



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 2VX2 / pdb_00002vx2
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 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 : 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

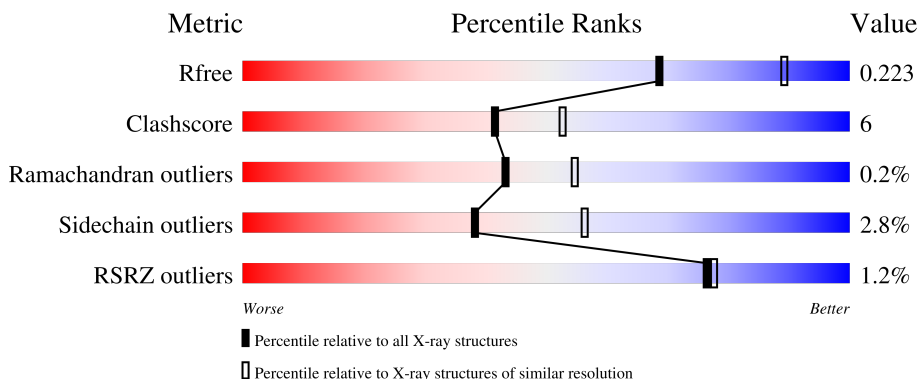
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	287	 67% 20% • 11%
1	B	287	 75% 12% • 11%
1	C	287	 77% 11% • 11%
1	D	287	 78% 10% • 11%
1	E	287	 79% 9% • 11%

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Mol	Chain	Length	Quality of chain
1	F	287	 73% 14% • 11%
1	G	287	 3% 74% 14% • 12%
1	H	287	 74% 14% • 11%
1	I	287	 2% 70% 17% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17539 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 DOMAIN-CONTAINING PROTEIN 3.

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

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.

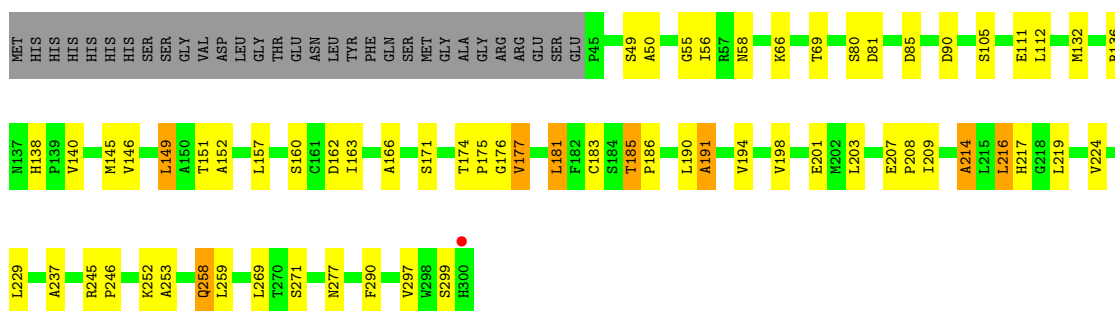
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	148	Total O 148 148	0	0
2	B	61	Total O 61 61	0	0
2	C	124	Total O 124 124	0	0
2	D	80	Total O 80 80	0	0
2	E	67	Total O 67 67	0	0
2	F	55	Total O 55 55	0	0
2	G	13	Total O 13 13	0	0
2	H	13	Total O 13 13	0	0
2	I	12	Total O 12 12	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

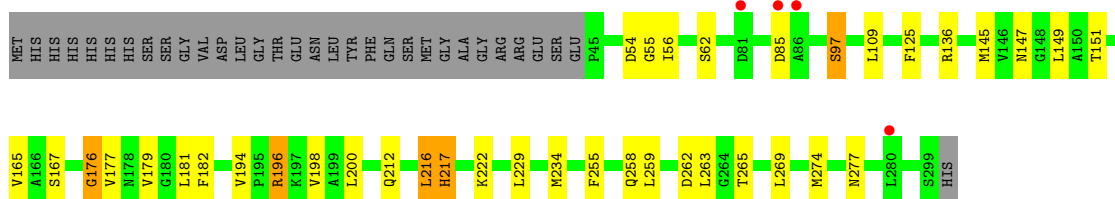
- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain A: 




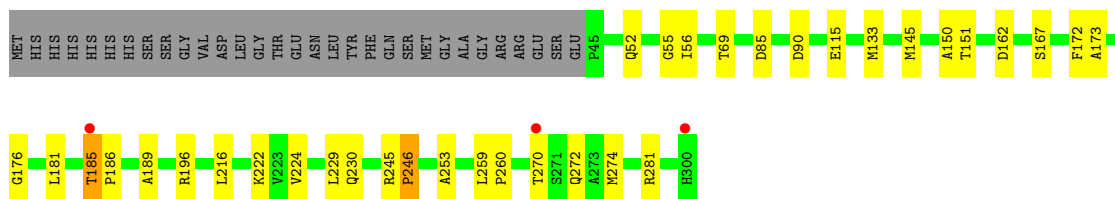
- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain B: 




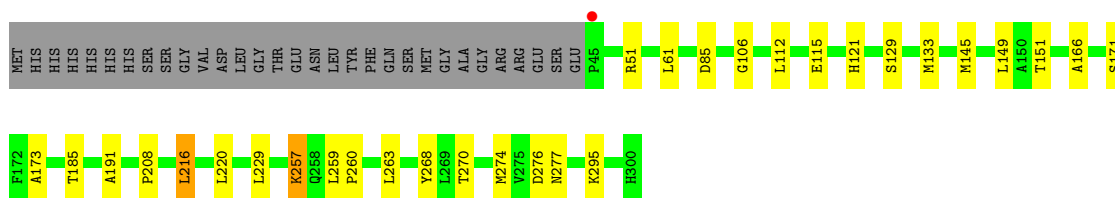
- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain C: 



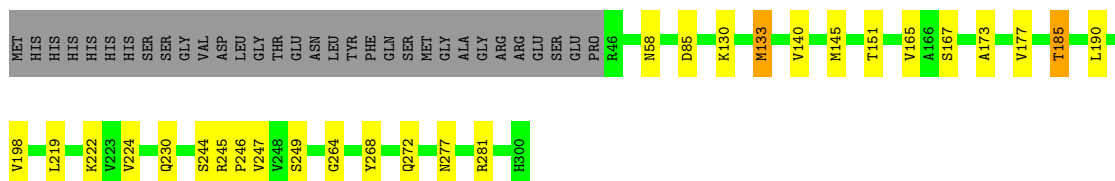
- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain D: 



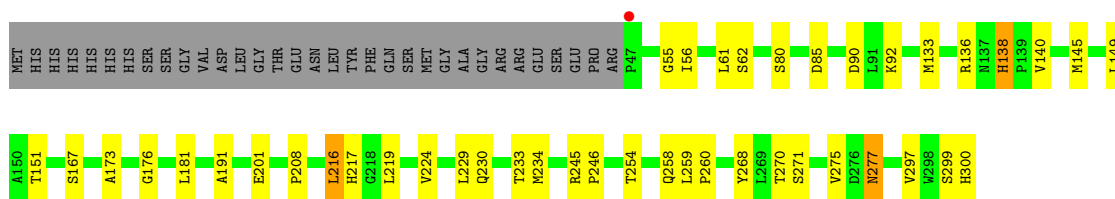
- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain E: 79% 9% 11%



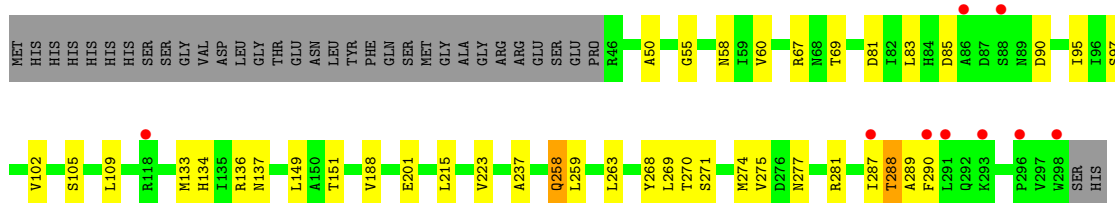
- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain F: 73% 14% 11%



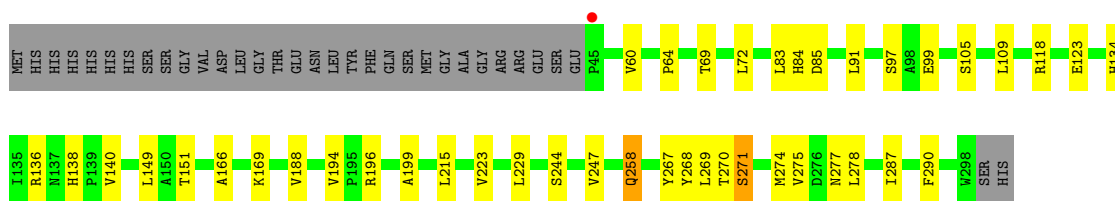
- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain G: 3% 74% 14% 12%

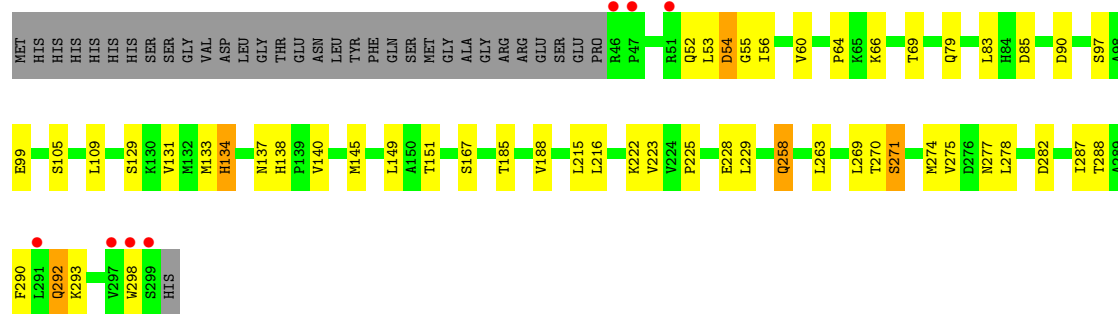


- Molecule 1: ENOYL-COA HYDRATASE DOMAIN-CONTAINING PROTEIN 3

Chain H: 74% 14% 11%



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.76Å 135.30Å 83.87Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	117.04 – 2.30 117.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (117.04-2.30) 99.4 (117.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.29Å)	Xtrriage
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 (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtrriage
Anisotropy	0.733	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17539	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage'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.*

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.

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	1.64	24/1985 (1.2%)	1.30	6/2688 (0.2%)
1	B	1.20	3/1939 (0.2%)	1.15	5/2634 (0.2%)
1	C	1.39	6/1964 (0.3%)	1.19	0/2664
1	D	1.20	2/1971 (0.1%)	1.11	4/2674 (0.1%)
1	E	1.18	7/1933 (0.4%)	1.11	2/2626 (0.1%)
1	F	1.12	2/1911 (0.1%)	1.11	2/2599 (0.1%)
1	G	0.88	0/1828	0.94	0/2499
1	H	0.91	0/1884	0.97	0/2566
1	I	0.90	1/1849 (0.1%)	0.95	2/2523 (0.1%)
All	All	1.19	45/17264 (0.3%)	1.10	21/23473 (0.1%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ALA	CA-CB	10.83	1.71	1.53
1	F	297	VAL	CA-CB	8.19	1.64	1.53
1	C	246	PRO	C-O	-7.40	1.15	1.24
1	A	224	VAL	C-O	-7.14	1.18	1.24
1	C	253	ALA	CA-CB	7.03	1.64	1.53
1	A	208	PRO	CA-C	6.90	1.61	1.52
1	A	149	LEU	CA-C	-6.90	1.43	1.52
1	A	152	ALA	N-CA	6.88	1.55	1.46
1	A	174	THR	N-CA	6.79	1.54	1.46
1	A	214	ALA	C-O	-6.75	1.15	1.24
1	C	162	ASP	C-O	6.67	1.31	1.24
1	A	181	LEU	C-O	-6.58	1.16	1.23
1	C	189	ALA	CA-CB	6.21	1.63	1.53
1	A	177	VAL	CA-CB	6.02	1.61	1.54
1	A	171	SER	N-CA	-5.93	1.38	1.46
1	A	259	LEU	CA-CB	-5.90	1.48	1.54
1	D	257	LYS	C-O	-5.84	1.17	1.24
1	E	130	LYS	C-O	-5.82	1.17	1.24
1	E	140	VAL	CA-CB	5.80	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	VAL	CA-CB	5.76	1.61	1.54
1	A	190	LEU	C-O	-5.70	1.17	1.24
1	A	163	ILE	N-CA	5.64	1.53	1.46
1	D	276	ASP	C-O	-5.54	1.17	1.24
1	E	165	VAL	CA-CB	5.49	1.61	1.54
1	B	176	GLY	C-O	-5.46	1.17	1.23
1	A	157	LEU	CA-C	-5.36	1.46	1.52
1	E	190	LEU	C-O	-5.35	1.17	1.24
1	A	258	GLN	CG-CD	-5.32	1.38	1.52
1	A	160	SER	C-O	-5.31	1.17	1.24
1	A	259	LEU	CA-C	5.30	1.58	1.52
1	B	198	VAL	C-O	-5.29	1.18	1.24
1	A	237	ALA	CA-CB	5.27	1.61	1.53
1	A	253	ALA	CA-CB	-5.26	1.45	1.53
1	E	198	VAL	C-O	-5.25	1.18	1.24
1	A	209	ILE	N-CA	-5.16	1.39	1.46
1	I	185	THR	CA-CB	5.16	1.60	1.53
1	A	81	ASP	C-O	-5.15	1.18	1.24
1	E	58	ASN	CG-OD1	5.14	1.33	1.23
1	C	69	THR	CA-CB	5.10	1.61	1.53
1	E	219	LEU	C-O	-5.09	1.17	1.24
1	B	196	ARG	C-O	-5.05	1.18	1.24
1	F	191	ALA	CA-C	5.05	1.59	1.52
1	C	272	GLN	CD-OE1	5.04	1.33	1.23
1	A	56	ILE	CA-CB	5.03	1.60	1.54
1	A	269	LEU	N-CA	-5.03	1.40	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	LEU	N-CA-C	7.82	119.58	111.14
1	D	185	THR	CA-C-N	-7.72	110.79	119.28
1	D	185	THR	C-N-CA	-7.72	110.79	119.28
1	I	134	HIS	CB-CG-CD2	-6.91	122.22	131.20
1	A	198	VAL	N-CA-C	-6.49	104.53	110.82
1	A	207	GLU	N-CA-C	6.24	117.52	109.65
1	A	224	VAL	CA-C-N	-6.10	112.22	119.84
1	A	224	VAL	C-N-CA	-6.10	112.22	119.84
1	F	138	HIS	CA-C-N	6.03	126.19	119.32
1	F	138	HIS	C-N-CA	6.03	126.19	119.32
1	D	115	GLU	N-CA-C	6.00	119.43	111.75
1	B	259	LEU	CA-C-N	-5.93	113.87	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	LEU	C-N-CA	-5.93	113.87	120.45
1	B	194	VAL	CA-C-N	-5.73	114.36	120.03
1	B	194	VAL	C-N-CA	-5.73	114.36	120.03
1	A	297	VAL	N-CA-C	-5.53	99.19	107.37
1	I	134	HIS	CB-CG-ND1	5.45	130.88	122.70
1	E	185	THR	CA-C-N	-5.41	113.33	119.28
1	E	185	THR	C-N-CA	-5.41	113.33	119.28
1	B	217	HIS	N-CA-C	5.33	119.78	113.16
1	D	106	GLY	N-CA-C	-5.17	104.68	112.84

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	1951	0	1997	33	0
1	B	1904	0	1918	30	0
1	C	1932	0	1961	29	0
1	D	1936	0	1963	18	0
1	E	1901	0	1905	17	0
1	F	1879	0	1873	37	0
1	G	1795	0	1715	29	0
1	H	1850	0	1815	25	0
1	I	1818	0	1750	31	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	217	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 6.

All (217) 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: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:F:145:MET:HE1	1:F:230:GLN:HA	1.56	0.88
1:A:111:GLU:CA	1:A:111:GLU:O	2.22	0.88
1:C:185:THR:OG1	1:C:186:PRO:HD3	1.76	0.84
1:C:216:LEU:HD23	1:C:216:LEU:O	1.81	0.81
1:F:151:THR:HG22	1:F:173:ALA:HB3	1.61	0.81
1:G:83:LEU:HD21	1:G:134:HIS:CD2	2.16	0.80
1:H:83:LEU:HD21	1:H:134:HIS:CD2	2.17	0.79
1:A:214:ALA:HB1	1:A:219:LEU:HB3	1.64	0.78
1:A:145:MET:HE3	1:A:229:LEU:HG	1.65	0.76
1:A:69[A]:THR:CG2	1:A:105:SER:OG	2.34	0.76
1:B:216:LEU:HD22	1:B:217:HIS:CE1	2.20	0.76
1:D:263:LEU:HD23	1:E:133:MET:HE1	1.69	0.75
1:B:149:LEU:HG	1:B:151:THR:HG23	1.70	0.73
1:B:274:MET:HE2	1:C:185:THR:OG1	1.89	0.73
1:F:145:MET:HE2	1:F:229:LEU:HG	1.70	0.71
1:E:264:GLY:HA2	1:F:133:MET:HE1	1.75	0.69
1:I:64:PRO:HG3	1:I:99:GLU:HB3	1.75	0.69
1:F:145:MET:HE3	1:F:233:THR:OG1	1.93	0.69
1:I:83:LEU:HD21	1:I:134:HIS:CD2	2.28	0.69
1:B:216:LEU:C	1:B:216:LEU:HD23	2.18	0.68
1:D:263:LEU:HD23	1:E:133:MET:CE	2.25	0.66
1:B:97:SER:HB3	1:B:145:MET:HE2	1.78	0.65
1:A:185:THR:OG1	1:A:186:PRO:HD3	1.95	0.65
1:C:216:LEU:HD23	1:C:216:LEU:C	2.22	0.65
1:B:216:LEU:HD23	1:B:216:LEU:O	1.97	0.65
1:I:145:MET:HE3	1:I:229:LEU:HG	1.78	0.65
1:I:53:LEU:O	1:I:54:ASP:HB2	1.97	0.64
1:A:69[A]:THR:HG22	1:A:105:SER:HG	1.58	0.64
1:C:185:THR:OG1	1:C:186:PRO:CD	2.44	0.63
1:E:268:TYR:CZ	1:E:272:GLN:OE1	2.51	0.63
1:E:151:THR:HG22	1:E:173:ALA:HB3	1.80	0.63
1:A:149:LEU:HG	1:A:151:THR:HG23	1.81	0.62
1:G:188:VAL:HG22	1:I:258:GLN:HG3	1.81	0.62
1:D:145:MET:HE3	1:D:229:LEU:HG	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:SER:HB2	1:B:125:PHE:HB3	1.81	0.60
1:D:191:ALA:HB1	1:F:259:LEU:CD1	2.32	0.60
1:A:185:THR:OG1	1:C:274:MET:HE2	2.01	0.60
1:I:69:THR:HG22	1:I:105:SER:OG	2.01	0.59
1:B:263:LEU:HD23	1:C:133:MET:SD	2.42	0.59
1:H:271:SER:O	1:H:275:VAL:HG23	2.01	0.59
1:F:145:MET:HE3	1:F:233:THR:CB	2.32	0.59
1:G:281:ARG:CB	2:G:2013:HOH:O	2.50	0.59
1:D:149:LEU:HD11	1:D:151:THR:CG2	2.31	0.59
1:C:176:GLY:HA3	1:C:181:LEU:O	2.03	0.58
1:B:147:ASN:HA	1:B:167:SER:OG	2.03	0.58
1:H:69:THR:HG22	1:H:105:SER:OG	2.03	0.58
1:F:145:MET:CE	1:F:230:GLN:HA	2.32	0.57
1:F:216:LEU:HD13	1:F:217:HIS:CE1	2.40	0.56
1:F:268:TYR:C	1:F:268:TYR:CD2	2.83	0.56
1:F:149:LEU:HD11	1:F:151:THR:HG23	1.86	0.56
1:D:268:TYR:C	1:D:268:TYR:CD2	2.83	0.56
1:A:136[B]:ARG:NH2	2:A:2058:HOH:O	2.39	0.55
1:B:167:SER:HB3	1:B:229:LEU:HD22	1.87	0.55
1:G:271:SER:O	1:G:275:VAL:HG23	2.07	0.55
1:F:92:LYS:HE3	1:F:300:HIS:CE1	2.42	0.55
1:G:69:THR:HG22	1:G:105:SER:OG	2.06	0.55
1:E:277:ASN:C	1:E:277:ASN:HD22	2.15	0.55
1:A:162:ASP:OD1	1:A:252:LYS:NZ	2.37	0.55
1:G:136:ARG:NH1	1:I:263:LEU:HD22	2.21	0.55
1:I:149:LEU:HG	1:I:151:THR:HG23	1.90	0.54
1:I:271:SER:O	1:I:275:VAL:HG23	2.07	0.54
1:F:55:GLY:HA2	1:F:90:ASP:O	2.08	0.53
1:G:201:GLU:OE2	1:I:222:LYS:NZ	2.40	0.53
1:G:270:THR:O	1:G:274:MET:HG2	2.08	0.53
1:D:277:ASN:C	1:D:277:ASN:HD22	2.17	0.53
1:C:259:LEU:HB3	1:C:260:PRO:HD3	1.91	0.52
1:F:136:ARG:NH2	2:F:2014:HOH:O	2.43	0.52
1:F:271:SER:O	1:F:275:VAL:HG23	2.10	0.52
1:H:60:VAL:HG22	1:H:97:SER:OG	2.09	0.52
1:D:216:LEU:HD11	1:F:216:LEU:HD23	1.93	0.51
1:H:277:ASN:HD22	1:H:277:ASN:C	2.18	0.51
1:A:185:THR:CB	1:A:186:PRO:HD3	2.40	0.51
1:C:145:MET:CE	1:C:229:LEU:HG	2.41	0.51
1:F:277:ASN:HD22	1:F:277:ASN:C	2.19	0.51
1:F:216:LEU:O	1:F:216:LEU:HD22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:VAL:HG22	1:I:97:SER:OG	2.10	0.51
1:G:263:LEU:HD22	1:H:136:ARG:NH1	2.26	0.51
1:A:176:GLY:HA3	1:A:181:LEU:O	2.11	0.50
1:G:83:LEU:HD21	1:G:134:HIS:HD2	1.73	0.50
1:A:245:ARG:HB3	1:A:246:PRO:HD3	1.93	0.50
1:G:149:LEU:HG	1:G:151:THR:HG23	1.93	0.50
1:B:216:LEU:C	1:B:216:LEU:CD2	2.84	0.50
1:G:215:LEU:HD22	1:G:223:VAL:HB	1.93	0.50
1:H:149:LEU:HG	1:H:151:THR:HG23	1.94	0.49
1:A:149:LEU:HG	1:A:151:THR:CG2	2.41	0.49
1:C:216:LEU:C	1:C:216:LEU:CD2	2.85	0.49
1:F:138:HIS:ND1	1:F:140:VAL:HG22	2.27	0.49
1:G:81:ASP:OD1	2:G:2001:HOH:O	2.18	0.49
1:B:255:PHE:O	1:B:258:GLN:HG3	2.13	0.49
1:F:259:LEU:HB3	1:F:260:PRO:HD3	1.94	0.49
1:A:191:ALA:HB1	1:C:259:LEU:CD1	2.42	0.49
1:I:79:GLN:HB2	1:I:131:VAL:HG22	1.94	0.49
1:D:263:LEU:CD2	1:E:133:MET:HE1	2.40	0.48
1:I:215:LEU:HD22	1:I:223:VAL:HB	1.94	0.48
1:A:277:ASN:C	1:A:277:ASN:HD22	2.20	0.48
1:H:194:VAL:HG23	1:H:199:ALA:HB2	1.94	0.48
1:H:267:TYR:O	1:H:271:SER:OG	2.32	0.48
1:I:225:PRO:HD2	1:I:228:GLU:OE1	2.13	0.48
1:A:290:PHE:CD2	1:B:109:LEU:HD12	2.49	0.48
1:C:145:MET:HE3	1:C:229:LEU:HG	1.96	0.48
1:G:50:ALA:HA	1:G:58:ASN:O	2.14	0.48
1:A:136[B]:ARG:HH12	1:B:196:ARG:HH12	1.61	0.47
1:G:277:ASN:C	1:G:277:ASN:HD22	2.22	0.47
1:H:258:GLN:HG3	1:I:188:VAL:HG22	1.96	0.47
1:C:176:GLY:C	1:C:181:LEU:O	2.57	0.47
1:D:270:THR:O	1:D:274:MET:HG2	2.14	0.47
1:A:111:GLU:N	1:A:112:LEU:N	2.61	0.47
1:A:55:GLY:HA2	1:A:90:ASP:O	2.15	0.47
1:C:270:THR:O	1:C:274:MET:HG2	2.15	0.47
1:D:166:ALA:HB3	1:D:220:LEU:HD13	1.97	0.47
1:F:149:LEU:CD1	1:F:151:THR:HG23	2.45	0.47
1:F:254:THR:HG22	1:F:270:THR:HG22	1.97	0.47
1:A:146:VAL:O	1:A:166:ALA:HA	2.15	0.46
1:E:264:GLY:HA2	1:F:133:MET:CE	2.44	0.46
1:C:151:THR:HG22	1:C:173:ALA:HB3	1.97	0.46
1:D:149:LEU:HD11	1:D:151:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:GLN:HG3	1:H:188:VAL:HG22	1.96	0.46
1:I:52:GLN:HA	1:I:56:ILE:O	2.15	0.46
1:I:66:LYS:O	1:I:69:THR:HG23	2.16	0.46
1:H:278:LEU:CD2	1:H:287:ILE:HD11	2.46	0.46
1:B:179:VAL:HG23	1:B:179:VAL:O	2.16	0.46
1:H:215:LEU:HD22	1:H:223:VAL:HB	1.96	0.46
1:F:167:SER:HA	1:F:224:VAL:O	2.16	0.46
1:F:259:LEU:HB3	1:F:260:PRO:CD	2.45	0.46
1:C:55:GLY:HA2	1:C:90:ASP:O	2.15	0.46
1:C:245:ARG:HB3	1:C:246:PRO:HD3	1.98	0.46
1:D:259:LEU:HB3	1:D:260:PRO:HD3	1.97	0.46
1:F:176:GLY:HA3	1:F:181:LEU:O	2.17	0.46
1:A:216:LEU:HD23	1:A:217:HIS:CE1	2.51	0.45
1:F:254:THR:CG2	1:F:270:THR:HG22	2.46	0.45
1:G:290:PHE:CD2	1:H:109:LEU:HD12	2.51	0.45
1:H:72:LEU:HD21	1:H:123:GLU:OE2	2.15	0.45
1:E:145:MET:HE1	1:E:230:GLN:OE1	2.15	0.45
1:G:95:ILE:HD11	1:G:237:ALA:HB2	1.98	0.45
1:C:185:THR:HG1	1:C:186:PRO:HD3	1.81	0.45
1:E:245:ARG:HB3	1:E:246:PRO:HD3	1.98	0.45
1:G:109:LEU:HD12	1:I:290:PHE:CD2	2.52	0.45
1:H:244:SER:OG	1:H:247:VAL:HG23	2.16	0.45
1:A:219:LEU:O	1:A:219:LEU:HD12	2.17	0.45
1:C:145:MET:CE	1:C:230:GLN:HA	2.47	0.45
1:B:165:VAL:HG13	1:B:222:LYS:HB2	1.99	0.45
1:B:277:ASN:HD22	1:B:277:ASN:C	2.25	0.45
1:I:278:LEU:CD2	1:I:287:ILE:HD11	2.47	0.45
1:C:176:GLY:CA	1:C:181:LEU:O	2.65	0.44
1:H:138:HIS:CE1	1:H:140:VAL:HG22	2.52	0.44
1:D:149:LEU:HG	1:D:151:THR:HG23	1.98	0.44
1:B:54:ASP:OD1	1:B:54:ASP:N	2.48	0.44
1:B:216:LEU:HD22	1:B:217:HIS:ND1	2.31	0.44
1:A:138:HIS:ND1	1:A:140:VAL:HG22	2.33	0.44
1:B:212:GLN:HG3	2:B:2043:HOH:O	2.17	0.44
1:B:56:ILE:HD13	1:B:234:MET:HE1	2.00	0.44
1:G:67:ARG:HD2	1:G:102:VAL:HG21	1.99	0.44
1:G:275:VAL:HG12	1:H:118:ARG:NH2	2.32	0.44
1:A:191:ALA:HB1	1:C:259:LEU:HD11	1.99	0.44
1:A:201:GLU:OE2	1:C:222:LYS:HE2	2.18	0.44
1:F:145:MET:HE3	1:F:233:THR:HB	1.98	0.44
1:I:129:SER:O	1:I:133:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:O	1:A:69[A]:THR:HG23	2.18	0.43
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.89	0.43
1:E:264:GLY:CA	1:F:133:MET:HE1	2.47	0.43
1:A:185:THR:HG1	1:C:274:MET:HE2	1.83	0.43
1:C:167:SER:HA	1:C:224:VAL:O	2.18	0.43
1:H:270:THR:O	1:H:274:MET:HG2	2.18	0.43
1:G:95:ILE:HD11	1:G:237:ALA:CB	2.49	0.43
1:C:150:ALA:O	1:C:172:PHE:HA	2.19	0.43
1:A:50:ALA:HA	1:A:58:ASN:O	2.19	0.43
1:B:176:GLY:HA3	1:B:181:LEU:O	2.19	0.43
1:E:245:ARG:O	1:E:249:SER:HB2	2.18	0.43
1:I:270:THR:O	1:I:274:MET:HG2	2.19	0.43
1:F:92:LYS:CE	1:F:300:HIS:CE1	3.02	0.42
1:E:167:SER:HA	1:E:224:VAL:O	2.19	0.42
1:F:245:ARG:HB3	1:F:246:PRO:HD3	2.01	0.42
1:I:288:THR:HG22	1:I:292:GLN:OE1	2.19	0.42
1:E:281:ARG:HE	1:E:281:ARG:HB2	1.63	0.42
1:B:262:ASP:OD2	1:B:265:THR:OG1	2.30	0.42
1:F:219:LEU:HD12	1:F:219:LEU:O	2.20	0.42
1:G:50:ALA:HB3	2:G:2001:HOH:O	2.18	0.42
1:H:166:ALA:C	1:H:229:LEU:HD13	2.45	0.42
1:I:138:HIS:CE1	1:I:140:VAL:HG22	2.55	0.42
1:C:52:GLN:HA	1:C:56:ILE:O	2.20	0.42
1:I:282:ASP:O	1:I:298:TRP:HZ3	2.01	0.42
1:E:244:SER:OG	1:E:247:VAL:HG23	2.20	0.42
1:G:259:LEU:HD21	1:H:196:ARG:NE	2.34	0.42
1:B:181:LEU:O	1:B:182:PHE:C	2.63	0.42
1:F:173:ALA:HB2	1:F:208:PRO:HB3	2.02	0.42
1:H:84:HIS:O	1:H:85:ASP:C	2.62	0.42
1:D:129:SER:O	1:D:133:MET:HG2	2.20	0.42
1:I:167:SER:HB3	1:I:229:LEU:HD22	2.02	0.42
1:B:216:LEU:CD2	1:B:217:HIS:CE1	2.96	0.42
1:E:222:LYS:HE2	1:F:201:GLU:OE1	2.20	0.41
1:G:60:VAL:HG22	1:G:97:SER:OG	2.20	0.41
1:H:268:TYR:CD2	1:H:268:TYR:C	2.96	0.41
1:B:136:ARG:HH12	1:C:196:ARG:HH12	1.69	0.41
1:B:149:LEU:HD11	1:B:151:THR:HG22	2.02	0.41
1:D:112:LEU:HA	1:D:121:HIS:CD2	2.55	0.41
1:G:55:GLY:HA2	1:G:90:ASP:O	2.20	0.41
1:H:64:PRO:HG3	1:H:99:GLU:HB3	2.02	0.41
1:C:281:ARG:HD3	1:C:281:ARG:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ALA:HB2	1:D:208:PRO:HB3	2.02	0.41
1:G:133:MET:O	1:G:137:ASN:ND2	2.52	0.41
1:I:66:LYS:CB	2:I:2002:HOH:O	2.69	0.41
1:I:277:ASN:C	1:I:277:ASN:HD22	2.29	0.41
1:B:149:LEU:CG	1:B:151:THR:HG23	2.46	0.41
1:F:56:ILE:CD1	1:F:234:MET:HE1	2.51	0.41
1:I:55:GLY:HA2	1:I:90:ASP:O	2.21	0.41
1:I:133:MET:O	1:I:137:ASN:ND2	2.53	0.41
1:G:268:TYR:CD2	1:G:268:TYR:C	2.99	0.40
1:F:299:SER:O	1:F:300:HIS:HB2	2.21	0.40
1:H:290:PHE:CD2	1:I:109:LEU:HD12	2.56	0.40
1:D:263:LEU:CG	1:E:133:MET:HE1	2.52	0.40
1:F:138:HIS:CE1	1:F:140:VAL:HG22	2.56	0.40
1:G:288:THR:HG22	1:G:289:ALA:N	2.36	0.40
1:I:216:LEU:HD12	1:I:216:LEU:HA	1.96	0.40

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	254/287 (88%)	246 (97%)	7 (3%)	1 (0%)	30	38
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%)	30	38
1	H	253/287 (88%)	243 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	252/287 (88%)	240 (95%)	9 (4%)	3 (1%)	10	12
All	All	2279/2583 (88%)	2201 (97%)	73 (3%)	5 (0%)	43	55

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 [i](#)

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%)	204 (95%)	10 (5%)	23	35
1	B	206/240 (86%)	200 (97%)	6 (3%)	37	55
1	C	210/240 (88%)	207 (99%)	3 (1%)	59	76
1	D	210/240 (88%)	202 (96%)	8 (4%)	29	44
1	E	203/240 (85%)	199 (98%)	4 (2%)	48	67
1	F	200/240 (83%)	193 (96%)	7 (4%)	32	48
1	G	178/240 (74%)	174 (98%)	4 (2%)	45	65
1	H	190/240 (79%)	185 (97%)	5 (3%)	40	59
1	I	183/240 (76%)	179 (98%)	4 (2%)	45	65
All	All	1794/2160 (83%)	1743 (97%)	51 (3%)	38	56

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	80	SER

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Mol	Chain	Res	Type
1	A	85	ASP
1	A	132	MET
1	A	175	PRO
1	A	177	VAL
1	A	185	THR
1	A	216	LEU
1	A	258	GLN
1	A	299	SER
1	B	62	SER
1	B	85	ASP
1	B	97	SER
1	B	177	VAL
1	B	216	LEU
1	B	269	LEU
1	C	85	ASP
1	C	115	GLU
1	C	185	THR
1	D	51[A]	ARG
1	D	51[B]	ARG
1	D	61	LEU
1	D	85	ASP
1	D	171	SER
1	D	216	LEU
1	D	257	LYS
1	D	295	LYS
1	E	85	ASP
1	E	133	MET
1	E	177	VAL
1	E	185	THR
1	F	61	LEU
1	F	62	SER
1	F	80	SER
1	F	85	ASP
1	F	216	LEU
1	F	258	GLN
1	F	277	ASN
1	G	258	GLN
1	G	269	LEU
1	G	287	ILE
1	G	288	THR
1	H	91	LEU
1	H	169	LYS

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Mol	Chain	Res	Type
1	H	258	GLN
1	H	269	LEU
1	H	271	SER
1	I	258	GLN
1	I	269	LEU
1	I	271	SER
1	I	292	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	147	ASN
1	A	156	GLN
1	A	277	ASN
1	B	147	ASN
1	C	156	GLN
1	C	230	GLN
1	C	292	GLN
1	D	79	GLN
1	D	116	GLN
1	D	134	HIS
1	D	272	GLN
1	D	292	GLN
1	E	79	GLN
1	E	134	HIS
1	E	292	GLN
1	F	79	GLN
1	G	58	ASN
1	G	261	GLN
1	G	277	ASN
1	H	58	ASN
1	H	79	GLN
1	H	137	ASN
1	H	277	ASN
1	I	58	ASN
1	I	134	HIS

5.3.3 RNA

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	256/287 (89%)	0.28	1 (0%) 88 89	8, 18, 25, 40	2 (0%)
1	B	255/287 (88%)	0.13	4 (1%) 70 72	12, 18, 25, 56	1 (0%)
1	C	256/287 (89%)	0.14	3 (1%) 76 77	10, 17, 26, 39	0
1	D	256/287 (89%)	-0.10	1 (0%) 88 89	12, 18, 26, 41	1 (0%)
1	E	255/287 (88%)	-0.16	0 100 100	13, 18, 26, 37	0
1	F	254/287 (88%)	-0.11	1 (0%) 88 89	12, 18, 25, 39	1 (0%)
1	G	253/287 (88%)	0.50	9 (3%) 46 48	12, 25, 50, 74	2 (0%)
1	H	254/287 (88%)	0.35	1 (0%) 88 89	15, 25, 31, 51	1 (0%)
1	I	254/287 (88%)	0.36	7 (2%) 55 57	21, 25, 61, 71	0
All	All	2293/2583 (88%)	0.16	27 (1%) 76 77	8, 20, 28, 74	8 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	118	ARG	7.3
1	H	45	PRO	4.8
1	I	299	SER	3.8
1	B	86	ALA	3.6
1	I	291	LEU	3.5
1	I	297	VAL	3.5
1	G	291	LEU	3.3
1	A	300	HIS	3.2
1	G	298	TRP	3.1
1	I	46	ARG	2.8
1	G	293	LYS	2.7
1	G	88	SER	2.7
1	I	47	PRO	2.7
1	G	290	PHE	2.6
1	G	86	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	47	PRO	2.3
1	C	270	THR	2.3
1	B	81	ASP	2.3
1	I	298	TRP	2.2
1	B	85	ASP	2.2
1	C	185	THR	2.2
1	G	287	ILE	2.1
1	B	280	LEU	2.1
1	C	300	HIS	2.1
1	I	51	ARG	2.1
1	G	296	PRO	2.0
1	D	45	PRO	2.0

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.