515	O 515	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.55Å 74.55Å 89.90Å 70.06° 79.95° 81.11°	Depositor
Resolution (Å)	36.66 – 1.84 36.66 – 1.84	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.66-1.84) 92.3 (36.66-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.252 0.221 , 0.252	Depositor DCC
R_{free} test set	7152 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8600	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.85% 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](#)

MolProbity failed to run properly - this section is therefore empty.

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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	BEZ	A	1529	-	9,9,9	1.16	1 (11%)	11,11,11	1.26	1 (9%)
2	BEZ	B	1529	-	9,9,9	1.43	1 (11%)	11,11,11	1.90	4 (36%)

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
2	BEZ	A	1529	-	-	0/4/4/4	0/1/1/1
2	BEZ	B	1529	-	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1529	BEZ	C1-C	2.27	1.54	1.49
2	A	1529	BEZ	C1-C	2.09	1.53	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1529	BEZ	C5-C6-C1	-3.45	116.97	120.36
2	B	1529	BEZ	C4-C3-C2	-3.07	116.45	120.24
2	B	1529	BEZ	C4-C5-C6	2.75	123.63	120.24
2	B	1529	BEZ	C3-C2-C1	2.75	123.06	120.36
2	A	1529	BEZ	C5-C6-C1	-2.28	118.12	120.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

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	489/529 (92%)	0.37	32 (6%) 25 26	15, 23, 40, 52	0
1	B	489/529 (92%)	0.33	26 (5%) 32 34	14, 24, 42, 51	0
All	All	978/1058 (92%)	0.35	58 (5%) 28 30	14, 24, 41, 52	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	TYR	7.0
1	B	153	PRO	6.3
1	A	153	PRO	6.0
1	A	141	ALA	5.2
1	B	141	ALA	4.9
1	A	465	GLY	4.8
1	B	464	HIS	4.7
1	A	160	LEU	4.4
1	B	22	LEU	4.3
1	A	22	LEU	4.1
1	A	464	HIS	3.9
1	A	351	TYR	3.8
1	B	160	LEU	3.8
1	B	152	GLN	3.2
1	A	503	TYR	3.2
1	A	75	ARG	3.1
1	A	467	LEU	3.1
1	B	498	LEU	3.1
1	B	351	TYR	3.1
1	B	433	LYS	3.0
1	A	225	ASN	3.0
1	A	369	ALA	2.8
1	A	463	ASP	2.8
1	A	373	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	501	HIS	2.7
1	B	467	LEU	2.7
1	B	369	ALA	2.7
1	A	370	GLY	2.7
1	A	417	LEU	2.7
1	A	371	HIS	2.6
1	B	503	TYR	2.6
1	A	500	PRO	2.6
1	B	368	GLU	2.6
1	A	145	GLY	2.5
1	B	140	SER	2.5
1	B	161	ALA	2.5
1	A	152	GLN	2.5
1	B	354	THR	2.4
1	B	500	PRO	2.4
1	A	66	ARG	2.4
1	A	415	CYS	2.4
1	B	528	GLU	2.4
1	B	260	ARG	2.3
1	A	221	GLY	2.3
1	A	376	GLY	2.3
1	A	260	ARG	2.2
1	A	378	VAL	2.2
1	B	373	VAL	2.2
1	B	501	HIS	2.2
1	A	315	GLU	2.2
1	A	140	SER	2.2
1	A	506	ASP	2.2
1	B	145	GLY	2.2
1	B	376	GLY	2.2
1	A	368	GLU	2.1
1	B	508	VAL	2.1
1	B	378	VAL	2.1
1	B	484	GLU	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BEZ	A	1529	9/9	0.96	0.06	14,16,18,18	0
2	BEZ	B	1529	9/9	0.97	0.05	15,16,19,19	0

5.5 Other polymers [i](#)

There are no such residues in this entry.