



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:35 PM UTC

PDB ID : 4KUE / pdb_00004kue
Title : Crystal structure of 3-hydroxybutylryl-CoA dehydrogenase from Clostridium butyricum
Authors : Kim, E.J.; Kim, S.; Kim, K.J.
Deposited on : 2013-05-22
Resolution : 2.00 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 ⓘ 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 : 4-5-2 with Phenix2.0
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

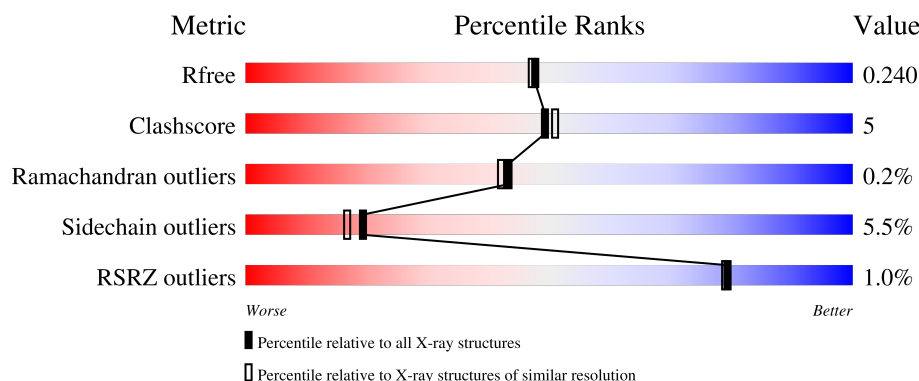
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	288	% 83% 12% ..
1	B	288	2% 74% 20% ..
1	C	288	83% 13% ..
1	D	288	84% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8855 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 3-hydroxybutyryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2114	1343	350	406	15			
1	B	280	Total	C	N	O	S	0	0	0
			2114	1343	350	406	15			
1	C	280	Total	C	N	O	S	0	0	0
			2114	1343	350	406	15			
1	D	280	Total	C	N	O	S	0	0	0
			2114	1343	350	406	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	SER	-	expression tag	UNP C4IEM5
A	282	LYS	-	expression tag	UNP C4IEM5
A	283	HIS	-	expression tag	UNP C4IEM5
A	284	HIS	-	expression tag	UNP C4IEM5
A	285	HIS	-	expression tag	UNP C4IEM5
A	286	HIS	-	expression tag	UNP C4IEM5
A	287	HIS	-	expression tag	UNP C4IEM5
A	288	HIS	-	expression tag	UNP C4IEM5
B	281	SER	-	expression tag	UNP C4IEM5
B	282	LYS	-	expression tag	UNP C4IEM5
B	283	HIS	-	expression tag	UNP C4IEM5
B	284	HIS	-	expression tag	UNP C4IEM5
B	285	HIS	-	expression tag	UNP C4IEM5
B	286	HIS	-	expression tag	UNP C4IEM5
B	287	HIS	-	expression tag	UNP C4IEM5
B	288	HIS	-	expression tag	UNP C4IEM5
C	281	SER	-	expression tag	UNP C4IEM5
C	282	LYS	-	expression tag	UNP C4IEM5
C	283	HIS	-	expression tag	UNP C4IEM5
C	284	HIS	-	expression tag	UNP C4IEM5
C	285	HIS	-	expression tag	UNP C4IEM5

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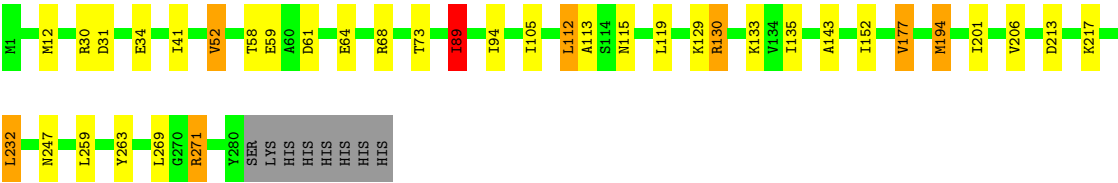
Chain	Residue	Modelled	Actual	Comment	Reference
C	286	HIS	-	expression tag	UNP C4IEM5
C	287	HIS	-	expression tag	UNP C4IEM5
C	288	HIS	-	expression tag	UNP C4IEM5
D	281	SER	-	expression tag	UNP C4IEM5
D	282	LYS	-	expression tag	UNP C4IEM5
D	283	HIS	-	expression tag	UNP C4IEM5
D	284	HIS	-	expression tag	UNP C4IEM5
D	285	HIS	-	expression tag	UNP C4IEM5
D	286	HIS	-	expression tag	UNP C4IEM5
D	287	HIS	-	expression tag	UNP C4IEM5
D	288	HIS	-	expression tag	UNP C4IEM5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	77	Total O 77 77	0	0
2	B	71	Total O 71 71	0	0
2	C	111	Total O 111 111	0	0
2	D	140	Total O 140 140	0	0

- Molecule 1: 3-hydroxybutyryl-CoA dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	144.11Å 144.11Å 205.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.87 – 2.00 29.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	80.9 (29.87-2.00) 81.0 (29.87-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.234 0.194 , 0.240	Depositor DCC
R_{free} test set	4395 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8855	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0225e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

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	1.04	2/2140 (0.1%)	1.16	5/2882 (0.2%)
1	B	1.10	5/2140 (0.2%)	1.18	5/2882 (0.2%)
1	C	1.24	6/2140 (0.3%)	1.25	10/2882 (0.3%)
1	D	1.25	0/2140	1.21	9/2882 (0.3%)
All	All	1.16	13/8560 (0.2%)	1.20	29/11528 (0.3%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	PHE	C-O	6.54	1.30	1.24
1	C	65	ILE	C-O	6.26	1.31	1.24
1	B	182	ALA	C-N	6.23	1.41	1.33
1	A	182	ALA	C-N	6.09	1.40	1.33
1	C	117	SER	C-O	-5.84	1.16	1.24

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	LEU	N-CA-C	8.51	120.88	110.41
1	C	105	ILE	N-CA-C	8.48	118.56	110.42
1	C	143	ALA	CA-C-N	-7.43	112.14	119.87
1	C	143	ALA	C-N-CA	-7.43	112.14	119.87
1	C	121	ILE	CB-CA-C	-6.62	101.90	112.16

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	2114	0	2193	24	0
1	B	2114	0	2193	38	0
1	C	2114	0	2193	16	0
1	D	2114	0	2193	26	0
2	A	77	0	0	1	0
2	B	71	0	0	3	0
2	C	111	0	0	0	0
2	D	140	0	0	2	0
All	All	8855	0	8772	93	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 5.

The worst 5 of 93 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:C:194:MET:HE2	1:D:194:MET:HE2	1.47	0.94
1:A:194:MET:HE2	1:B:194:MET:HE2	1.52	0.91
1:C:1:MET:HE3	1:C:168:MET:HB2	1.57	0.87
1:A:194:MET:HE2	1:B:194:MET:CE	2.12	0.79
1:D:58:THR:HG22	1:D:61:ASP:CG	2.11	0.74

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	278/288 (96%)	270 (97%)	7 (2%)	1 (0%)	30 27
1	B	278/288 (96%)	267 (96%)	10 (4%)	1 (0%)	30 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	278/288 (96%)	268 (96%)	10 (4%)	0	100	100
1	D	278/288 (96%)	272 (98%)	6 (2%)	0	100	100
All	All	1112/1152 (96%)	1077 (97%)	33 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	B	10	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	226/234 (97%)	212 (94%)	14 (6%)	16	13
1	B	226/234 (97%)	211 (93%)	15 (7%)	15	12
1	C	226/234 (97%)	216 (96%)	10 (4%)	25	24
1	D	226/234 (97%)	215 (95%)	11 (5%)	22	20
All	All	904/936 (97%)	854 (94%)	50 (6%)	19	17

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	262	LYS
1	C	112	LEU
1	D	269	LEU
1	C	2	LYS
1	C	56	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	141	ASN

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 oligosaccharides 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](#)

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	280/288 (97%)	0.07	4 (1%) 73 73	26, 41, 66, 75	0
1	B	280/288 (97%)	-0.01	6 (2%) 63 63	25, 39, 71, 97	0
1	C	280/288 (97%)	-0.23	1 (0%) 88 88	19, 32, 58, 73	0
1	D	280/288 (97%)	-0.40	0 100 100	18, 28, 46, 62	0
All	All	1120/1152 (97%)	-0.14	11 (0%) 79 79	18, 35, 62, 97	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	ILE	2.9
1	B	52	VAL	2.8
1	B	118	SER	2.7
1	A	104	GLY	2.7
1	C	33	LYS	2.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.