



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 06:07 am BST

PDB ID : 4QFE  
Title : Crystal Structure of an Enoyl-CoA hydratase from Mycobacterium smegmatis  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2014-05-20  
Resolution : 1.95 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

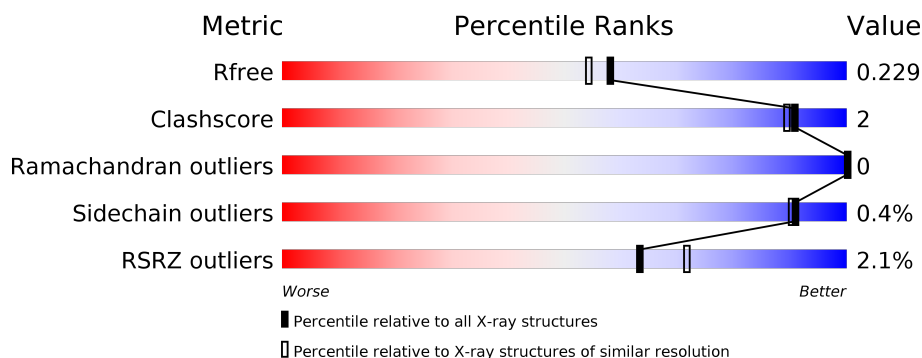
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	259	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>• • 13%</div> </div> </div>
1	B	259	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>• 12%</div> </div> </div>
1	C	259	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>• 12%</div> </div> </div>
1	D	259	<div> <div></div> <div> <div>84%</div> <div>• • 11%</div> </div> </div>
1	E	259	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>• • 13%</div> </div> </div>
1	F	259	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>• 13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	259	<div><div><div>%</div><div><div></div><div>82%</div><div><div></div><div></div><div></div></div><div>12%</div></div></div></div>
1	H	259	<div><div><div>2%</div><div><div></div><div>85%</div><div><div></div><div></div><div></div></div><div>12%</div></div></div></div>
1	I	259	<div><div><div>%</div><div><div></div><div>83%</div><div><div></div><div></div><div></div></div><div>12%</div></div></div></div>
1	J	259	<div><div><div>%</div><div><div></div><div>84%</div><div><div></div><div></div><div></div></div><div>12%</div></div></div></div>
1	K	259	<div><div><div>5%</div><div><div></div><div>85%</div><div><div></div><div></div><div></div></div><div>12%</div></div></div></div>
1	L	259	<div><div><div>7%</div><div><div></div><div>87%</div><div><div></div><div></div><div></div></div><div>12%</div></div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21505 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	2	0
			1630	1013	292	315	10			
1	B	228	Total	C	N	O	S	0	2	0
			1668	1036	304	318	10			
1	C	229	Total	C	N	O	S	0	1	0
			1655	1026	302	317	10			
1	D	230	Total	C	N	O	S	0	1	0
			1666	1034	300	322	10			
1	E	225	Total	C	N	O	S	0	2	0
			1620	1005	290	315	10			
1	F	226	Total	C	N	O	S	0	1	0
			1669	1036	305	318	10			
1	G	227	Total	C	N	O	S	0	1	0
			1659	1035	298	316	10			
1	H	227	Total	C	N	O	S	0	1	0
			1639	1020	298	311	10			
1	I	228	Total	C	N	O	S	0	2	0
			1675	1040	302	323	10			
1	J	228	Total	C	N	O	S	0	2	0
			1691	1056	306	319	10			
1	K	229	Total	C	N	O	S	0	1	0
			1668	1036	300	322	10			
1	L	229	Total	C	N	O	S	0	0	0
			1626	1014	296	306	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
A	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
A	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
A	-1	SER	-	EXPRESSION TAG	UNP A0QS88
A	0	MET	-	EXPRESSION TAG	UNP A0QS88

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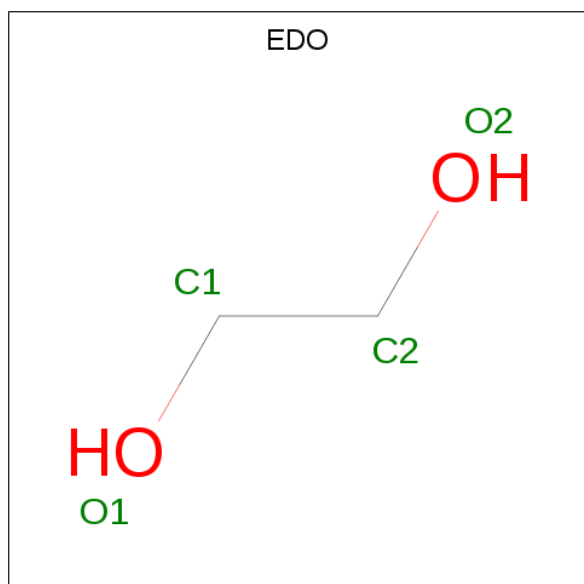
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	EXPRESSION TAG	UNP A0QS88
B	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
B	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
B	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
B	-1	SER	-	EXPRESSION TAG	UNP A0QS88
B	0	MET	-	EXPRESSION TAG	UNP A0QS88
B	1	VAL	-	EXPRESSION TAG	UNP A0QS88
C	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
C	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
C	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
C	-1	SER	-	EXPRESSION TAG	UNP A0QS88
C	0	MET	-	EXPRESSION TAG	UNP A0QS88
C	1	VAL	-	EXPRESSION TAG	UNP A0QS88
D	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
D	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
D	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
D	-1	SER	-	EXPRESSION TAG	UNP A0QS88
D	0	MET	-	EXPRESSION TAG	UNP A0QS88
D	1	VAL	-	EXPRESSION TAG	UNP A0QS88
E	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
E	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
E	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
E	-1	SER	-	EXPRESSION TAG	UNP A0QS88
E	0	MET	-	EXPRESSION TAG	UNP A0QS88
E	1	VAL	-	EXPRESSION TAG	UNP A0QS88
F	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
F	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
F	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
F	-1	SER	-	EXPRESSION TAG	UNP A0QS88
F	0	MET	-	EXPRESSION TAG	UNP A0QS88
F	1	VAL	-	EXPRESSION TAG	UNP A0QS88
G	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
G	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
G	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
G	-1	SER	-	EXPRESSION TAG	UNP A0QS88
G	0	MET	-	EXPRESSION TAG	UNP A0QS88
G	1	VAL	-	EXPRESSION TAG	UNP A0QS88
H	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
H	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
H	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
H	-1	SER	-	EXPRESSION TAG	UNP A0QS88
H	0	MET	-	EXPRESSION TAG	UNP A0QS88

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1	VAL	-	EXPRESSION TAG	UNP A0QS88
I	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
I	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
I	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
I	-1	SER	-	EXPRESSION TAG	UNP A0QS88
I	0	MET	-	EXPRESSION TAG	UNP A0QS88
I	1	VAL	-	EXPRESSION TAG	UNP A0QS88
J	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
J	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
J	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
J	-1	SER	-	EXPRESSION TAG	UNP A0QS88
J	0	MET	-	EXPRESSION TAG	UNP A0QS88
J	1	VAL	-	EXPRESSION TAG	UNP A0QS88
K	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
K	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
K	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
K	-1	SER	-	EXPRESSION TAG	UNP A0QS88
K	0	MET	-	EXPRESSION TAG	UNP A0QS88
K	1	VAL	-	EXPRESSION TAG	UNP A0QS88
L	-4	GLY	-	EXPRESSION TAG	UNP A0QS88
L	-3	PRO	-	EXPRESSION TAG	UNP A0QS88
L	-2	GLY	-	EXPRESSION TAG	UNP A0QS88
L	-1	SER	-	EXPRESSION TAG	UNP A0QS88
L	0	MET	-	EXPRESSION TAG	UNP A0QS88
L	1	VAL	-	EXPRESSION TAG	UNP A0QS88

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	E	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	J	1	Total 4	C 2	O 2	0	0

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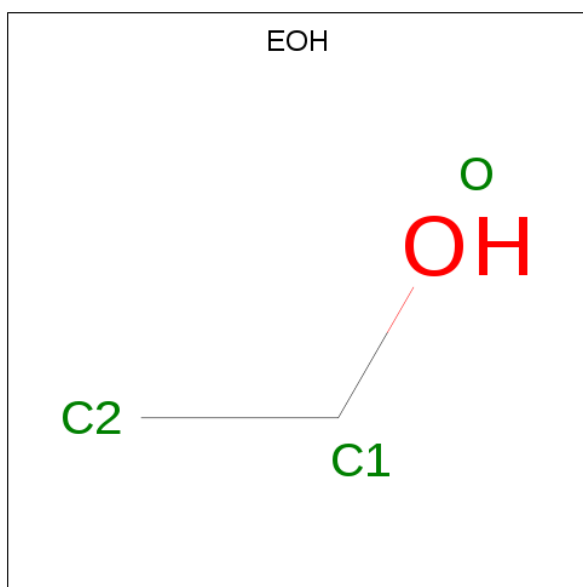
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	J	1	Total Na 1 1	0	0

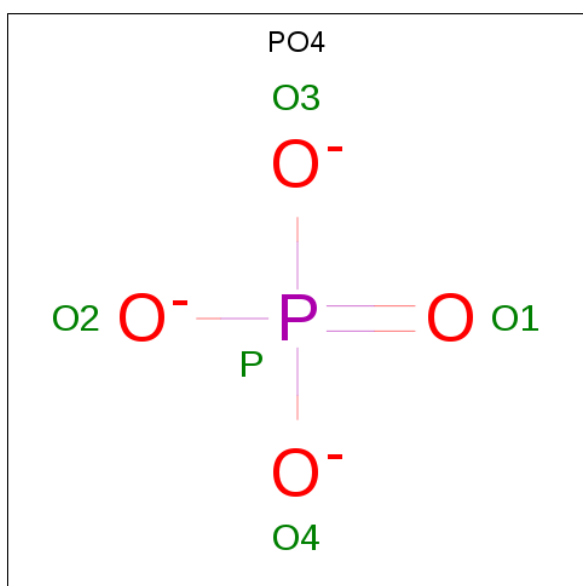
- Molecule 4 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	2	1		
4	I	1	Total	C	O	0	0
			3	2	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		

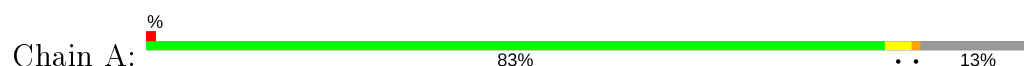
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	155	Total	O		0	0
			155	155			
6	B	119	Total	O		0	1
			120	120			
6	C	139	Total	O		0	1
			140	140			
6	D	137	Total	O		0	1
			138	138			
6	E	141	Total	O		0	0
			141	141			
6	F	108	Total	O		0	1
			109	109			
6	G	122	Total	O		0	0
			122	122			
6	H	85	Total	O		0	0
			85	85			
6	I	132	Total	O		0	2
			134	134			
6	J	146	Total	O		0	0
			146	146			
6	K	110	Total	O		0	0
			110	110			
6	L	81	Total	O		0	0
			81	81			

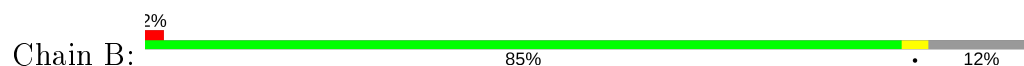
### 3 Residue-property plots [i](#)

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

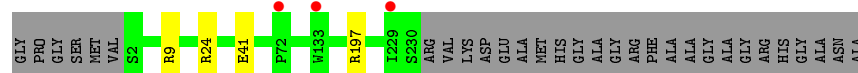
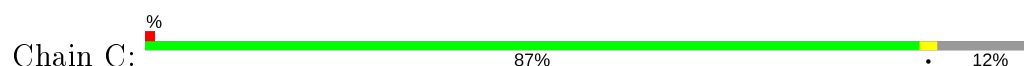
- Molecule 1: Enoyl-CoA hydratase



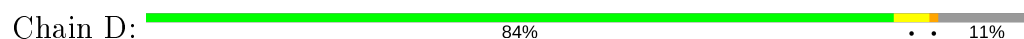
- Molecule 1: Enoyl-CoA hydratase



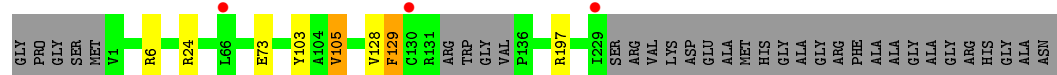
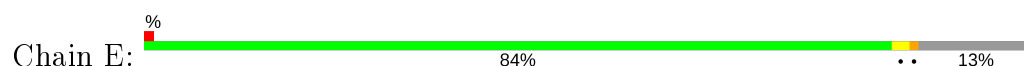
- Molecule 1: Enoyl-CoA hydratase



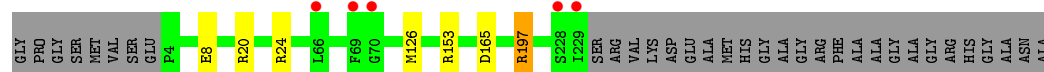
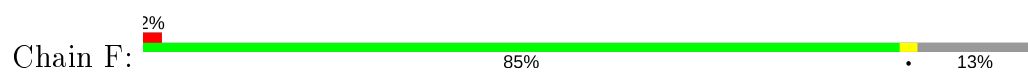
- Molecule 1: Enoyl-CoA hydratase



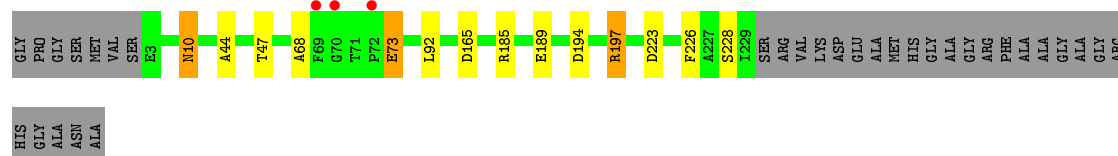
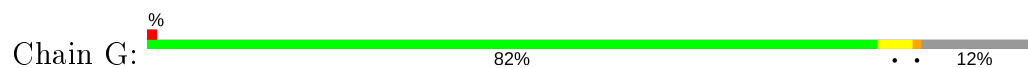
- Molecule 1: Enoyl-CoA hydratase



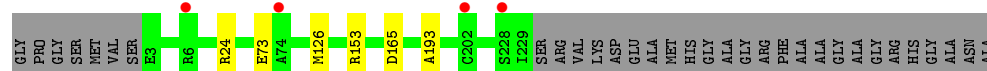
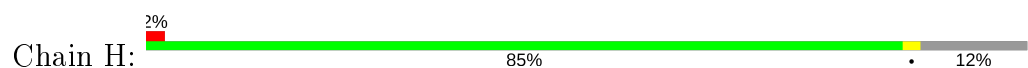
- Molecule 1: Enoyl-CoA hydratase



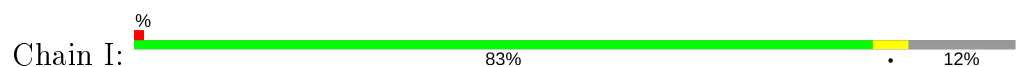
- Molecule 1: Enoyl-CoA hydratase



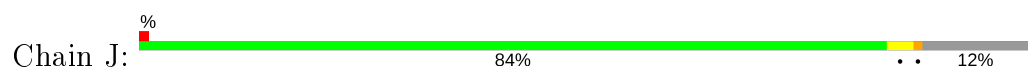
- Molecule 1: Enoyl-CoA hydratase



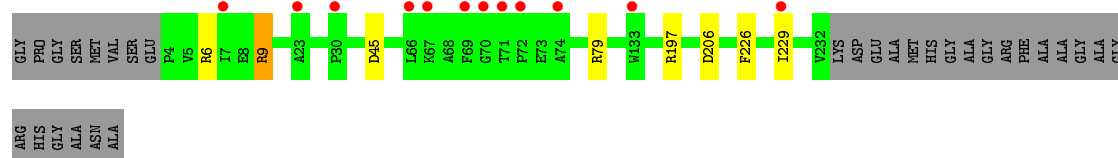
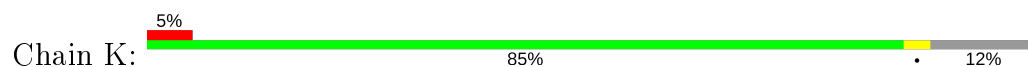
- Molecule 1: Enoyl-CoA hydratase



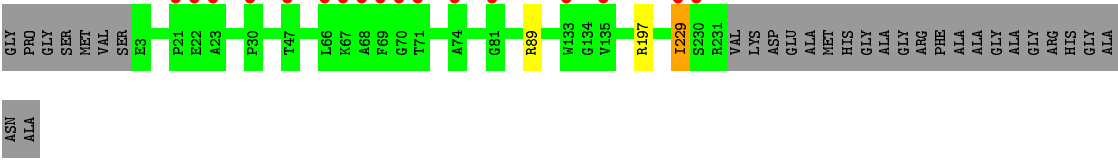
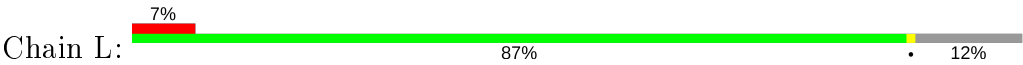
- Molecule 1: Enoyl-CoA hydratase



- Molecule 1: Enoyl-CoA hydratase



- Molecule 1: Enoyl-CoA hydratase



ASN  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.29 Å   86.58 Å   106.16 Å 84.96°   73.62°   83.18°	Depositor
Resolution (Å)	46.32 – 1.95 46.32 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.2 (46.32-1.95) 96.3 (46.32-1.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.197   ,   0.223 0.204   ,   0.229	Depositor DCC
$R_{free}$ test set	9247 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, EOH, EDO

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	0.67	1/1663 (0.1%)	0.84	5/2265 (0.2%)
1	B	0.57	0/1704	0.79	3/2322 (0.1%)
1	C	0.59	0/1686	0.83	8/2298 (0.3%)
1	D	0.67	1/1698 (0.1%)	0.81	4/2315 (0.2%)
1	E	0.68	1/1653 (0.1%)	0.92	8/2253 (0.4%)
1	F	0.59	0/1699	0.90	12/2313 (0.5%)
1	G	0.56	0/1693	0.82	4/2307 (0.2%)
1	H	0.52	0/1672	0.76	4/2280 (0.2%)
1	I	0.60	0/1711	0.82	4/2331 (0.2%)
1	J	0.64	0/1731	0.84	5/2357 (0.2%)
1	K	0.56	0/1701	0.83	9/2318 (0.4%)
1	L	0.55	1/1656 (0.1%)	0.91	4/2262 (0.2%)
All	All	0.60	4/20267 (0.0%)	0.84	70/27621 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	197	ARG	CZ-NH1	-5.62	1.25	1.33
1	A	129	PHE	N-CA	5.59	1.57	1.46
1	E	129	PHE	N-CA	5.20	1.56	1.46
1	D	216	GLU	CG-CD	-5.01	1.44	1.51

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	197	ARG	NE-CZ-NH1	-18.38	111.11	120.30
1	L	197	ARG	NE-CZ-NH2	17.56	129.08	120.30
1	B	197	ARG	NE-CZ-NH1	12.61	126.60	120.30
1	G	197	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	J	197	ARG	NE-CZ-NH1	12.37	126.48	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1630	0	1584	7	0
1	B	1668	0	1620	5	0
1	C	1655	0	1600	1	0
1	D	1666	0	1607	10	0
1	E	1620	0	1552	2	0
1	F	1669	0	1632	3	0
1	G	1659	0	1611	14	0
1	H	1639	0	1580	5	0
1	I	1675	0	1625	15	0
1	J	1691	0	1669	11	0
1	K	1668	0	1611	3	0
1	L	1626	0	1558	1	0
2	A	16	0	24	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
2	F	8	0	12	0	0
2	G	12	0	18	2	0
2	I	24	0	36	2	0
2	J	24	0	36	4	0
2	K	12	0	18	0	0
2	L	8	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
4	B	3	0	6	0	0
4	I	3	0	6	0	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	155	0	0	1	0
6	B	120	0	0	1	0
6	C	140	0	0	0	0
6	D	138	0	0	1	0
6	E	141	0	0	0	0
6	F	109	0	0	0	0
6	G	122	0	0	1	0
6	H	85	0	0	3	0
6	I	134	0	0	7	0
6	J	146	0	0	4	0
6	K	110	0	0	0	0
6	L	81	0	0	0	0
All	All	21505	0	19453	68	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 2.

The worst 5 of 68 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:I:9:ARG:NH2	6:I:487:HOH:O	1.90	1.02
1:H:153[A]:ARG:HH11	1:H:153[A]:ARG:HG2	1.39	0.85
1:I:73:GLU:HB3	6:I:450:HOH:O	1.79	0.82
1:I:137:LEU:O	1:I:138[A]:ILE:HD13	1.83	0.78
1:J:76:GLN:NE2	6:J:521:HOH:O	2.27	0.68

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	223/259 (86%)	217 (97%)	6 (3%)	0	100	100
1	B	228/259 (88%)	220 (96%)	8 (4%)	0	100	100
1	C	228/259 (88%)	222 (97%)	6 (3%)	0	100	100
1	D	229/259 (88%)	221 (96%)	8 (4%)	0	100	100
1	E	223/259 (86%)	217 (97%)	6 (3%)	0	100	100
1	F	225/259 (87%)	218 (97%)	7 (3%)	0	100	100
1	G	226/259 (87%)	220 (97%)	6 (3%)	0	100	100
1	H	226/259 (87%)	220 (97%)	6 (3%)	0	100	100
1	I	228/259 (88%)	223 (98%)	5 (2%)	0	100	100
1	J	229/259 (88%)	224 (98%)	5 (2%)	0	100	100
1	K	228/259 (88%)	222 (97%)	6 (3%)	0	100	100
1	L	227/259 (88%)	222 (98%)	5 (2%)	0	100	100
All	All	2720/3108 (88%)	2646 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	159/185 (86%)	156 (98%)	3 (2%)	57	50
1	B	162/185 (88%)	162 (100%)	0	100	100
1	C	159/185 (86%)	159 (100%)	0	100	100
1	D	161/185 (87%)	160 (99%)	1 (1%)	86	85
1	E	155/185 (84%)	155 (100%)	0	100	100
1	F	164/185 (89%)	164 (100%)	0	100	100
1	G	161/185 (87%)	159 (99%)	2 (1%)	71	68
1	H	156/185 (84%)	156 (100%)	0	100	100
1	I	164/185 (89%)	163 (99%)	1 (1%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	168/185 (91%)	167 (99%)	1 (1%)	86	85
1	K	162/185 (88%)	162 (100%)	0	100	100
1	L	152/185 (82%)	151 (99%)	1 (1%)	84	82
All	All	1923/2220 (87%)	1914 (100%)	9 (0%)	91	88

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	10	ASN
1	L	229	ILE
1	I	79	ARG
1	A	10[B]	ASN
1	G	73	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	B	201	GLN
1	C	201	GLN
1	G	10	ASN
1	J	10	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 42 ligands modelled in this entry, 4 are monoatomic - leaving 38 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	$\# Z  > 2$
2	EDO	J	306	-	3,3,3	0.53	0	2,2,2	0.35	0
2	EDO	A	301	-	3,3,3	0.66	0	2,2,2	0.13	0
5	PO4	B	304	-	4,4,4	0.72	0	6,6,6	0.97	0
2	EDO	F	301	-	3,3,3	0.55	0	2,2,2	0.82	0
2	EDO	F	302	-	3,3,3	0.44	0	2,2,2	0.67	0
5	PO4	H	301	-	4,4,4	0.77	0	6,6,6	0.45	0
2	EDO	A	302	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	E	301	-	3,3,3	0.50	0	2,2,2	0.18	0
2	EDO	I	306	-	3,3,3	0.51	0	2,2,2	0.48	0
2	EDO	C	301	-	3,3,3	0.47	0	2,2,2	0.09	0
2	EDO	A	304	-	3,3,3	0.22	0	2,2,2	0.48	0
2	EDO	K	301	-	3,3,3	0.58	0	2,2,2	0.10	0
5	PO4	D	301	-	4,4,4	0.68	0	6,6,6	0.92	0
5	PO4	G	305	-	4,4,4	0.75	0	6,6,6	0.80	0
2	EDO	K	303	-	3,3,3	0.43	0	2,2,2	0.42	0
2	EDO	B	303	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	J	302	-	3,3,3	0.44	0	2,2,2	0.45	0
2	EDO	I	302	-	3,3,3	0.52	0	2,2,2	0.31	0
2	EDO	J	303	-	3,3,3	0.62	0	2,2,2	0.16	0
2	EDO	A	303	-	3,3,3	0.40	0	2,2,2	0.24	0
2	EDO	G	302	-	3,3,3	0.61	0	2,2,2	0.27	0
2	EDO	I	307	-	3,3,3	0.32	0	2,2,2	0.49	0
2	EDO	C	302	-	3,3,3	0.45	0	2,2,2	0.54	0
2	EDO	J	305	-	3,3,3	0.64	0	2,2,2	0.35	0
2	EDO	I	303	-	3,3,3	0.49	0	2,2,2	0.35	0
2	EDO	J	301	-	3,3,3	0.35	0	2,2,2	0.45	0
2	EDO	G	301	-	3,3,3	0.62	0	2,2,2	0.18	0
4	EOH	B	301	-	2,2,2	0.46	0	1,1,1	0.61	0
2	EDO	I	305	-	3,3,3	0.48	0	2,2,2	0.46	0
2	EDO	I	304	-	3,3,3	0.42	0	2,2,2	0.78	0
2	EDO	J	304	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	G	303	-	3,3,3	0.27	0	2,2,2	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	L	301	-	3,3,3	0.31	0	2,2,2	0.63	0
4	EOH	I	301	-	2,2,2	0.40	0	1,1,1	0.13	0
2	EDO	D	302	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	B	302	-	3,3,3	0.60	0	2,2,2	0.06	0
2	EDO	L	302	-	3,3,3	0.35	0	2,2,2	0.26	0
2	EDO	K	302	-	3,3,3	0.37	0	2,2,2	0.86	0

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	EDO	J	306	-	-	0/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	F	301	-	-	1/1/1/1	-
2	EDO	F	302	-	-	0/1/1/1	-
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	E	301	-	-	0/1/1/1	-
2	EDO	I	306	-	-	0/1/1/1	-
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	A	304	-	-	1/1/1/1	-
2	EDO	K	301	-	-	1/1/1/1	-
2	EDO	K	303	-	-	0/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	J	302	-	-	1/1/1/1	-
2	EDO	I	302	-	-	0/1/1/1	-
2	EDO	J	303	-	-	0/1/1/1	-
2	EDO	A	303	-	-	0/1/1/1	-
2	EDO	G	302	-	-	1/1/1/1	-
2	EDO	I	307	-	-	1/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
2	EDO	J	305	-	-	0/1/1/1	-
2	EDO	I	303	-	-	0/1/1/1	-
2	EDO	J	301	-	-	1/1/1/1	-
2	EDO	G	301	-	-	1/1/1/1	-
2	EDO	I	305	-	-	0/1/1/1	-
2	EDO	I	304	-	-	1/1/1/1	-
2	EDO	J	304	-	-	0/1/1/1	-
2	EDO	G	303	-	-	0/1/1/1	-
2	EDO	L	301	-	-	1/1/1/1	-
2	EDO	D	302	-	-	1/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	L	302	-	-	0/1/1/1	-
2	EDO	K	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	EDO	O1-C1-C2-O2
2	A	302	EDO	O1-C1-C2-O2
2	G	302	EDO	O1-C1-C2-O2
2	J	301	EDO	O1-C1-C2-O2
2	A	304	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	306	EDO	1	0
2	I	307	EDO	2	0
2	J	305	EDO	2	0
2	J	301	EDO	1	0
2	G	301	EDO	1	0
2	G	303	EDO	1	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 ⓘ

### 6.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	225/259 (86%)	0.03	2 (0%) 84 89	11, 18, 38, 49	0
1	B	228/259 (88%)	0.04	4 (1%) 68 76	12, 22, 38, 48	0
1	C	229/259 (88%)	-0.03	3 (1%) 77 83	13, 22, 40, 50	0
1	D	230/259 (88%)	-0.08	1 (0%) 92 95	12, 19, 36, 46	0
1	E	225/259 (86%)	0.01	3 (1%) 77 83	12, 19, 37, 55	0
1	F	226/259 (87%)	0.13	5 (2%) 62 70	12, 23, 41, 46	0
1	G	227/259 (87%)	0.01	3 (1%) 77 83	14, 22, 41, 56	0
1	H	227/259 (87%)	0.24	4 (1%) 68 76	13, 27, 44, 56	0
1	I	228/259 (88%)	-0.01	2 (0%) 84 89	14, 22, 42, 53	0
1	J	228/259 (88%)	-0.16	2 (0%) 84 89	11, 18, 33, 68	0
1	K	229/259 (88%)	0.33	12 (5%) 27 37	14, 27, 51, 65	0
1	L	229/259 (88%)	0.41	17 (7%) 14 22	13, 30, 58, 70	0
All	All	2731/3108 (87%)	0.08	58 (2%) 63 72	11, 22, 44, 70	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	66	LEU	5.3
1	L	74	ALA	4.8
1	K	70	GLY	4.4
1	L	66	LEU	4.4
1	D	70	GLY	4.3

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	EDO	F	301	4/4	0.71	0.17	43,45,46,48	0
2	EDO	K	301	4/4	0.74	0.23	53,54,54,54	0
2	EDO	I	304	4/4	0.74	0.14	43,46,47,50	0
2	EDO	I	302	4/4	0.76	0.24	53,53,55,57	0
5	PO4	H	301	5/5	0.76	0.26	63,68,71,75	0
4	EOH	I	301	3/3	0.77	0.18	40,40,42,42	0
2	EDO	A	301	4/4	0.79	0.19	39,39,42,45	0
2	EDO	D	302	4/4	0.82	0.17	45,46,48,48	0
2	EDO	J	306	4/4	0.83	0.18	36,36,39,40	0
2	EDO	A	302	4/4	0.83	0.16	41,43,45,45	0
4	EOH	B	301	3/3	0.84	0.21	25,25,28,28	0
2	EDO	A	304	4/4	0.84	0.18	31,35,35,40	0
2	EDO	G	302	4/4	0.84	0.15	43,44,44,47	0
2	EDO	J	305	4/4	0.84	0.16	33,34,34,36	0
2	EDO	I	307	4/4	0.85	0.25	37,41,41,41	0
5	PO4	G	305	5/5	0.85	0.21	75,76,83,83	0
2	EDO	I	306	4/4	0.86	0.14	27,27,29,30	0
2	EDO	C	301	4/4	0.87	0.14	41,41,42,45	0
2	EDO	G	301	4/4	0.88	0.17	35,35,36,38	0
2	EDO	J	303	4/4	0.89	0.13	33,33,33,34	0
5	PO4	D	301	5/5	0.90	0.24	42,43,52,52	0
2	EDO	C	302	4/4	0.90	0.19	31,33,34,37	0
5	PO4	B	304	5/5	0.90	0.23	55,56,60,62	0
2	EDO	K	303	4/4	0.90	0.19	39,40,40,42	0
2	EDO	F	302	4/4	0.91	0.11	26,29,31,35	0
2	EDO	B	302	4/4	0.91	0.14	34,38,39,41	0
2	EDO	L	302	4/4	0.91	0.14	23,24,25,26	0
2	EDO	L	301	4/4	0.92	0.11	27,28,28,30	0
3	NA	B	305	1/1	0.93	0.17	26,26,26,26	0
2	EDO	I	303	4/4	0.94	0.11	20,21,22,23	0
2	EDO	J	304	4/4	0.94	0.14	23,23,23,26	0
2	EDO	J	301	4/4	0.95	0.10	25,27,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	J	302	4/4	0.95	0.11	18,18,19,19	0
2	EDO	B	303	4/4	0.95	0.09	22,22,22,24	0
2	EDO	G	303	4/4	0.95	0.13	21,21,23,23	0
2	EDO	K	302	4/4	0.95	0.13	20,22,24,24	0
2	EDO	E	301	4/4	0.96	0.08	21,21,22,22	0
2	EDO	I	305	4/4	0.96	0.15	25,28,28,30	0
2	EDO	A	303	4/4	0.97	0.08	16,17,17,18	0
3	NA	A	305	1/1	0.98	0.13	18,18,18,18	0
3	NA	G	304	1/1	0.98	0.12	23,23,23,23	0
3	NA	J	307	1/1	0.99	0.03	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.