



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:01 am BST

PDB ID : 5VE2
Title : Crystal structure of enoyl-CoA hydratase/isomerase from *Pseudoalteromonas atlantica* T6c at 2.3 Å resolution.
Authors : Siuda, M.K.; Shabalin, I.G.; Cooper, D.R.; Chapman, H.C.; Tkaczuk, K.L.; Bonanno, J.; Almo, S.C.; Minor, W.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2017-04-03
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 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

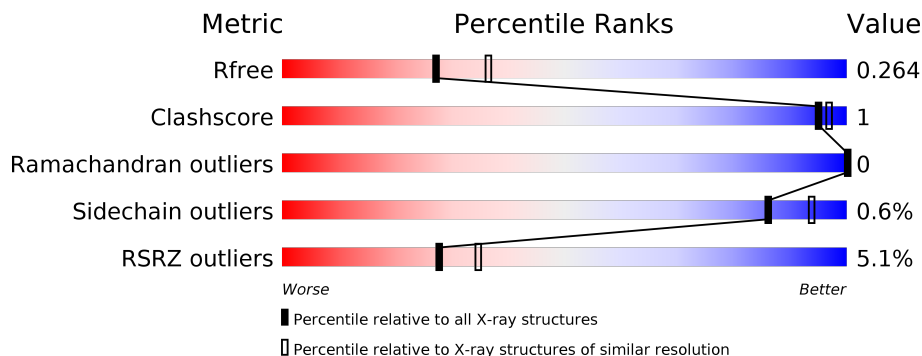
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



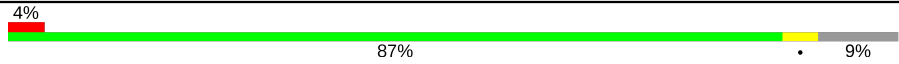

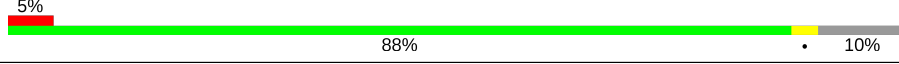



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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	275	
1	B	275	
1	C	275	
1	D	275	
1	E	275	
1	F	275	

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Mol	Chain	Length	Quality of chain
1	G	275	
1	H	275	
1	I	275	
1	J	275	
1	K	275	
1	L	275	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24561 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
			Total	C	N	O	S	Se			
1	A	251	Total 1863	C 1179	N 326	O 352	S 2	Se 4	0	0	0
1	B	251	Total 1864	C 1177	N 327	O 354	S 2	Se 4	0	0	0
1	C	251	Total 1883	C 1190	N 330	O 357	S 2	Se 4	0	0	0
1	D	251	Total 1880	C 1187	N 330	O 357	S 2	Se 4	0	0	0
1	E	251	Total 1869	C 1182	N 326	O 355	S 2	Se 4	0	0	0
1	F	251	Total 1872	C 1180	N 329	O 357	S 2	Se 4	0	0	0
1	G	251	Total 1890	C 1194	N 331	O 359	S 2	Se 4	0	0	0
1	H	251	Total 1884	C 1189	N 330	O 359	S 2	Se 4	0	0	0
1	I	248	Total 1859	C 1173	N 325	O 355	S 2	Se 4	0	0	0
1	J	251	Total 1881	C 1190	N 328	O 357	S 2	Se 4	0	0	0
1	K	251	Total 1866	C 1171	N 330	O 359	S 2	Se 4	0	0	0
1	L	251	Total 1885	C 1189	N 331	O 359	S 2	Se 4	0	0	0

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	initiating methionine	UNP Q15VV3
A	-20	HIS	-	expression tag	UNP Q15VV3
A	-19	HIS	-	expression tag	UNP Q15VV3
A	-18	HIS	-	expression tag	UNP Q15VV3
A	-17	HIS	-	expression tag	UNP Q15VV3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP Q15VV3
A	-15	HIS	-	expression tag	UNP Q15VV3
A	-14	SER	-	expression tag	UNP Q15VV3
A	-13	SER	-	expression tag	UNP Q15VV3
A	-12	GLY	-	expression tag	UNP Q15VV3
A	-11	VAL	-	expression tag	UNP Q15VV3
A	-10	ASP	-	expression tag	UNP Q15VV3
A	-9	LEU	-	expression tag	UNP Q15VV3
A	-8	GLY	-	expression tag	UNP Q15VV3
A	-7	THR	-	expression tag	UNP Q15VV3
A	-6	GLU	-	expression tag	UNP Q15VV3
A	-5	ASN	-	expression tag	UNP Q15VV3
A	-4	LEU	-	expression tag	UNP Q15VV3
A	-3	TYR	-	expression tag	UNP Q15VV3
A	-2	PHE	-	expression tag	UNP Q15VV3
A	-1	GLN	-	expression tag	UNP Q15VV3
A	0	SER	-	expression tag	UNP Q15VV3
B	-21	MSE	-	initiating methionine	UNP Q15VV3
B	-20	HIS	-	expression tag	UNP Q15VV3
B	-19	HIS	-	expression tag	UNP Q15VV3
B	-18	HIS	-	expression tag	UNP Q15VV3
B	-17	HIS	-	expression tag	UNP Q15VV3
B	-16	HIS	-	expression tag	UNP Q15VV3
B	-15	HIS	-	expression tag	UNP Q15VV3
B	-14	SER	-	expression tag	UNP Q15VV3
B	-13	SER	-	expression tag	UNP Q15VV3
B	-12	GLY	-	expression tag	UNP Q15VV3
B	-11	VAL	-	expression tag	UNP Q15VV3
B	-10	ASP	-	expression tag	UNP Q15VV3
B	-9	LEU	-	expression tag	UNP Q15VV3
B	-8	GLY	-	expression tag	UNP Q15VV3
B	-7	THR	-	expression tag	UNP Q15VV3
B	-6	GLU	-	expression tag	UNP Q15VV3
B	-5	ASN	-	expression tag	UNP Q15VV3
B	-4	LEU	-	expression tag	UNP Q15VV3
B	-3	TYR	-	expression tag	UNP Q15VV3
B	-2	PHE	-	expression tag	UNP Q15VV3
B	-1	GLN	-	expression tag	UNP Q15VV3
B	0	SER	-	expression tag	UNP Q15VV3
C	-21	MSE	-	initiating methionine	UNP Q15VV3
C	-20	HIS	-	expression tag	UNP Q15VV3
C	-19	HIS	-	expression tag	UNP Q15VV3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP Q15VV3
C	-17	HIS	-	expression tag	UNP Q15VV3
C	-16	HIS	-	expression tag	UNP Q15VV3
C	-15	HIS	-	expression tag	UNP Q15VV3
C	-14	SER	-	expression tag	UNP Q15VV3
C	-13	SER	-	expression tag	UNP Q15VV3
C	-12	GLY	-	expression tag	UNP Q15VV3
C	-11	VAL	-	expression tag	UNP Q15VV3
C	-10	ASP	-	expression tag	UNP Q15VV3
C	-9	LEU	-	expression tag	UNP Q15VV3
C	-8	GLY	-	expression tag	UNP Q15VV3
C	-7	THR	-	expression tag	UNP Q15VV3
C	-6	GLU	-	expression tag	UNP Q15VV3
C	-5	ASN	-	expression tag	UNP Q15VV3
C	-4	LEU	-	expression tag	UNP Q15VV3
C	-3	TYR	-	expression tag	UNP Q15VV3
C	-2	PHE	-	expression tag	UNP Q15VV3
C	-1	GLN	-	expression tag	UNP Q15VV3
C	0	SER	-	expression tag	UNP Q15VV3
D	-21	MSE	-	initiating methionine	UNP Q15VV3
D	-20	HIS	-	expression tag	UNP Q15VV3
D	-19	HIS	-	expression tag	UNP Q15VV3
D	-18	HIS	-	expression tag	UNP Q15VV3
D	-17	HIS	-	expression tag	UNP Q15VV3
D	-16	HIS	-	expression tag	UNP Q15VV3
D	-15	HIS	-	expression tag	UNP Q15VV3
D	-14	SER	-	expression tag	UNP Q15VV3
D	-13	SER	-	expression tag	UNP Q15VV3
D	-12	GLY	-	expression tag	UNP Q15VV3
D	-11	VAL	-	expression tag	UNP Q15VV3
D	-10	ASP	-	expression tag	UNP Q15VV3
D	-9	LEU	-	expression tag	UNP Q15VV3
D	-8	GLY	-	expression tag	UNP Q15VV3
D	-7	THR	-	expression tag	UNP Q15VV3
D	-6	GLU	-	expression tag	UNP Q15VV3
D	-5	ASN	-	expression tag	UNP Q15VV3
D	-4	LEU	-	expression tag	UNP Q15VV3
D	-3	TYR	-	expression tag	UNP Q15VV3
D	-2	PHE	-	expression tag	UNP Q15VV3
D	-1	GLN	-	expression tag	UNP Q15VV3
D	0	SER	-	expression tag	UNP Q15VV3
E	-21	MSE	-	initiating methionine	UNP Q15VV3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	HIS	-	expression tag	UNP Q15VV3
E	-19	HIS	-	expression tag	UNP Q15VV3
E	-18	HIS	-	expression tag	UNP Q15VV3
E	-17	HIS	-	expression tag	UNP Q15VV3
E	-16	HIS	-	expression tag	UNP Q15VV3
E	-15	HIS	-	expression tag	UNP Q15VV3
E	-14	SER	-	expression tag	UNP Q15VV3
E	-13	SER	-	expression tag	UNP Q15VV3
E	-12	GLY	-	expression tag	UNP Q15VV3
E	-11	VAL	-	expression tag	UNP Q15VV3
E	-10	ASP	-	expression tag	UNP Q15VV3
E	-9	LEU	-	expression tag	UNP Q15VV3
E	-8	GLY	-	expression tag	UNP Q15VV3
E	-7	THR	-	expression tag	UNP Q15VV3
E	-6	GLU	-	expression tag	UNP Q15VV3
E	-5	ASN	-	expression tag	UNP Q15VV3
E	-4	LEU	-	expression tag	UNP Q15VV3
E	-3	TYR	-	expression tag	UNP Q15VV3
E	-2	PHE	-	expression tag	UNP Q15VV3
E	-1	GLN	-	expression tag	UNP Q15VV3
E	0	SER	-	expression tag	UNP Q15VV3
F	-21	MSE	-	initiating methionine	UNP Q15VV3
F	-20	HIS	-	expression tag	UNP Q15VV3
F	-19	HIS	-	expression tag	UNP Q15VV3
F	-18	HIS	-	expression tag	UNP Q15VV3
F	-17	HIS	-	expression tag	UNP Q15VV3
F	-16	HIS	-	expression tag	UNP Q15VV3
F	-15	HIS	-	expression tag	UNP Q15VV3
F	-14	SER	-	expression tag	UNP Q15VV3
F	-13	SER	-	expression tag	UNP Q15VV3
F	-12	GLY	-	expression tag	UNP Q15VV3
F	-11	VAL	-	expression tag	UNP Q15VV3
F	-10	ASP	-	expression tag	UNP Q15VV3
F	-9	LEU	-	expression tag	UNP Q15VV3
F	-8	GLY	-	expression tag	UNP Q15VV3
F	-7	THR	-	expression tag	UNP Q15VV3
F	-6	GLU	-	expression tag	UNP Q15VV3
F	-5	ASN	-	expression tag	UNP Q15VV3
F	-4	LEU	-	expression tag	UNP Q15VV3
F	-3	TYR	-	expression tag	UNP Q15VV3
F	-2	PHE	-	expression tag	UNP Q15VV3
F	-1	GLN	-	expression tag	UNP Q15VV3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP Q15VV3
G	-21	MSE	-	initiating methionine	UNP Q15VV3
G	-20	HIS	-	expression tag	UNP Q15VV3
G	-19	HIS	-	expression tag	UNP Q15VV3
G	-18	HIS	-	expression tag	UNP Q15VV3
G	-17	HIS	-	expression tag	UNP Q15VV3
G	-16	HIS	-	expression tag	UNP Q15VV3
G	-15	HIS	-	expression tag	UNP Q15VV3
G	-14	SER	-	expression tag	UNP Q15VV3
G	-13	SER	-	expression tag	UNP Q15VV3
G	-12	GLY	-	expression tag	UNP Q15VV3
G	-11	VAL	-	expression tag	UNP Q15VV3
G	-10	ASP	-	expression tag	UNP Q15VV3
G	-9	LEU	-	expression tag	UNP Q15VV3
G	-8	GLY	-	expression tag	UNP Q15VV3
G	-7	THR	-	expression tag	UNP Q15VV3
G	-6	GLU	-	expression tag	UNP Q15VV3
G	-5	ASN	-	expression tag	UNP Q15VV3
G	-4	LEU	-	expression tag	UNP Q15VV3
G	-3	TYR	-	expression tag	UNP Q15VV3
G	-2	PHE	-	expression tag	UNP Q15VV3
G	-1	GLN	-	expression tag	UNP Q15VV3
G	0	SER	-	expression tag	UNP Q15VV3
H	-21	MSE	-	initiating methionine	UNP Q15VV3
H	-20	HIS	-	expression tag	UNP Q15VV3
H	-19	HIS	-	expression tag	UNP Q15VV3
H	-18	HIS	-	expression tag	UNP Q15VV3
H	-17	HIS	-	expression tag	UNP Q15VV3
H	-16	HIS	-	expression tag	UNP Q15VV3
H	-15	HIS	-	expression tag	UNP Q15VV3
H	-14	SER	-	expression tag	UNP Q15VV3
H	-13	SER	-	expression tag	UNP Q15VV3
H	-12	GLY	-	expression tag	UNP Q15VV3
H	-11	VAL	-	expression tag	UNP Q15VV3
H	-10	ASP	-	expression tag	UNP Q15VV3
H	-9	LEU	-	expression tag	UNP Q15VV3
H	-8	GLY	-	expression tag	UNP Q15VV3
H	-7	THR	-	expression tag	UNP Q15VV3
H	-6	GLU	-	expression tag	UNP Q15VV3
H	-5	ASN	-	expression tag	UNP Q15VV3
H	-4	LEU	-	expression tag	UNP Q15VV3
H	-3	TYR	-	expression tag	UNP Q15VV3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	PHE	-	expression tag	UNP Q15VV3
H	-1	GLN	-	expression tag	UNP Q15VV3
H	0	SER	-	expression tag	UNP Q15VV3
I	-21	MSE	-	initiating methionine	UNP Q15VV3
I	-20	HIS	-	expression tag	UNP Q15VV3
I	-19	HIS	-	expression tag	UNP Q15VV3
I	-18	HIS	-	expression tag	UNP Q15VV3
I	-17	HIS	-	expression tag	UNP Q15VV3
I	-16	HIS	-	expression tag	UNP Q15VV3
I	-15	HIS	-	expression tag	UNP Q15VV3
I	-14	SER	-	expression tag	UNP Q15VV3
I	-13	SER	-	expression tag	UNP Q15VV3
I	-12	GLY	-	expression tag	UNP Q15VV3
I	-11	VAL	-	expression tag	UNP Q15VV3
I	-10	ASP	-	expression tag	UNP Q15VV3
I	-9	LEU	-	expression tag	UNP Q15VV3
I	-8	GLY	-	expression tag	UNP Q15VV3
I	-7	THR	-	expression tag	UNP Q15VV3
I	-6	GLU	-	expression tag	UNP Q15VV3
I	-5	ASN	-	expression tag	UNP Q15VV3
I	-4	LEU	-	expression tag	UNP Q15VV3
I	-3	TYR	-	expression tag	UNP Q15VV3
I	-2	PHE	-	expression tag	UNP Q15VV3
I	-1	GLN	-	expression tag	UNP Q15VV3
I	0	SER	-	expression tag	UNP Q15VV3
J	-21	MSE	-	initiating methionine	UNP Q15VV3
J	-20	HIS	-	expression tag	UNP Q15VV3
J	-19	HIS	-	expression tag	UNP Q15VV3
J	-18	HIS	-	expression tag	UNP Q15VV3
J	-17	HIS	-	expression tag	UNP Q15VV3
J	-16	HIS	-	expression tag	UNP Q15VV3
J	-15	HIS	-	expression tag	UNP Q15VV3
J	-14	SER	-	expression tag	UNP Q15VV3
J	-13	SER	-	expression tag	UNP Q15VV3
J	-12	GLY	-	expression tag	UNP Q15VV3
J	-11	VAL	-	expression tag	UNP Q15VV3
J	-10	ASP	-	expression tag	UNP Q15VV3
J	-9	LEU	-	expression tag	UNP Q15VV3
J	-8	GLY	-	expression tag	UNP Q15VV3
J	-7	THR	-	expression tag	UNP Q15VV3
J	-6	GLU	-	expression tag	UNP Q15VV3
J	-5	ASN	-	expression tag	UNP Q15VV3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	LEU	-	expression tag	UNP Q15VV3
J	-3	TYR	-	expression tag	UNP Q15VV3
J	-2	PHE	-	expression tag	UNP Q15VV3
J	-1	GLN	-	expression tag	UNP Q15VV3
J	0	SER	-	expression tag	UNP Q15VV3
K	-21	MSE	-	initiating methionine	UNP Q15VV3
K	-20	HIS	-	expression tag	UNP Q15VV3
K	-19	HIS	-	expression tag	UNP Q15VV3
K	-18	HIS	-	expression tag	UNP Q15VV3
K	-17	HIS	-	expression tag	UNP Q15VV3
K	-16	HIS	-	expression tag	UNP Q15VV3
K	-15	HIS	-	expression tag	UNP Q15VV3
K	-14	SER	-	expression tag	UNP Q15VV3
K	-13	SER	-	expression tag	UNP Q15VV3
K	-12	GLY	-	expression tag	UNP Q15VV3
K	-11	VAL	-	expression tag	UNP Q15VV3
K	-10	ASP	-	expression tag	UNP Q15VV3
K	-9	LEU	-	expression tag	UNP Q15VV3
K	-8	GLY	-	expression tag	UNP Q15VV3
K	-7	THR	-	expression tag	UNP Q15VV3
K	-6	GLU	-	expression tag	UNP Q15VV3
K	-5	ASN	-	expression tag	UNP Q15VV3
K	-4	LEU	-	expression tag	UNP Q15VV3
K	-3	TYR	-	expression tag	UNP Q15VV3
K	-2	PHE	-	expression tag	UNP Q15VV3
K	-1	GLN	-	expression tag	UNP Q15VV3
K	0	SER	-	expression tag	UNP Q15VV3
L	-21	MSE	-	initiating methionine	UNP Q15VV3
L	-20	HIS	-	expression tag	UNP Q15VV3
L	-19	HIS	-	expression tag	UNP Q15VV3
L	-18	HIS	-	expression tag	UNP Q15VV3
L	-17	HIS	-	expression tag	UNP Q15VV3
L	-16	HIS	-	expression tag	UNP Q15VV3
L	-15	HIS	-	expression tag	UNP Q15VV3
L	-14	SER	-	expression tag	UNP Q15VV3
L	-13	SER	-	expression tag	UNP Q15VV3
L	-12	GLY	-	expression tag	UNP Q15VV3
L	-11	VAL	-	expression tag	UNP Q15VV3
L	-10	ASP	-	expression tag	UNP Q15VV3
L	-9	LEU	-	expression tag	UNP Q15VV3
L	-8	GLY	-	expression tag	UNP Q15VV3
L	-7	THR	-	expression tag	UNP Q15VV3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	GLU	-	expression tag	UNP Q15VV3
L	-5	ASN	-	expression tag	UNP Q15VV3
L	-4	LEU	-	expression tag	UNP Q15VV3
L	-3	TYR	-	expression tag	UNP Q15VV3
L	-2	PHE	-	expression tag	UNP Q15VV3
L	-1	GLN	-	expression tag	UNP Q15VV3
L	0	SER	-	expression tag	UNP Q15VV3

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	K	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



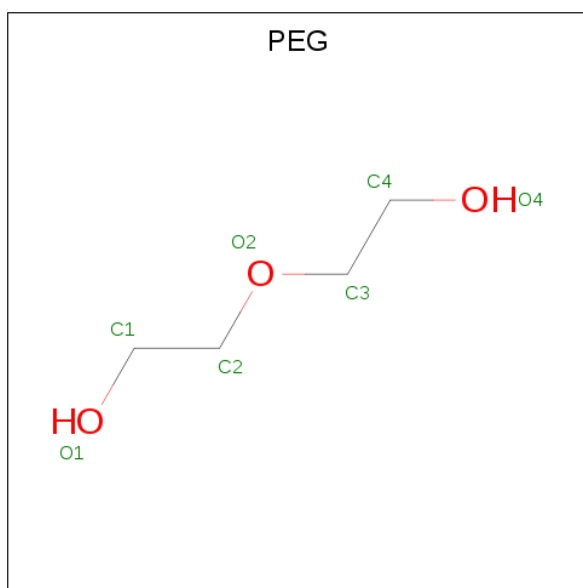
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			7	4	3		
5	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total	O	0	0
			176	176		
6	B	156	Total	O	0	0
			156	156		
6	C	209	Total	O	0	0
			209	209		
6	D	182	Total	O	0	0
			182	182		
6	E	155	Total	O	0	0
			155	155		
6	F	169	Total	O	0	0
			169	169		
6	G	165	Total	O	0	0
			165	165		
6	H	167	Total	O	0	0
			167	167		
6	I	146	Total	O	0	0
			146	146		

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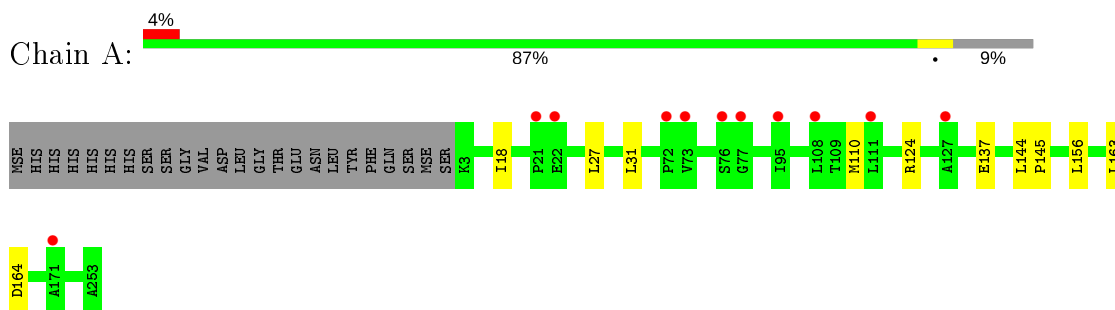
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	167	Total 167	O 167	0	0
6	K	150	Total 150	O 150	0	0
6	L	156	Total 156	O 156	0	0

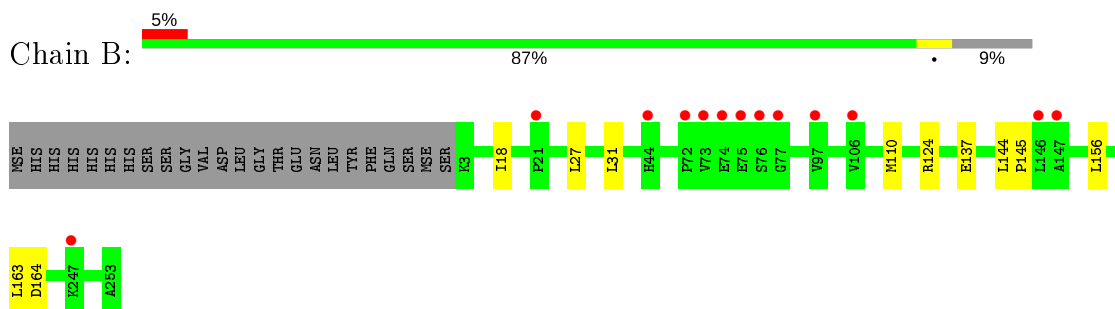
3 Residue-property plots [i](#)

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.

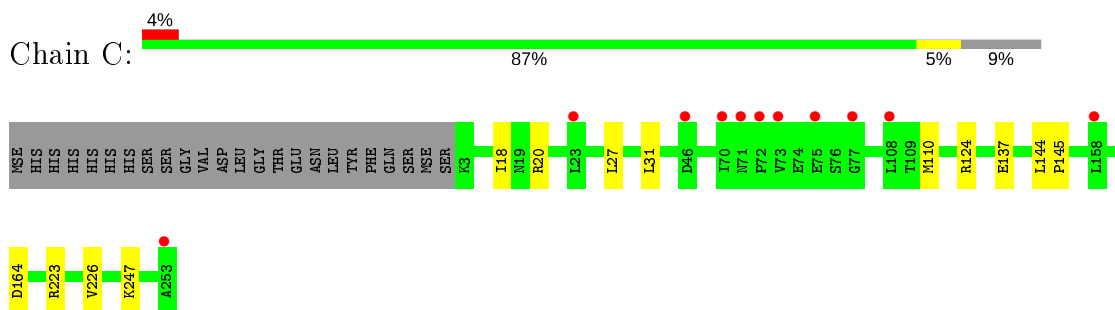
- Molecule 1: Enoyl-CoA hydratase



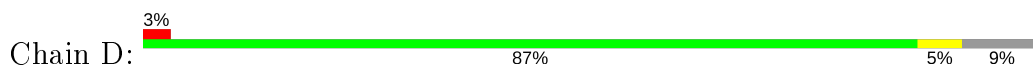
- Molecule 1: Enoyl-CoA hydratase

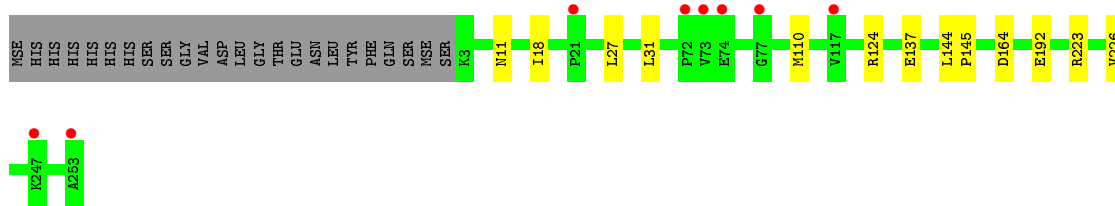


- Molecule 1: Enoyl-CoA hydratase

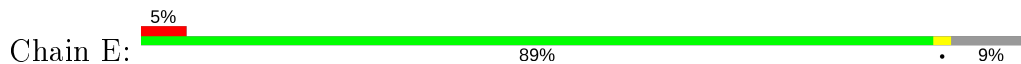


- Molecule 1: Enoyl-CoA hydratase

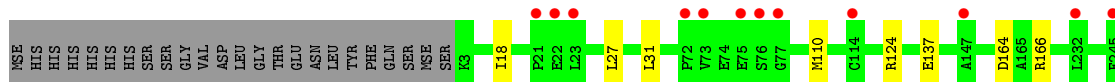
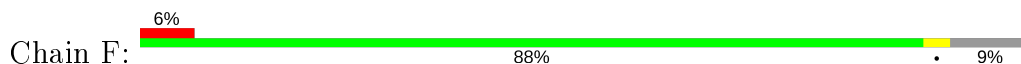




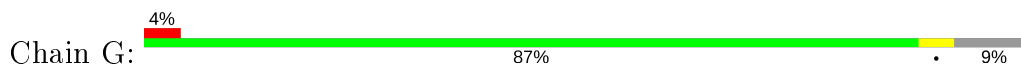
• Molecule 1: Enoyl-CoA hydratase



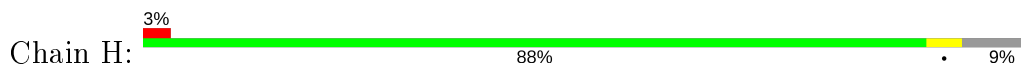
• Molecule 1: Enoyl-CoA hydratase



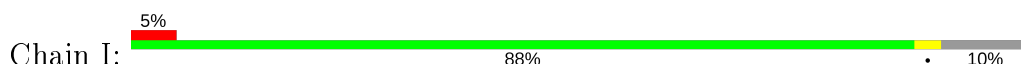
• Molecule 1: Enoyl-CoA hydratase

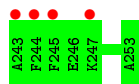


• Molecule 1: Enoyl-CoA hydratase

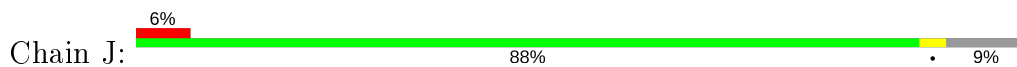


• Molecule 1: Enoyl-CoA hydratase

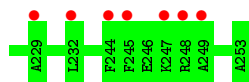
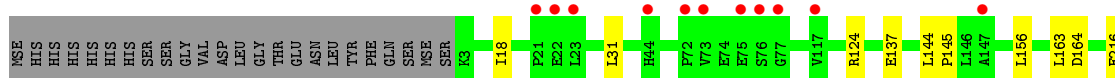
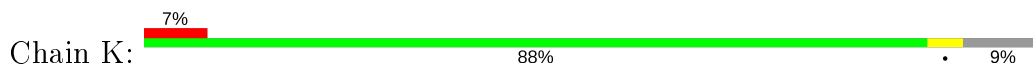




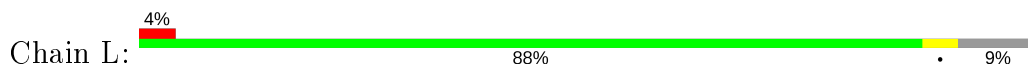
- Molecule 1: Enoyl-CoA hydratase



- Molecule 1: Enoyl-CoA hydratase



- Molecule 1: Enoyl-CoA hydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 160.14Å 136.27Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	38.00 – 2.30 37.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (38.00-2.30) 95.2 (37.77-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.205 , 0.258 0.218 , 0.264	Depositor DCC
R_{free} test set	7178 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtrriage
Anisotropy	0.421	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24561	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9664e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, 1PE, NA

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	0.58	0/1887	0.71	0/2558
1	B	0.58	0/1887	0.71	0/2557
1	C	0.59	0/1907	0.72	1/2583 (0.0%)
1	D	0.60	0/1904	0.72	0/2579
1	E	0.59	0/1893	0.70	0/2567
1	F	0.59	0/1895	0.71	0/2568
1	G	0.61	0/1914	0.73	2/2591 (0.1%)
1	H	0.58	0/1908	0.72	1/2584 (0.0%)
1	I	0.61	0/1880	0.73	0/2544
1	J	0.59	0/1905	0.72	0/2580
1	K	0.60	0/1887	0.72	1/2557 (0.0%)
1	L	0.58	0/1909	0.73	0/2585
All	All	0.59	0/22776	0.72	5/30853 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	216	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	H	166	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	K	216	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	C	20	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	G	223	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1863	0	1849	5	0
1	B	1864	0	1855	5	0
1	C	1883	0	1881	6	0
1	D	1880	0	1872	6	0
1	E	1869	0	1855	3	0
1	F	1872	0	1858	3	0
1	G	1890	0	1894	6	0
1	H	1884	0	1876	4	0
1	I	1859	0	1855	3	0
1	J	1881	0	1881	4	0
1	K	1866	0	1855	4	0
1	L	1885	0	1881	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	C	16	0	22	0	0
3	D	13	0	17	0	0
4	E	12	0	16	0	0
5	G	7	0	10	0	0
5	H	7	0	10	0	0
6	A	176	0	0	0	0
6	B	156	0	0	0	0
6	C	209	0	0	1	0
6	D	182	0	0	0	0
6	E	155	0	0	0	0
6	F	169	0	0	0	0
6	G	165	0	0	0	0
6	H	167	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	146	0	0	0	0
6	J	167	0	0	0	0
6	K	150	0	0	0	0
6	L	156	0	0	0	0
All	All	24561	0	22487	53	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 1.

All (53) 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:D:223:ARG:O	1:D:226:VAL:HG12	2.12	0.49
1:C:223:ARG:O	1:C:226:VAL:HG12	2.13	0.48
1:F:18:ILE:HG23	1:F:31:LEU:HD21	1.97	0.47
1:G:27:LEU:HD21	1:G:110:MSE:HE1	1.96	0.46
1:E:18:ILE:HG23	1:E:31:LEU:HD21	1.98	0.46
1:J:18:ILE:HG23	1:J:31:LEU:HD21	1.98	0.46
1:D:18:ILE:HG23	1:D:31:LEU:HD21	1.98	0.45
1:I:18:ILE:HG23	1:I:31:LEU:HD21	1.98	0.45
1:K:18:ILE:HG23	1:K:31:LEU:HD21	1.98	0.45
1:B:18:ILE:HG23	1:B:31:LEU:HD21	1.98	0.45
1:C:247:LYS:NZ	6:C:406:HOH:O	2.49	0.45
1:E:124:ARG:HD3	1:E:164:ASP:HA	1.99	0.45
1:F:124:ARG:HD3	1:F:164:ASP:HA	1.99	0.45
1:I:124:ARG:HD3	1:I:164:ASP:HA	1.99	0.45
1:J:124:ARG:HD3	1:J:164:ASP:HA	1.99	0.45
1:D:124:ARG:HD3	1:D:164:ASP:HA	1.99	0.44
1:L:18:ILE:HG23	1:L:31:LEU:HD21	1.98	0.44
1:G:18:ILE:HG23	1:G:31:LEU:HD21	1.97	0.44
1:A:18:ILE:HG23	1:A:31:LEU:HD21	1.98	0.44
1:C:124:ARG:HD3	1:C:164:ASP:HA	1.99	0.44
1:B:124:ARG:HD3	1:B:164:ASP:HA	1.99	0.44
1:K:124:ARG:HD3	1:K:164:ASP:HA	1.99	0.44
1:G:124:ARG:HD3	1:G:164:ASP:HA	1.99	0.44
1:H:18:ILE:HG23	1:H:31:LEU:HD21	1.99	0.44
1:C:18:ILE:HG23	1:C:31:LEU:HD21	1.99	0.43
1:H:124:ARG:HD3	1:H:164:ASP:HA	1.99	0.43
1:A:27:LEU:HD11	1:A:110:MSE:HE1	2.01	0.43
1:L:124:ARG:HD3	1:L:164:ASP:HA	2.00	0.43
1:A:124:ARG:HD3	1:A:164:ASP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:HD11	1:C:110:MSE:HE1	2.01	0.42
1:G:27:LEU:CD1	1:G:61:THR:OG1	2.67	0.42
1:E:27:LEU:HD11	1:E:110:MSE:HE1	2.01	0.42
1:G:27:LEU:HD11	1:G:61:THR:OG1	2.20	0.42
1:F:27:LEU:HD11	1:F:110:MSE:HE1	2.02	0.42
1:J:144:LEU:HB3	1:J:145:PRO:HD3	2.02	0.42
1:L:156:LEU:HD21	1:L:163:LEU:HD13	2.02	0.41
1:I:144:LEU:HB3	1:I:145:PRO:HD3	2.03	0.41
1:A:144:LEU:HB3	1:A:145:PRO:HD3	2.03	0.41
1:B:144:LEU:HB3	1:B:145:PRO:HD3	2.03	0.41
1:J:27:LEU:HD11	1:J:110:MSE:HE1	2.01	0.41
1:B:27:LEU:HD11	1:B:110:MSE:HE1	2.02	0.41
1:D:27:LEU:HD11	1:D:110:MSE:HE1	2.03	0.41
1:K:156:LEU:HD21	1:K:163:LEU:HD13	2.03	0.41
1:K:144:LEU:HB3	1:K:145:PRO:HD3	2.03	0.41
1:L:144:LEU:HB3	1:L:145:PRO:HD3	2.03	0.41
1:D:144:LEU:HB3	1:D:145:PRO:HD3	2.03	0.41
1:G:144:LEU:HB3	1:G:145:PRO:HD3	2.03	0.40
1:C:144:LEU:HB3	1:C:145:PRO:HD3	2.03	0.40
1:H:156:LEU:HD21	1:H:163:LEU:HD13	2.04	0.40
1:H:144:LEU:HB3	1:H:145:PRO:HD3	2.03	0.40
1:A:156:LEU:HD21	1:A:163:LEU:HD13	2.04	0.40
1:B:156:LEU:HD21	1:B:163:LEU:HD13	2.04	0.40
1:D:11:ASN:ND2	1:D:192:GLU:OE1	2.50	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	249/275 (90%)	244 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	C	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	D	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	E	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	F	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	G	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	H	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	I	244/275 (89%)	240 (98%)	4 (2%)	0	100	100
1	J	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	K	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
1	L	249/275 (90%)	244 (98%)	5 (2%)	0	100	100
All	All	2983/3300 (90%)	2924 (98%)	59 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	189/221 (86%)	188 (100%)	1 (0%)	88	95
1	B	190/221 (86%)	189 (100%)	1 (0%)	88	95
1	C	194/221 (88%)	193 (100%)	1 (0%)	88	95
1	D	193/221 (87%)	192 (100%)	1 (0%)	88	95
1	E	191/221 (86%)	191 (100%)	0	100	100
1	F	191/221 (86%)	189 (99%)	2 (1%)	76	87
1	G	196/221 (89%)	195 (100%)	1 (0%)	88	95
1	H	194/221 (88%)	193 (100%)	1 (0%)	88	95
1	I	191/221 (86%)	190 (100%)	1 (0%)	88	95
1	J	194/221 (88%)	193 (100%)	1 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	191/221 (86%)	190 (100%)	1 (0%)	88	95
1	L	195/221 (88%)	193 (99%)	2 (1%)	76	87
All	All	2309/2652 (87%)	2296 (99%)	13 (1%)	86	94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	B	137	GLU
1	C	137	GLU
1	D	137	GLU
1	F	137	GLU
1	F	166	ARG
1	G	137	GLU
1	H	137	GLU
1	I	137	GLU
1	J	137	GLU
1	K	137	GLU
1	L	137	GLU
1	L	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\# Z > 2$
5	PEG	H	302	-	6,6,6	0.60	0	5,5,5	0.52	0
4	GOL	E	302	-	5,5,5	0.57	0	5,5,5	0.42	0
4	GOL	E	301	-	5,5,5	0.49	0	5,5,5	0.54	0
3	1PE	C	302	-	15,15,15	0.50	0	14,14,14	0.41	0
3	1PE	D	302	-	12,12,15	0.53	0	11,11,14	0.33	0
5	PEG	G	302	-	6,6,6	0.59	0	5,5,5	0.29	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
5	PEG	H	302	-	-	2/4/4/4	-
4	GOL	E	302	-	-	2/4/4/4	-
4	GOL	E	301	-	-	3/4/4/4	-
3	1PE	C	302	-	-	5/13/13/13	-
3	1PE	D	302	-	-	7/10/10/13	-
5	PEG	G	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	302	GOL	C1-C2-C3-O3
4	E	302	GOL	O2-C2-C3-O3
3	C	302	1PE	OH4-C13-C23-OH3
3	C	302	1PE	OH6-C15-C25-OH5
5	H	302	PEG	O1-C1-C2-O2
3	D	302	1PE	OH7-C16-C26-OH6

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Mol	Chain	Res	Type	Atoms
4	E	301	GOL	O1-C1-C2-C3
4	E	301	GOL	C1-C2-C3-O3
5	H	302	PEG	O2-C3-C4-O4
3	D	302	1PE	OH4-C13-C23-OH3
4	E	301	GOL	O2-C2-C3-O3
3	C	302	1PE	C25-C15-OH6-C26
3	C	302	1PE	C13-C23-OH3-C22
5	G	302	PEG	O1-C1-C2-O2
3	D	302	1PE	OH6-C15-C25-OH5
3	D	302	1PE	C14-C24-OH4-C13
3	D	302	1PE	OH5-C14-C24-OH4
3	D	302	1PE	C15-C25-OH5-C14
3	D	302	1PE	C23-C13-OH4-C24
3	C	302	1PE	OH5-C14-C24-OH4
5	G	302	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	247/275 (89%)	0.14	11 (4%) 33 40	27, 40, 79, 143	0
1	B	247/275 (89%)	0.30	13 (5%) 26 33	27, 42, 96, 177	0
1	C	247/275 (89%)	0.01	11 (4%) 33 40	25, 38, 76, 113	0
1	D	247/275 (89%)	-0.01	8 (3%) 47 54	25, 39, 75, 115	0
1	E	247/275 (89%)	0.16	13 (5%) 26 33	24, 40, 88, 141	0
1	F	247/275 (89%)	0.32	16 (6%) 18 24	23, 41, 101, 166	0
1	G	247/275 (89%)	0.04	12 (4%) 29 36	26, 40, 78, 119	0
1	H	247/275 (89%)	0.06	8 (3%) 47 54	23, 40, 79, 117	0
1	I	244/275 (88%)	0.24	13 (5%) 26 33	26, 43, 94, 139	0
1	J	247/275 (89%)	0.18	16 (6%) 18 24	25, 41, 86, 155	0
1	K	247/275 (89%)	0.24	18 (7%) 15 20	28, 41, 97, 195	0
1	L	247/275 (89%)	0.12	11 (4%) 33 40	27, 41, 86, 165	0
All	All	2961/3300 (89%)	0.15	150 (5%) 28 35	23, 41, 87, 195	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	72	PRO	10.7
1	K	72	PRO	9.4
1	J	72	PRO	8.6
1	I	76	SER	7.7
1	J	73	VAL	7.1
1	F	72	PRO	6.8
1	E	72	PRO	5.9
1	D	73	VAL	5.5
1	B	72	PRO	5.5
1	D	72	PRO	5.3
1	J	76	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	73	VAL	5.2
1	I	77	GLY	5.1
1	H	77	GLY	5.0
1	C	72	PRO	4.9
1	I	245	PHE	4.8
1	H	76	SER	4.8
1	C	73	VAL	4.6
1	F	21	PRO	4.6
1	F	73	VAL	4.6
1	L	76	SER	4.5
1	F	77	GLY	4.5
1	A	72	PRO	4.4
1	F	76	SER	4.3
1	K	76	SER	4.3
1	J	75	GLU	4.2
1	A	73	VAL	4.1
1	F	23	LEU	4.0
1	E	77	GLY	4.0
1	J	77	GLY	3.9
1	J	74	GLU	3.9
1	F	253	ALA	3.9
1	E	69	PHE	3.8
1	J	71	ASN	3.8
1	I	23	LEU	3.7
1	G	76	SER	3.7
1	E	76	SER	3.7
1	H	72	PRO	3.7
1	G	77	GLY	3.6
1	C	253	ALA	3.6
1	K	247	LYS	3.6
1	E	75	GLU	3.5
1	A	108	LEU	3.5
1	B	147	ALA	3.3
1	E	73	VAL	3.3
1	L	73	VAL	3.3
1	D	253	ALA	3.3
1	F	251	HIS	3.2
1	D	21	PRO	3.2
1	F	232	LEU	3.2
1	G	73	VAL	3.2
1	G	72	PRO	3.2
1	A	76	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	69	PHE	3.1
1	K	147	ALA	3.1
1	I	21	PRO	3.1
1	B	247	LYS	3.1
1	K	23	LEU	3.0
1	H	108	LEU	2.9
1	A	77	GLY	2.9
1	D	74	GLU	2.9
1	L	69	PHE	2.9
1	F	247	LYS	2.9
1	E	108	LEU	2.8
1	G	21	PRO	2.8
1	B	106	VAL	2.8
1	B	74	GLU	2.8
1	E	74	GLU	2.8
1	G	147	ALA	2.7
1	L	21	PRO	2.7
1	F	245	PHE	2.7
1	G	108	LEU	2.7
1	I	68	ASP	2.7
1	B	77	GLY	2.7
1	B	44	HIS	2.7
1	K	44	HIS	2.6
1	I	247	LYS	2.6
1	I	232	LEU	2.6
1	K	22	GLU	2.6
1	L	108	LEU	2.6
1	L	77	GLY	2.6
1	E	78	THR	2.5
1	E	245	PHE	2.5
1	C	23	LEU	2.5
1	H	23	LEU	2.5
1	F	147	ALA	2.5
1	C	46	ASP	2.5
1	F	249	ALA	2.5
1	J	108	LEU	2.5
1	B	76	SER	2.5
1	G	106	VAL	2.4
1	E	21	PRO	2.4
1	C	108	LEU	2.4
1	K	75	GLU	2.4
1	J	68	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	75	GLU	2.4
1	E	171	ALA	2.4
1	J	22	GLU	2.4
1	K	77	GLY	2.4
1	K	248	ARG	2.4
1	G	109	THR	2.4
1	I	109	THR	2.4
1	J	70	ILE	2.4
1	L	253	ALA	2.4
1	I	70	ILE	2.3
1	B	146	LEU	2.3
1	C	75	GLU	2.3
1	K	117	VAL	2.3
1	B	21	PRO	2.3
1	K	229	ALA	2.3
1	A	171	ALA	2.3
1	D	247	LYS	2.3
1	K	249	ALA	2.3
1	K	232	LEU	2.3
1	A	95	ILE	2.3
1	F	114	CYS	2.3
1	J	46	ASP	2.2
1	D	117	VAL	2.2
1	J	78	THR	2.2
1	A	21	PRO	2.2
1	I	114	CYS	2.2
1	F	22	GLU	2.2
1	I	244	PHE	2.2
1	J	111	LEU	2.2
1	I	243	ALA	2.2
1	H	73	VAL	2.1
1	H	69	PHE	2.1
1	G	253	ALA	2.1
1	B	75	GLU	2.1
1	F	75	GLU	2.1
1	K	73	VAL	2.1
1	K	245	PHE	2.1
1	A	111	LEU	2.1
1	A	22	GLU	2.1
1	C	158	LEU	2.1
1	C	71	ASN	2.1
1	B	97	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	77	GLY	2.1
1	A	127	ALA	2.1
1	K	21	PRO	2.1
1	L	74	GLU	2.0
1	C	70	ILE	2.0
1	E	111	LEU	2.0
1	H	109	THR	2.0
1	D	77	GLY	2.0
1	J	245	PHE	2.0
1	K	244	PHE	2.0
1	G	68	ASP	2.0
1	G	226	VAL	2.0
1	L	158	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th 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(\AA^2)	Q<0.9
3	1PE	D	302	13/16	0.83	0.20	32,55,73,77	0
4	GOL	E	301	6/6	0.84	0.12	58,71,90,98	0
4	GOL	E	302	6/6	0.84	0.16	44,56,66,67	0
3	1PE	C	302	16/16	0.86	0.17	44,60,79,79	0
2	NA	B	301	1/1	0.89	0.07	38,38,38,38	0
5	PEG	H	302	7/7	0.90	0.15	40,58,68,85	0
2	NA	D	301	1/1	0.90	0.07	38,38,38,38	0
2	NA	G	301	1/1	0.91	0.08	29,29,29,29	0
5	PEG	G	302	7/7	0.91	0.15	43,62,76,90	0
2	NA	H	301	1/1	0.91	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	J	301	1/1	0.92	0.12	41,41,41,41	0
2	NA	F	301	1/1	0.94	0.08	33,33,33,33	0
2	NA	E	303	1/1	0.94	0.09	36,36,36,36	0
2	NA	C	301	1/1	0.94	0.05	40,40,40,40	0
2	NA	I	301	1/1	0.95	0.12	41,41,41,41	0
2	NA	K	301	1/1	0.96	0.06	39,39,39,39	0
2	NA	L	301	1/1	0.97	0.04	39,39,39,39	0
2	NA	A	301	1/1	0.97	0.07	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.