



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 04:59 AM EDT

PDB ID : 3Q0G / pdb_00003q0g
Title : Crystal Structure of the Mycobacterium tuberculosis Crotonase Bound to a Reaction Intermediate Derived from Crotonyl CoA
Authors : Bruning, J.B.; Delgado, E.; Ghosh, S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2010-12-15
Resolution : 2.38 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	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 2.38 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12127 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.

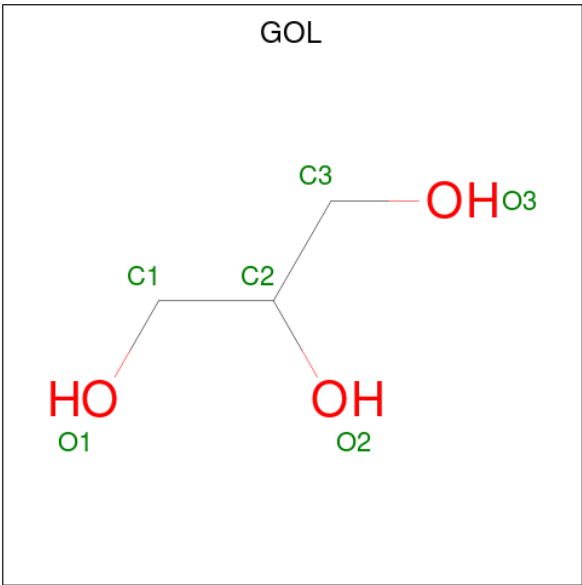
- Molecule 1 is a protein called enoyl-CoA hydratase echA8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	1	0
			1840	1147	321	361	11			
1	B	253	Total	C	N	O	S	0	0	0
			1866	1164	322	368	12			
1	C	255	Total	C	N	O	S	0	1	0
			1878	1172	324	370	12			
1	D	250	Total	C	N	O	S	0	1	0
			1831	1140	318	362	11			
1	E	253	Total	C	N	O	S	0	2	0
			1857	1158	323	364	12			
1	F	254	Total	C	N	O	S	0	3	0
			1885	1176	326	371	12			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

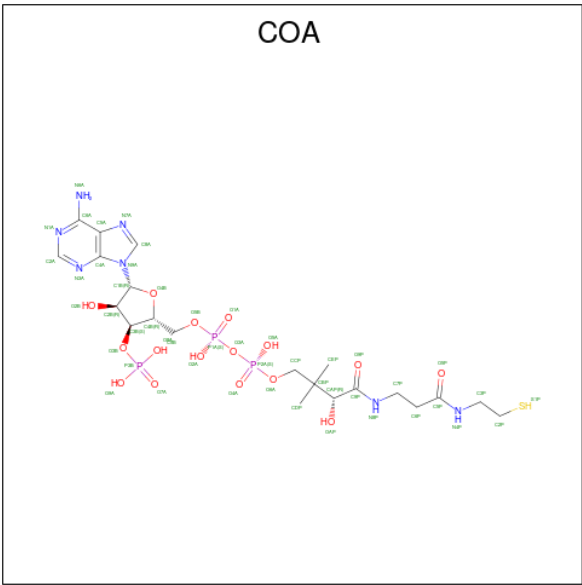
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



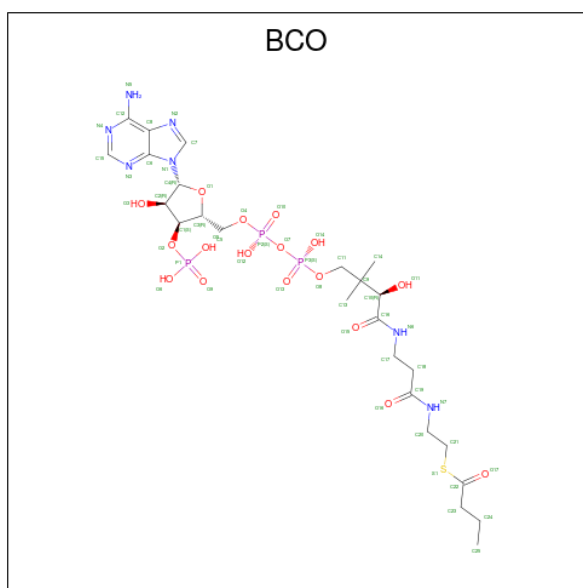
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 5 is Butyryl Coenzyme A (CCD ID: BCO) (formula: $C_{25}H_{42}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	140	Total	O	0	0
			140	140		
6	C	152	Total	O	0	0
			152	152		
6	D	141	Total	O	0	0
			141	141		
6	E	144	Total	O	0	0
			144	144		
6	F	149	Total	O	0	0
			149	149		

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

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.64Å 133.17Å 133.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.38	Depositor
% Data completeness (in resolution range)	93.0 (19.87-2.38)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.233 , 0.288	Depositor
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.133	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
Total number of atoms	12127	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 73.46 % 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 1.8312e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

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](#)

validation-pack failed to run properly - this section is therefore empty.

4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

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

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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