



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 06:44 AM GMT

PDB ID : 2VX2  
Title : CRYSTAL STRUCTURE OF HUMAN ENOYL COENZYME A HYDRATASE DOMAIN-CONTAINING PROTEIN 3 (ECHDC3)  
Authors : Yue, W.W.; Guo, K.; Kochan, G.; Pilka, E.; Murray, J.W.; Salah, E.; Cocking, R.; Sun, Z.; Roos, A.K.; Pike, A.C.W.; Filippakopoulos, P.; Arrowsmith, C.; Wikstrom, M.; Edwards, A.; Bountra, C.; Oppermann, U.  
Deposited on : 2008-06-30  
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
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A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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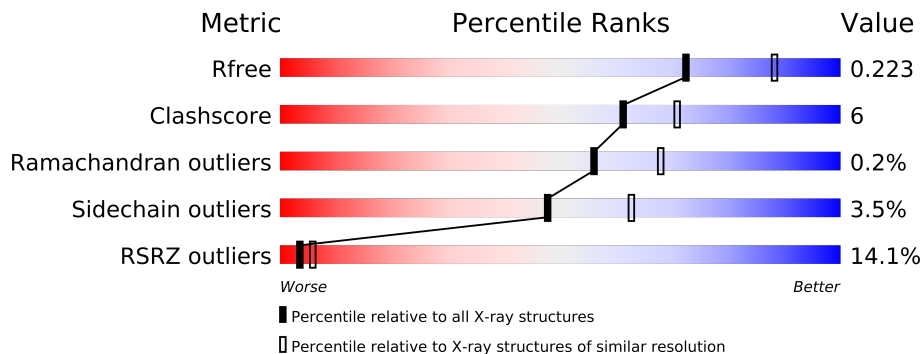
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	287	
1	B	287	
1	C	287	
1	D	287	
1	E	287	
1	F	287	
1	G	287	
1	H	287	
1	I	287	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17539 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DOMAIN-CONTAINING PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	2	0
			1951	1228	345	367	11			
1	B	255	Total	C	N	O	S	0	1	0
			1904	1200	329	364	11			
1	C	256	Total	C	N	O	S	0	0	0
			1932	1215	341	365	11			
1	D	256	Total	C	N	O	S	0	1	0
			1936	1217	343	365	11			
1	E	255	Total	C	N	O	S	0	0	0
			1901	1199	329	362	11			
1	F	254	Total	C	N	O	S	0	0	0
			1879	1184	326	358	11			
1	G	253	Total	C	N	O	S	0	1	0
			1795	1129	313	342	11			
1	H	254	Total	C	N	O	S	0	1	0
			1850	1165	324	350	11			
1	I	254	Total	C	N	O	S	0	0	0
			1818	1144	315	348	11			

There are 225 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	EXPRESSION TAG	UNP Q96DC8
A	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
A	21	SER	-	EXPRESSION TAG	UNP Q96DC8
A	22	SER	-	EXPRESSION TAG	UNP Q96DC8
A	23	GLY	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
A	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
A	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
A	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
A	28	THR	-	EXPRESSION TAG	UNP Q96DC8
A	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
A	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
A	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
A	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
A	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
A	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
A	35	SER	-	EXPRESSION TAG	UNP Q96DC8
A	36	MET	-	EXPRESSION TAG	UNP Q96DC8
A	69	THR	ALA	CONFLICT	UNP Q96DC8
A	151	THR	ALA	CONFLICT	UNP Q96DC8
B	14	MET	-	EXPRESSION TAG	UNP Q96DC8
B	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
B	21	SER	-	EXPRESSION TAG	UNP Q96DC8
B	22	SER	-	EXPRESSION TAG	UNP Q96DC8
B	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
B	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
B	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
B	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
B	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
B	28	THR	-	EXPRESSION TAG	UNP Q96DC8
B	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
B	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
B	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
B	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
B	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
B	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
B	35	SER	-	EXPRESSION TAG	UNP Q96DC8
B	36	MET	-	EXPRESSION TAG	UNP Q96DC8
B	69	THR	ALA	CONFLICT	UNP Q96DC8
B	151	THR	ALA	CONFLICT	UNP Q96DC8
C	14	MET	-	EXPRESSION TAG	UNP Q96DC8
C	15	HIS	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
C	21	SER	-	EXPRESSION TAG	UNP Q96DC8
C	22	SER	-	EXPRESSION TAG	UNP Q96DC8
C	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
C	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
C	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
C	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
C	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
C	28	THR	-	EXPRESSION TAG	UNP Q96DC8
C	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
C	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
C	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
C	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
C	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
C	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
C	35	SER	-	EXPRESSION TAG	UNP Q96DC8
C	36	MET	-	EXPRESSION TAG	UNP Q96DC8
C	69	THR	ALA	CONFLICT	UNP Q96DC8
C	151	THR	ALA	CONFLICT	UNP Q96DC8
D	14	MET	-	EXPRESSION TAG	UNP Q96DC8
D	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
D	21	SER	-	EXPRESSION TAG	UNP Q96DC8
D	22	SER	-	EXPRESSION TAG	UNP Q96DC8
D	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
D	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
D	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
D	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
D	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
D	28	THR	-	EXPRESSION TAG	UNP Q96DC8
D	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
D	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
D	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
D	32	TYR	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
D	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
D	35	SER	-	EXPRESSION TAG	UNP Q96DC8
D	36	MET	-	EXPRESSION TAG	UNP Q96DC8
D	69	THR	ALA	CONFLICT	UNP Q96DC8
D	151	THR	ALA	CONFLICT	UNP Q96DC8
E	14	MET	-	EXPRESSION TAG	UNP Q96DC8
E	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
E	21	SER	-	EXPRESSION TAG	UNP Q96DC8
E	22	SER	-	EXPRESSION TAG	UNP Q96DC8
E	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
E	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
E	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
E	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
E	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
E	28	THR	-	EXPRESSION TAG	UNP Q96DC8
E	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
E	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
E	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
E	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
E	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
E	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
E	35	SER	-	EXPRESSION TAG	UNP Q96DC8
E	36	MET	-	EXPRESSION TAG	UNP Q96DC8
E	69	THR	ALA	CONFLICT	UNP Q96DC8
E	151	THR	ALA	CONFLICT	UNP Q96DC8
F	14	MET	-	EXPRESSION TAG	UNP Q96DC8
F	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
F	21	SER	-	EXPRESSION TAG	UNP Q96DC8
F	22	SER	-	EXPRESSION TAG	UNP Q96DC8
F	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
F	24	VAL	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
F	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
F	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
F	28	THR	-	EXPRESSION TAG	UNP Q96DC8
F	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
F	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
F	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
F	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
F	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
F	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
F	35	SER	-	EXPRESSION TAG	UNP Q96DC8
F	36	MET	-	EXPRESSION TAG	UNP Q96DC8
F	69	THR	ALA	CONFLICT	UNP Q96DC8
F	151	THR	ALA	CONFLICT	UNP Q96DC8
G	14	MET	-	EXPRESSION TAG	UNP Q96DC8
G	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
G	21	SER	-	EXPRESSION TAG	UNP Q96DC8
G	22	SER	-	EXPRESSION TAG	UNP Q96DC8
G	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
G	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
G	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
G	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
G	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
G	28	THR	-	EXPRESSION TAG	UNP Q96DC8
G	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
G	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
G	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
G	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
G	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
G	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
G	35	SER	-	EXPRESSION TAG	UNP Q96DC8
G	36	MET	-	EXPRESSION TAG	UNP Q96DC8
G	69	THR	ALA	CONFLICT	UNP Q96DC8
G	151	THR	ALA	CONFLICT	UNP Q96DC8
H	14	MET	-	EXPRESSION TAG	UNP Q96DC8
H	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	16	HIS	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
H	21	SER	-	EXPRESSION TAG	UNP Q96DC8
H	22	SER	-	EXPRESSION TAG	UNP Q96DC8
H	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
H	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
H	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
H	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
H	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
H	28	THR	-	EXPRESSION TAG	UNP Q96DC8
H	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
H	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
H	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
H	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
H	33	PHE	-	EXPRESSION TAG	UNP Q96DC8
H	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
H	35	SER	-	EXPRESSION TAG	UNP Q96DC8
H	36	MET	-	EXPRESSION TAG	UNP Q96DC8
H	69	THR	ALA	CONFLICT	UNP Q96DC8
H	151	THR	ALA	CONFLICT	UNP Q96DC8
I	14	MET	-	EXPRESSION TAG	UNP Q96DC8
I	15	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	16	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	17	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	18	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	19	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	20	HIS	-	EXPRESSION TAG	UNP Q96DC8
I	21	SER	-	EXPRESSION TAG	UNP Q96DC8
I	22	SER	-	EXPRESSION TAG	UNP Q96DC8
I	23	GLY	-	EXPRESSION TAG	UNP Q96DC8
I	24	VAL	-	EXPRESSION TAG	UNP Q96DC8
I	25	ASP	-	EXPRESSION TAG	UNP Q96DC8
I	26	LEU	-	EXPRESSION TAG	UNP Q96DC8
I	27	GLY	-	EXPRESSION TAG	UNP Q96DC8
I	28	THR	-	EXPRESSION TAG	UNP Q96DC8
I	29	GLU	-	EXPRESSION TAG	UNP Q96DC8
I	30	ASN	-	EXPRESSION TAG	UNP Q96DC8
I	31	LEU	-	EXPRESSION TAG	UNP Q96DC8
I	32	TYR	-	EXPRESSION TAG	UNP Q96DC8
I	33	PHE	-	EXPRESSION TAG	UNP Q96DC8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	34	GLN	-	EXPRESSION TAG	UNP Q96DC8
I	35	SER	-	EXPRESSION TAG	UNP Q96DC8
I	36	MET	-	EXPRESSION TAG	UNP Q96DC8
I	69	THR	ALA	CONFLICT	UNP Q96DC8
I	151	THR	ALA	CONFLICT	UNP Q96DC8

- Molecule 2 is water.

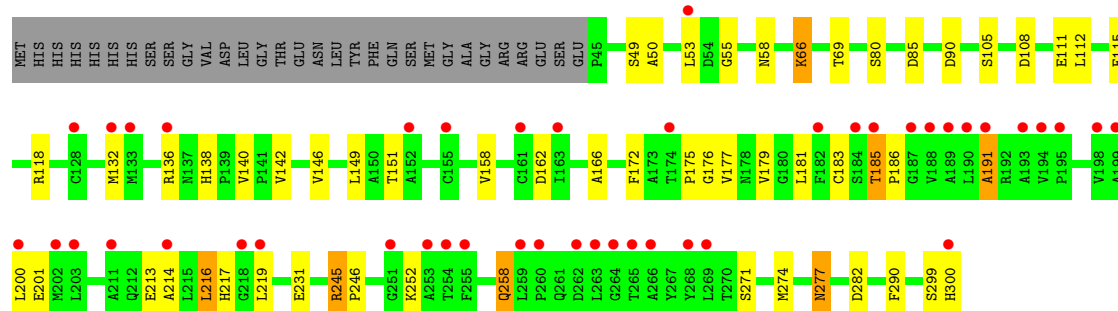
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	148	Total O 148 148	0	0
2	B	61	Total O 61 61	0	0
2	C	124	Total O 124 124	0	0
2	D	80	Total O 80 80	0	0
2	E	67	Total O 67 67	0	0
2	F	55	Total O 55 55	0	0
2	G	13	Total O 13 13	0	0
2	H	13	Total O 13 13	0	0
2	I	12	Total O 12 12	0	0

### 3 Residue-property plots

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

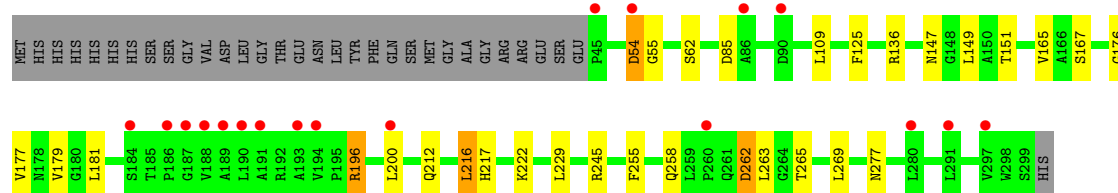
#### • Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain A: 



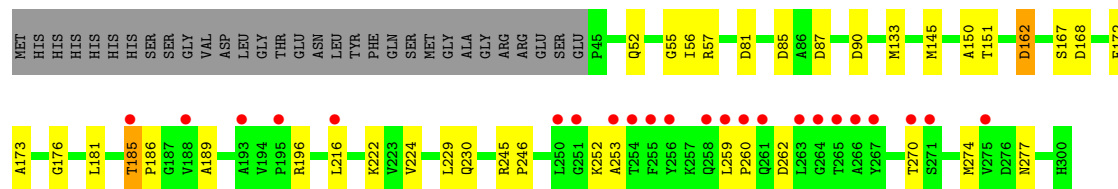
#### • Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain B: 



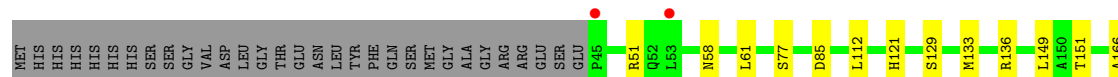
#### • Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

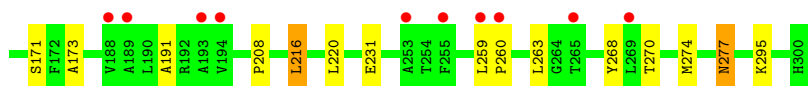
Chain C: 



#### • Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

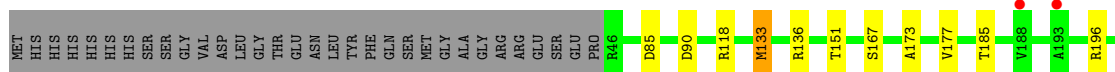
Chain D: 





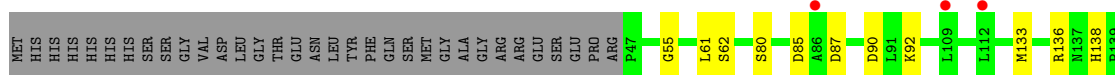
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain E:



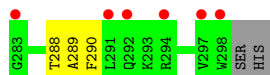
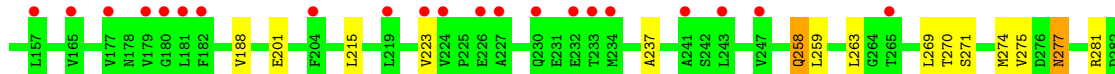
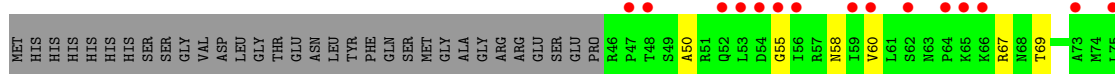
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain F:



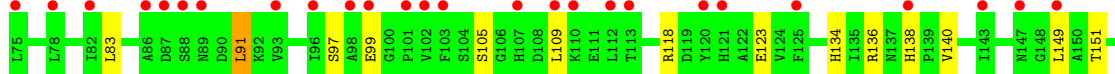
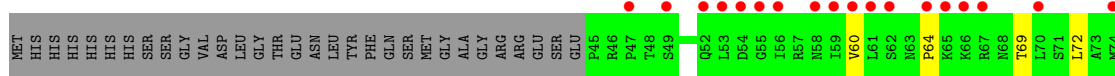
• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

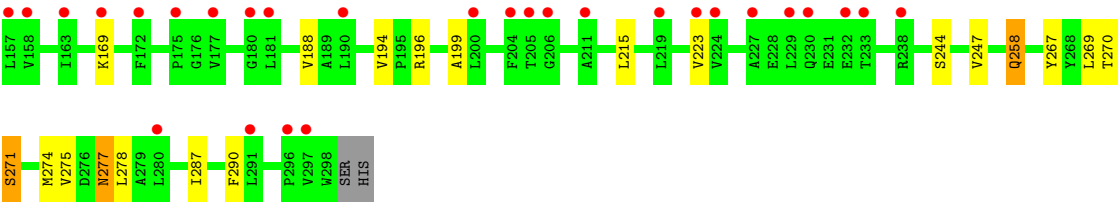
Chain G:



• Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

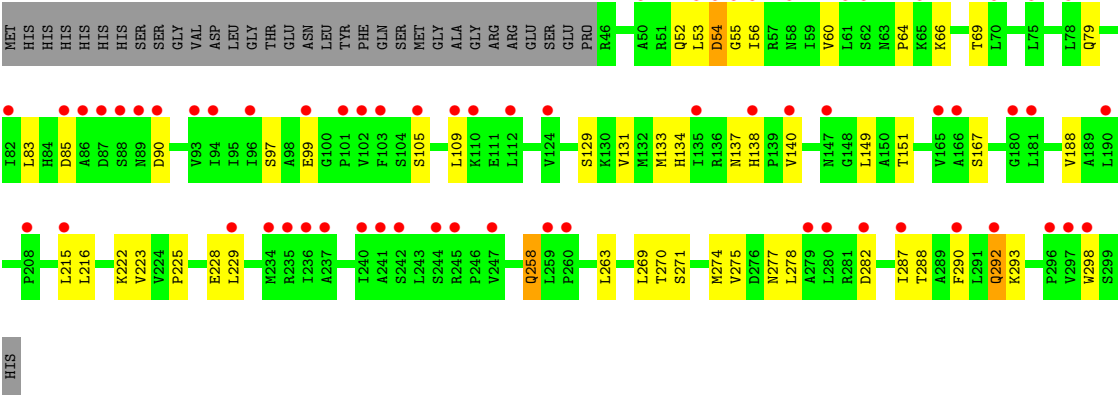
Chain H:





● Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain I:



HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.76Å 135.30Å 83.87Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	117.04 – 2.30 52.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (117.04-2.30) 99.4 (52.41-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.170 , 0.220 0.176 , 0.223	Depositor DCC
$R_{free}$ test set	5767 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 8.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 114561 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1.31	11/1985 (0.6%)	1.07	8/2688 (0.3%)
1	B	0.90	0/1939	0.86	2/2634 (0.1%)
1	C	1.09	3/1964 (0.2%)	0.97	5/2664 (0.2%)
1	D	0.93	1/1971 (0.1%)	0.85	1/2674 (0.0%)
1	E	0.89	0/1933	0.86	3/2626 (0.1%)
1	F	0.84	1/1911 (0.1%)	0.82	1/2599 (0.0%)
1	G	0.62	0/1828	0.61	0/2499
1	H	0.65	0/1884	0.63	1/2566 (0.0%)
1	I	0.62	0/1849	0.62	0/2523
All	All	0.90	16/17264 (0.1%)	0.83	21/23473 (0.1%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ALA	CA-CB	8.88	1.71	1.52
1	A	158	VAL	CB-CG1	-7.10	1.38	1.52
1	D	231	GLU	CG-CD	6.87	1.62	1.51
1	A	179	VAL	CB-CG1	6.82	1.67	1.52
1	A	115	GLU	CD-OE1	6.49	1.32	1.25

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	118	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	245	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	53	LEU	CB-CG-CD2	-6.36	100.18	111.00
1	A	274	MET	CG-SD-CE	6.06	109.89	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1951	0	1997	30	0
1	B	1904	0	1918	25	0
1	C	1932	0	1961	26	0
1	D	1936	0	1963	15	0
1	E	1901	0	1905	13	0
1	F	1879	0	1873	34	0
1	G	1795	0	1715	28	0
1	H	1850	0	1815	22	0
1	I	1818	0	1750	29	0
2	A	148	0	0	1	0
2	B	61	0	0	1	0
2	C	124	0	0	0	0
2	D	80	0	0	0	0
2	E	67	0	0	0	0
2	F	55	0	0	1	0
2	G	13	0	0	3	0
2	H	13	0	0	0	0
2	I	12	0	0	1	0
All	All	17539	0	16897	196	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 196 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69[A]:THR:HG22	1:A:105:SER:OG	1.57	1.03
1:A:111:GLU:CA	1:A:112:LEU:N	2.22	1.02
1:A:111:GLU:O	1:A:112:LEU:N	1.97	0.98
1:A:111:GLU:O	1:A:111:GLU:CA	2.22	0.88
1:C:185:THR:OG1	1:C:186:PRO:HD3	1.76	0.84

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	254/287 (88%)	246 (97%)	7 (3%)	1 (0%)	43	52
1	B	254/287 (88%)	248 (98%)	6 (2%)	0	100	100
1	C	254/287 (88%)	245 (96%)	9 (4%)	0	100	100
1	D	255/287 (89%)	248 (97%)	7 (3%)	0	100	100
1	E	253/287 (88%)	248 (98%)	5 (2%)	0	100	100
1	F	252/287 (88%)	244 (97%)	8 (3%)	0	100	100
1	G	252/287 (88%)	239 (95%)	12 (5%)	1 (0%)	43	52
1	H	253/287 (88%)	243 (96%)	10 (4%)	0	100	100
1	I	252/287 (88%)	240 (95%)	9 (4%)	3 (1%)	19	19
All	All	2279/2583 (88%)	2201 (97%)	73 (3%)	5 (0%)	56	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	85	ASP
1	I	54	ASP
1	I	293	LYS
1	A	183	CYS
1	I	85	ASP

### 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	214/240 (89%)	201 (94%)	13 (6%)	26	34
1	B	206/240 (86%)	198 (96%)	8 (4%)	43	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	210/240 (88%)	207 (99%)	3 (1%)	78	90
1	D	210/240 (88%)	200 (95%)	10 (5%)	35	46
1	E	203/240 (85%)	195 (96%)	8 (4%)	43	57
1	F	200/240 (83%)	192 (96%)	8 (4%)	42	56
1	G	178/240 (74%)	174 (98%)	4 (2%)	64	81
1	H	190/240 (79%)	184 (97%)	6 (3%)	51	67
1	I	183/240 (76%)	179 (98%)	4 (2%)	64	81
All	All	1794/2160 (83%)	1730 (96%)	64 (4%)	48	61

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	77	SER
1	E	133	MET
1	H	277	ASN
1	D	85	ASP
1	D	277	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	63	ASN
1	C	261	GLN
1	I	134	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	256/287 (89%)	0.99	44 (17%) 2 4	11, 18, 25, 40	0
1	B	255/287 (88%)	0.71	18 (7%) 16 23	12, 18, 25, 56	0
1	C	256/287 (89%)	0.73	23 (8%) 10 16	10, 17, 26, 39	0
1	D	256/287 (89%)	0.55	12 (4%) 30 40	12, 18, 26, 41	0
1	E	255/287 (88%)	0.47	4 (1%) 68 77	13, 18, 26, 37	0
1	F	254/287 (88%)	0.57	11 (4%) 34 44	12, 18, 25, 39	1 (0%)
1	G	253/287 (88%)	1.47	75 (29%) 1 1	21, 25, 50, 74	1 (0%)
1	H	254/287 (88%)	1.36	72 (28%) 1 1	21, 25, 31, 51	0
1	I	254/287 (88%)	1.23	64 (25%) 1 2	21, 25, 61, 71	0
All	All	2293/2583 (88%)	0.89	323 (14%) 3 6	10, 20, 28, 74	2 (0%)

The worst 5 of 323 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	112	LEU	7.7
1	I	297	VAL	6.9
1	H	109	LEU	5.6
1	G	53	LEU	5.5
1	H	102	VAL	5.2

### 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.