



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:22 PM UTC

PDB ID : 4W61 / pdb_00004w61
Title : Crystal structure of beta-ketoacyl thiolase B (BktB) from *Ralstonia eutropha*
Authors : Fage, C.D.; Keatinge-Clay, A.T.
Deposited on : 2014-08-19
Resolution : 2.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

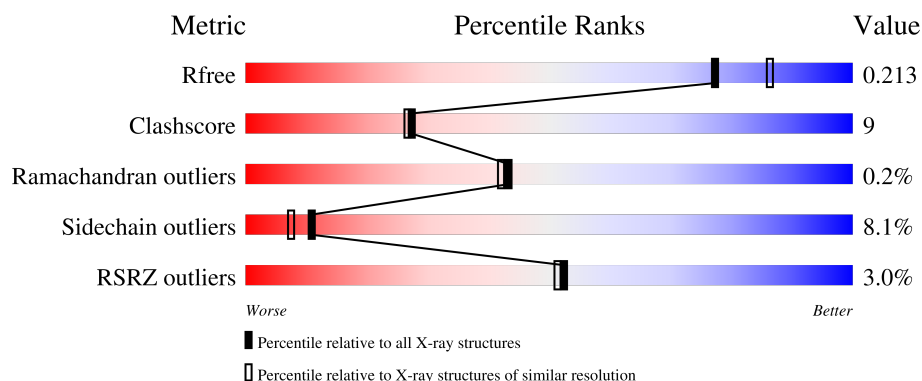
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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.



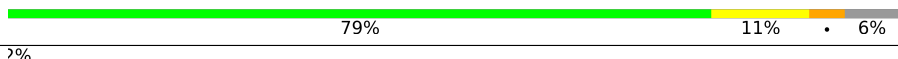
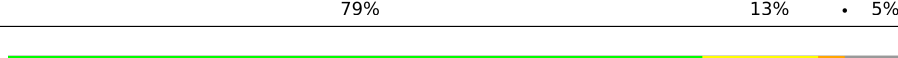
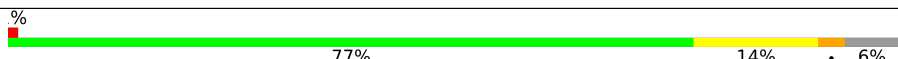
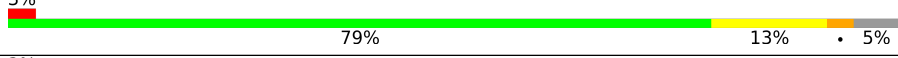
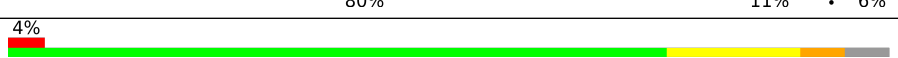
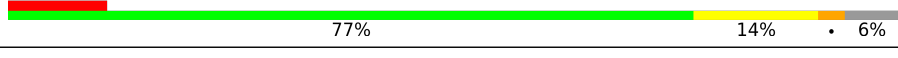
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	414	0% 79% 13% • 5%
1	B	414	3% 79% 12% • 6%
1	C	414	0% 80% 11% • 6%
1	D	414	80% 11% • 6%
1	E	414	5% 78% 13% • 7%

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Mol	Chain	Length	Quality of chain
1	F	414	 79% 13% • 6%
1	G	414	 79% 11% • 6%
1	H	414	 79% 13% • 5%
1	I	414	 78% 13% • 6%
1	J	414	 77% 14% • 6%
1	K	414	 79% 13% • 5%
1	L	414	 80% 11% • 6%
1	M	414	 80% 11% • 6%
1	N	414	 74% 15% 5% 6%
1	O	414	 80% 11% • 6%
1	P	414	 77% 14% • 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46062 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 Beta-ketothiolase BktB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			2859	1776	526	542	15			
1	B	391	Total	C	N	O	S	0	1	0
			2855	1775	525	541	14			
1	C	389	Total	C	N	O	S	0	1	0
			2837	1763	521	539	14			
1	D	390	Total	C	N	O	S	0	0	0
			2836	1763	520	539	14			
1	E	386	Total	C	N	O	S	0	0	0
			2806	1744	513	535	14			
1	F	388	Total	C	N	O	S	0	0	0
			2823	1755	517	537	14			
1	G	389	Total	C	N	O	S	0	0	0
			2831	1760	518	538	15			
1	H	392	Total	C	N	O	S	0	0	0
			2848	1771	522	541	14			
1	I	390	Total	C	N	O	S	0	1	0
			2847	1770	521	541	15			
1	J	389	Total	C	N	O	S	0	0	0
			2827	1757	518	538	14			
1	K	392	Total	C	N	O	S	0	0	0
			2850	1771	524	541	14			
1	L	390	Total	C	N	O	S	0	1	0
			2842	1765	523	540	14			
1	M	390	Total	C	N	O	S	0	0	0
			2835	1763	519	539	14			
1	N	392	Total	C	N	O	S	0	0	0
			2851	1771	525	541	14			
1	O	388	Total	C	N	O	S	0	0	0
			2823	1755	517	537	14			
1	P	388	Total	C	N	O	S	0	0	0
			2818	1751	516	537	14			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q0KBP1
A	-18	GLY	-	expression tag	UNP Q0KBP1
A	-17	SER	-	expression tag	UNP Q0KBP1
A	-16	SER	-	expression tag	UNP Q0KBP1
A	-15	HIS	-	expression tag	UNP Q0KBP1
A	-14	HIS	-	expression tag	UNP Q0KBP1
A	-13	HIS	-	expression tag	UNP Q0KBP1
A	-12	HIS	-	expression tag	UNP Q0KBP1
A	-11	HIS	-	expression tag	UNP Q0KBP1
A	-10	HIS	-	expression tag	UNP Q0KBP1
A	-9	SER	-	expression tag	UNP Q0KBP1
A	-8	SER	-	expression tag	UNP Q0KBP1
A	-7	GLY	-	expression tag	UNP Q0KBP1
A	-6	LEU	-	expression tag	UNP Q0KBP1
A	-5	VAL	-	expression tag	UNP Q0KBP1
A	-4	PRO	-	expression tag	UNP Q0KBP1
A	-3	ARG	-	expression tag	UNP Q0KBP1
A	-2	GLY	-	expression tag	UNP Q0KBP1
A	-1	SER	-	expression tag	UNP Q0KBP1
A	0	HIS	-	expression tag	UNP Q0KBP1
B	-19	MET	-	initiating methionine	UNP Q0KBP1
B	-18	GLY	-	expression tag	UNP Q0KBP1
B	-17	SER	-	expression tag	UNP Q0KBP1
B	-16	SER	-	expression tag	UNP Q0KBP1
B	-15	HIS	-	expression tag	UNP Q0KBP1
B	-14	HIS	-	expression tag	UNP Q0KBP1
B	-13	HIS	-	expression tag	UNP Q0KBP1
B	-12	HIS	-	expression tag	UNP Q0KBP1
B	-11	HIS	-	expression tag	UNP Q0KBP1
B	-10	HIS	-	expression tag	UNP Q0KBP1
B	-9	SER	-	expression tag	UNP Q0KBP1
B	-8	SER	-	expression tag	UNP Q0KBP1
B	-7	GLY	-	expression tag	UNP Q0KBP1
B	-6	LEU	-	expression tag	UNP Q0KBP1
B	-5	VAL	-	expression tag	UNP Q0KBP1
B	-4	PRO	-	expression tag	UNP Q0KBP1
B	-3	ARG	-	expression tag	UNP Q0KBP1
B	-2	GLY	-	expression tag	UNP Q0KBP1
B	-1	SER	-	expression tag	UNP Q0KBP1
B	0	HIS	-	expression tag	UNP Q0KBP1
C	-19	MET	-	initiating methionine	UNP Q0KBP1
C	-18	GLY	-	expression tag	UNP Q0KBP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP Q0KBP1
C	-16	SER	-	expression tag	UNP Q0KBP1
C	-15	HIS	-	expression tag	UNP Q0KBP1
C	-14	HIS	-	expression tag	UNP Q0KBP1
C	-13	HIS	-	expression tag	UNP Q0KBP1
C	-12	HIS	-	expression tag	UNP Q0KBP1
C	-11	HIS	-	expression tag	UNP Q0KBP1
C	-10	HIS	-	expression tag	UNP Q0KBP1
C	-9	SER	-	expression tag	UNP Q0KBP1
C	-8	SER	-	expression tag	UNP Q0KBP1
C	-7	GLY	-	expression tag	UNP Q0KBP1
C	-6	LEU	-	expression tag	UNP Q0KBP1
C	-5	VAL	-	expression tag	UNP Q0KBP1
C	-4	PRO	-	expression tag	UNP Q0KBP1
C	-3	ARG	-	expression tag	UNP Q0KBP1
C	-2	GLY	-	expression tag	UNP Q0KBP1
C	-1	SER	-	expression tag	UNP Q0KBP1
C	0	HIS	-	expression tag	UNP Q0KBP1
D	-19	MET	-	initiating methionine	UNP Q0KBP1
D	-18	GLY	-	expression tag	UNP Q0KBP1
D	-17	SER	-	expression tag	UNP Q0KBP1
D	-16	SER	-	expression tag	UNP Q0KBP1
D	-15	HIS	-	expression tag	UNP Q0KBP1
D	-14	HIS	-	expression tag	UNP Q0KBP1
D	-13	HIS	-	expression tag	UNP Q0KBP1
D	-12	HIS	-	expression tag	UNP Q0KBP1
D	-11	HIS	-	expression tag	UNP Q0KBP1
D	-10	HIS	-	expression tag	UNP Q0KBP1
D	-9	SER	-	expression tag	UNP Q0KBP1
D	-8	SER	-	expression tag	UNP Q0KBP1
D	-7	GLY	-	expression tag	UNP Q0KBP1
D	-6	LEU	-	expression tag	UNP Q0KBP1
D	-5	VAL	-	expression tag	UNP Q0KBP1
D	-4	PRO	-	expression tag	UNP Q0KBP1
D	-3	ARG	-	expression tag	UNP Q0KBP1
D	-2	GLY	-	expression tag	UNP Q0KBP1
D	-1	SER	-	expression tag	UNP Q0KBP1
D	0	HIS	-	expression tag	UNP Q0KBP1
E	-19	MET	-	initiating methionine	UNP Q0KBP1
E	-18	GLY	-	expression tag	UNP Q0KBP1
E	-17	SER	-	expression tag	UNP Q0KBP1
E	-16	SER	-	expression tag	UNP Q0KBP1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q0KBP1
E	-14	HIS	-	expression tag	UNP Q0KBP1
E	-13	HIS	-	expression tag	UNP Q0KBP1
E	-12	HIS	-	expression tag	UNP Q0KBP1
E	-11	HIS	-	expression tag	UNP Q0KBP1
E	-10	HIS	-	expression tag	UNP Q0KBP1
E	-9	SER	-	expression tag	UNP Q0KBP1
E	-8	SER	-	expression tag	UNP Q0KBP1
E	-7	GLY	-	expression tag	UNP Q0KBP1
E	-6	LEU	-	expression tag	UNP Q0KBP1
E	-5	VAL	-	expression tag	UNP Q0KBP1
E	-4	PRO	-	expression tag	UNP Q0KBP1
E	-3	ARG	-	expression tag	UNP Q0KBP1
E	-2	GLY	-	expression tag	UNP Q0KBP1
E	-1	SER	-	expression tag	UNP Q0KBP1
E	0	HIS	-	expression tag	UNP Q0KBP1
F	-19	MET	-	initiating methionine	UNP Q0KBP1
F	-18	GLY	-	expression tag	UNP Q0KBP1
F	-17	SER	-	expression tag	UNP Q0KBP1
F	-16	SER	-	expression tag	UNP Q0KBP1
F	-15	HIS	-	expression tag	UNP Q0KBP1
F	-14	HIS	-	expression tag	UNP Q0KBP1
F	-13	HIS	-	expression tag	UNP Q0KBP1
F	-12	HIS	-	expression tag	UNP Q0KBP1
F	-11	HIS	-	expression tag	UNP Q0KBP1
F	-10	HIS	-	expression tag	UNP Q0KBP1
F	-9	SER	-	expression tag	UNP Q0KBP1
F	-8	SER	-	expression tag	UNP Q0KBP1
F	-7	GLY	-	expression tag	UNP Q0KBP1
F	-6	LEU	-	expression tag	UNP Q0KBP1
F	-5	VAL	-	expression tag	UNP Q0KBP1
F	-4	PRO	-	expression tag	UNP Q0KBP1
F	-3	ARG	-	expression tag	UNP Q0KBP1
F	-2	GLY	-	expression tag	UNP Q0KBP1
F	-1	SER	-	expression tag	UNP Q0KBP1
F	0	HIS	-	expression tag	UNP Q0KBP1
G	-19	MET	-	initiating methionine	UNP Q0KBP1
G	-18	GLY	-	expression tag	UNP Q0KBP1
G	-17	SER	-	expression tag	UNP Q0KBP1
G	-16	SER	-	expression tag	UNP Q0KBP1
G	-15	HIS	-	expression tag	UNP Q0KBP1
G	-14	HIS	-	expression tag	UNP Q0KBP1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP Q0KBP1
G	-12	HIS	-	expression tag	UNP Q0KBP1
G	-11	HIS	-	expression tag	UNP Q0KBP1
G	-10	HIS	-	expression tag	UNP Q0KBP1
G	-9	SER	-	expression tag	UNP Q0KBP1
G	-8	SER	-	expression tag	UNP Q0KBP1
G	-7	GLY	-	expression tag	UNP Q0KBP1
G	-6	LEU	-	expression tag	UNP Q0KBP1
G	-5	VAL	-	expression tag	UNP Q0KBP1
G	-4	PRO	-	expression tag	UNP Q0KBP1
G	-3	ARG	-	expression tag	UNP Q0KBP1
G	-2	GLY	-	expression tag	UNP Q0KBP1
G	-1	SER	-	expression tag	UNP Q0KBP1
G	0	HIS	-	expression tag	UNP Q0KBP1
H	-19	MET	-	initiating methionine	UNP Q0KBP1
H	-18	GLY	-	expression tag	UNP Q0KBP1
H	-17	SER	-	expression tag	UNP Q0KBP1
H	-16	SER	-	expression tag	UNP Q0KBP1
H	-15	HIS	-	expression tag	UNP Q0KBP1
H	-14	HIS	-	expression tag	UNP Q0KBP1
H	-13	HIS	-	expression tag	UNP Q0KBP1
H	-12	HIS	-	expression tag	UNP Q0KBP1
H	-11	HIS	-	expression tag	UNP Q0KBP1
H	-10	HIS	-	expression tag	UNP Q0KBP1
H	-9	SER	-	expression tag	UNP Q0KBP1
H	-8	SER	-	expression tag	UNP Q0KBP1
H	-7	GLY	-	expression tag	UNP Q0KBP1
H	-6	LEU	-	expression tag	UNP Q0KBP1
H	-5	VAL	-	expression tag	UNP Q0KBP1
H	-4	PRO	-	expression tag	UNP Q0KBP1
H	-3	ARG	-	expression tag	UNP Q0KBP1
H	-2	GLY	-	expression tag	UNP Q0KBP1
H	-1	SER	-	expression tag	UNP Q0KBP1
H	0	HIS	-	expression tag	UNP Q0KBP1
I	-19	MET	-	initiating methionine	UNP Q0KBP1
I	-18	GLY	-	expression tag	UNP Q0KBP1
I	-17	SER	-	expression tag	UNP Q0KBP1
I	-16	SER	-	expression tag	UNP Q0KBP1
I	-15	HIS	-	expression tag	UNP Q0KBP1
I	-14	HIS	-	expression tag	UNP Q0KBP1
I	-13	HIS	-	expression tag	UNP Q0KBP1
I	-12	HIS	-	expression tag	UNP Q0KBP1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP Q0KBP1
I	-10	HIS	-	expression tag	UNP Q0KBP1
I	-9	SER	-	expression tag	UNP Q0KBP1
I	-8	SER	-	expression tag	UNP Q0KBP1
I	-7	GLY	-	expression tag	UNP Q0KBP1
I	-6	LEU	-	expression tag	UNP Q0KBP1
I	-5	VAL	-	expression tag	UNP Q0KBP1
I	-4	PRO	-	expression tag	UNP Q0KBP1
I	-3	ARG	-	expression tag	UNP Q0KBP1
I	-2	GLY	-	expression tag	UNP Q0KBP1
I	-1	SER	-	expression tag	UNP Q0KBP1
I	0	HIS	-	expression tag	UNP Q0KBP1
J	-19	MET	-	initiating methionine	UNP Q0KBP1
J	-18	GLY	-	expression tag	UNP Q0KBP1
J	-17	SER	-	expression tag	UNP Q0KBP1
J	-16	SER	-	expression tag	UNP Q0KBP1
J	-15	HIS	-	expression tag	UNP Q0KBP1
J	-14	HIS	-	expression tag	UNP Q0KBP1
J	-13	HIS	-	expression tag	UNP Q0KBP1
J	-12	HIS	-	expression tag	UNP Q0KBP1
J	-11	HIS	-	expression tag	UNP Q0KBP1
J	-10	HIS	-	expression tag	UNP Q0KBP1
J	-9	SER	-	expression tag	UNP Q0KBP1
J	-8	SER	-	expression tag	UNP Q0KBP1
J	-7	GLY	-	expression tag	UNP Q0KBP1
J	-6	LEU	-	expression tag	UNP Q0KBP1
J	-5	VAL	-	expression tag	UNP Q0KBP1
J	-4	PRO	-	expression tag	UNP Q0KBP1
J	-3	ARG	-	expression tag	UNP Q0KBP1
J	-2	GLY	-	expression tag	UNP Q0KBP1
J	-1	SER	-	expression tag	UNP Q0KBP1
J	0	HIS	-	expression tag	UNP Q0KBP1
K	-19	MET	-	initiating methionine	UNP Q0KBP1
K	-18	GLY	-	expression tag	UNP Q0KBP1
K	-17	SER	-	expression tag	UNP Q0KBP1
K	-16	SER	-	expression tag	UNP Q0KBP1
K	-15	HIS	-	expression tag	UNP Q0KBP1
K	-14	HIS	-	expression tag	UNP Q0KBP1
K	-13	HIS	-	expression tag	UNP Q0KBP1
K	-12	HIS	-	expression tag	UNP Q0KBP1
K	-11	HIS	-	expression tag	UNP Q0KBP1
K	-10	HIS	-	expression tag	UNP Q0KBP1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	expression tag	UNP Q0KBP1
K	-8	SER	-	expression tag	UNP Q0KBP1
K	-7	GLY	-	expression tag	UNP Q0KBP1
K	-6	LEU	-	expression tag	UNP Q0KBP1
K	-5	VAL	-	expression tag	UNP Q0KBP1
K	-4	PRO	-	expression tag	UNP Q0KBP1
K	-3	ARG	-	expression tag	UNP Q0KBP1
K	-2	GLY	-	expression tag	UNP Q0KBP1
K	-1	SER	-	expression tag	UNP Q0KBP1
K	0	HIS	-	expression tag	UNP Q0KBP1
L	-19	MET	-	initiating methionine	UNP Q0KBP1
L	-18	GLY	-	expression tag	UNP Q0KBP1
L	-17	SER	-	expression tag	UNP Q0KBP1
L	-16	SER	-	expression tag	UNP Q0KBP1
L	-15	HIS	-	expression tag	UNP Q0KBP1
L	-14	HIS	-	expression tag	UNP Q0KBP1
L	-13	HIS	-	expression tag	UNP Q0KBP1
L	-12	HIS	-	expression tag	UNP Q0KBP1
L	-11	HIS	-	expression tag	UNP Q0KBP1
L	-10	HIS	-	expression tag	UNP Q0KBP1
L	-9	SER	-	expression tag	UNP Q0KBP1
L	-8	SER	-	expression tag	UNP Q0KBP1
L	-7	GLY	-	expression tag	UNP Q0KBP1
L	-6	LEU	-	expression tag	UNP Q0KBP1
L	-5	VAL	-	expression tag	UNP Q0KBP1
L	-4	PRO	-	expression tag	UNP Q0KBP1
L	-3	ARG	-	expression tag	UNP Q0KBP1
L	-2	GLY	-	expression tag	UNP Q0KBP1
L	-1	SER	-	expression tag	UNP Q0KBP1
L	0	HIS	-	expression tag	UNP Q0KBP1
M	-19	MET	-	initiating methionine	UNP Q0KBP1
M	-18	GLY	-	expression tag	UNP Q0KBP1
M	-17	SER	-	expression tag	UNP Q0KBP1
M	-16	SER	-	expression tag	UNP Q0KBP1
M	-15	HIS	-	expression tag	UNP Q0KBP1
M	-14	HIS	-	expression tag	UNP Q0KBP1
M	-13	HIS	-	expression tag	UNP Q0KBP1
M	-12	HIS	-	expression tag	UNP Q0KBP1
M	-11	HIS	-	expression tag	UNP Q0KBP1
M	-10	HIS	-	expression tag	UNP Q0KBP1
M	-9	SER	-	expression tag	UNP Q0KBP1
M	-8	SER	-	expression tag	UNP Q0KBP1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLY	-	expression tag	UNP Q0KBP1
M	-6	LEU	-	expression tag	UNP Q0KBP1
M	-5	VAL	-	expression tag	UNP Q0KBP1
M	-4	PRO	-	expression tag	UNP Q0KBP1
M	-3	ARG	-	expression tag	UNP Q0KBP1
M	-2	GLY	-	expression tag	UNP Q0KBP1
M	-1	SER	-	expression tag	UNP Q0KBP1
M	0	HIS	-	expression tag	UNP Q0KBP1
N	-19	MET	-	initiating methionine	UNP Q0KBP1
N	-18	GLY	-	expression tag	UNP Q0KBP1
N	-17	SER	-	expression tag	UNP Q0KBP1
N	-16	SER	-	expression tag	UNP Q0KBP1
N	-15	HIS	-	expression tag	UNP Q0KBP1
N	-14	HIS	-	expression tag	UNP Q0KBP1
N	-13	HIS	-	expression tag	UNP Q0KBP1
N	-12	HIS	-	expression tag	UNP Q0KBP1
N	-11	HIS	-	expression tag	UNP Q0KBP1
N	-10	HIS	-	expression tag	UNP Q0KBP1
N	-9	SER	-	expression tag	UNP Q0KBP1
N	-8	SER	-	expression tag	UNP Q0KBP1
N	-7	GLY	-	expression tag	UNP Q0KBP1
N	-6	LEU	-	expression tag	UNP Q0KBP1
N	-5	VAL	-	expression tag	UNP Q0KBP1
N	-4	PRO	-	expression tag	UNP Q0KBP1
N	-3	ARG	-	expression tag	UNP Q0KBP1
N	-2	GLY	-	expression tag	UNP Q0KBP1
N	-1	SER	-	expression tag	UNP Q0KBP1
N	0	HIS	-	expression tag	UNP Q0KBP1
O	-19	MET	-	initiating methionine	UNP Q0KBP1
O	-18	GLY	-	expression tag	UNP Q0KBP1
O	-17	SER	-	expression tag	UNP Q0KBP1
O	-16	SER	-	expression tag	UNP Q0KBP1
O	-15	HIS	-	expression tag	UNP Q0KBP1
O	-14	HIS	-	expression tag	UNP Q0KBP1
O	-13	HIS	-	expression tag	UNP Q0KBP1
O	-12	HIS	-	expression tag	UNP Q0KBP1
O	-11	HIS	-	expression tag	UNP Q0KBP1
O	-10	HIS	-	expression tag	UNP Q0KBP1
O	-9	SER	-	expression tag	UNP Q0KBP1
O	-8	SER	-	expression tag	UNP Q0KBP1
O	-7	GLY	-	expression tag	UNP Q0KBP1
O	-6	LEU	-	expression tag	UNP Q0KBP1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	VAL	-	expression tag	UNP Q0KBP1
O	-4	PRO	-	expression tag	UNP Q0KBP1
O	-3	ARG	-	expression tag	UNP Q0KBP1
O	-2	GLY	-	expression tag	UNP Q0KBP1
O	-1	SER	-	expression tag	UNP Q0KBP1
O	0	HIS	-	expression tag	UNP Q0KBP1
P	-19	MET	-	initiating methionine	UNP Q0KBP1
P	-18	GLY	-	expression tag	UNP Q0KBP1
P	-17	SER	-	expression tag	UNP Q0KBP1
P	-16	SER	-	expression tag	UNP Q0KBP1
P	-15	HIS	-	expression tag	UNP Q0KBP1
P	-14	HIS	-	expression tag	UNP Q0KBP1
P	-13	HIS	-	expression tag	UNP Q0KBP1
P	-12	HIS	-	expression tag	UNP Q0KBP1
P	-11	HIS	-	expression tag	UNP Q0KBP1
P	-10	HIS	-	expression tag	UNP Q0KBP1
P	-9	SER	-	expression tag	UNP Q0KBP1
P	-8	SER	-	expression tag	UNP Q0KBP1
P	-7	GLY	-	expression tag	UNP Q0KBP1
P	-6	LEU	-	expression tag	UNP Q0KBP1
P	-5	VAL	-	expression tag	UNP Q0KBP1
P	-4	PRO	-	expression tag	UNP Q0KBP1
P	-3	ARG	-	expression tag	UNP Q0KBP1
P	-2	GLY	-	expression tag	UNP Q0KBP1
P	-1	SER	-	expression tag	UNP Q0KBP1
P	0	HIS	-	expression tag	UNP Q0KBP1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	63	Total O 63 63	0	0
2	B	59	Total O 59 59	0	0
2	C	60	Total O 60 60	0	0
2	D	53	Total O 53 53	0	0
2	E	44	Total O 44 44	0	0
2	F	32	Total O 32 32	0	0

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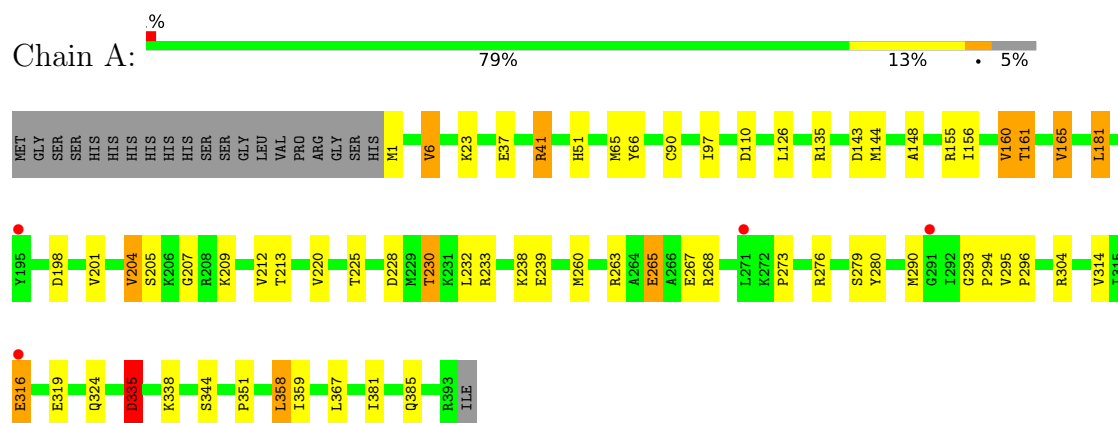
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	66	Total 66	O 66	0	0
2	H	50	Total 51	O 51	0	1
2	I	49	Total 49	O 49	0	0
2	J	30	Total 30	O 30	0	0
2	K	18	Total 18	O 18	0	0
2	L	25	Total 25	O 25	0	0
2	M	36	Total 36	O 36	0	0
2	N	24	Total 24	O 24	0	0
2	O	29	Total 29	O 29	0	0
2	P	35	Total 35	O 35	0	0

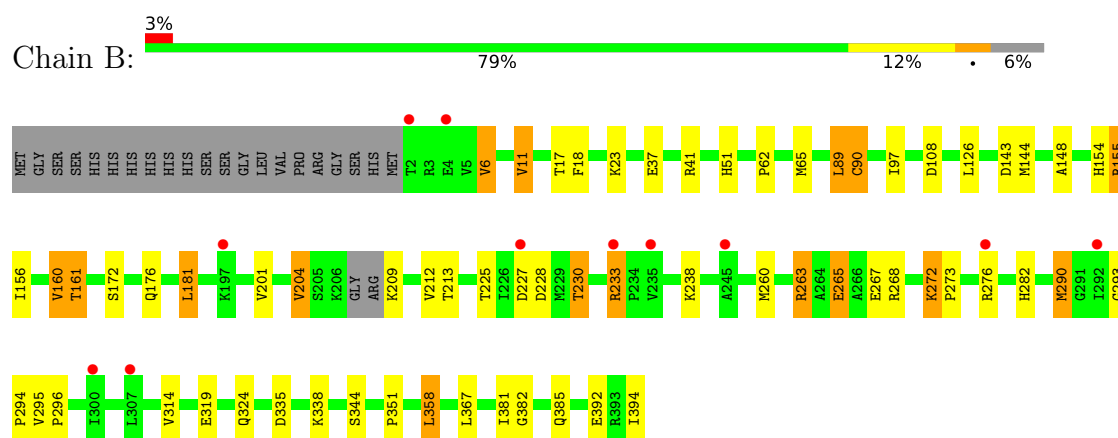
3 Residue-property plots [i](#)

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.

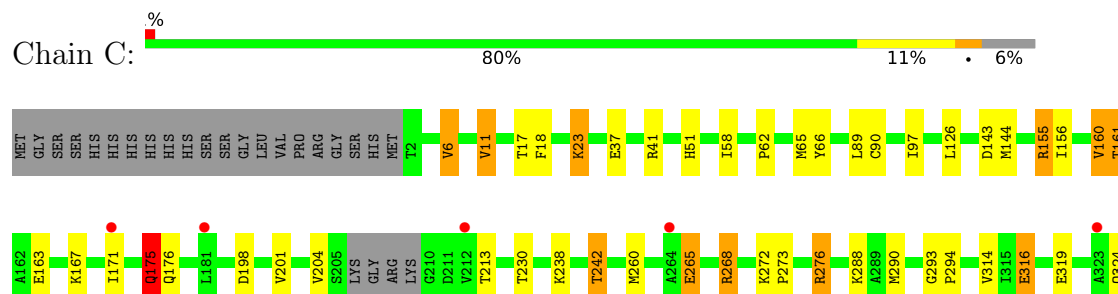
• Molecule 1: Beta-ketothiolase BktB



• Molecule 1: Beta-ketothiolase BktB



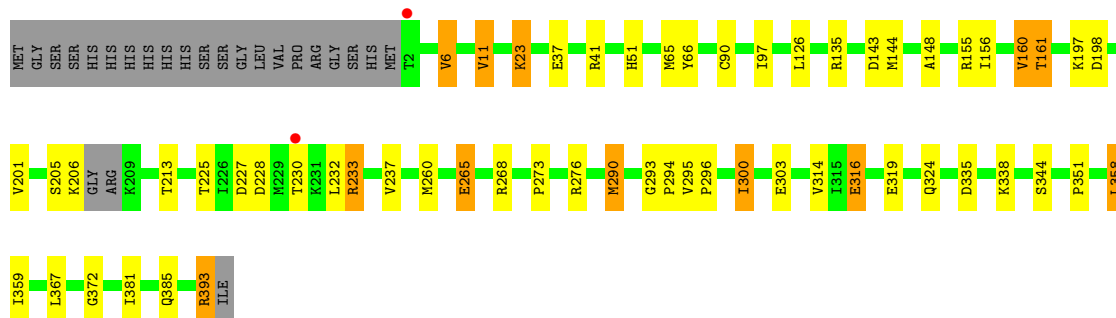
• Molecule 1: Beta-ketothiolase BktB





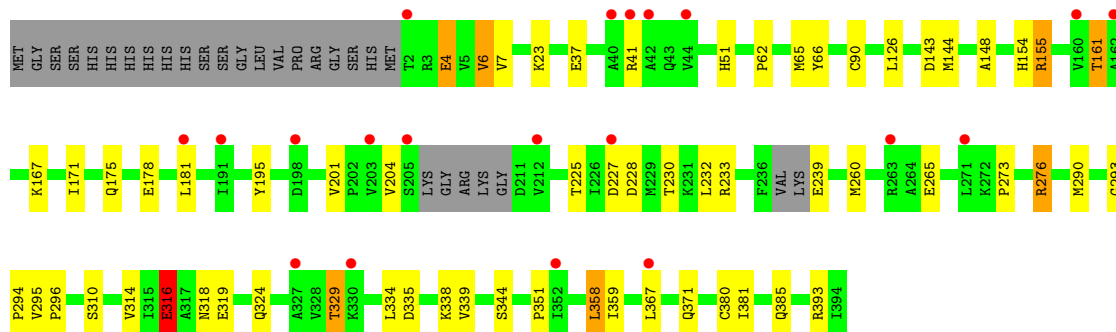
• Molecule 1: Beta-ketothiolase BktB

Chain D: 80% 11% 6%



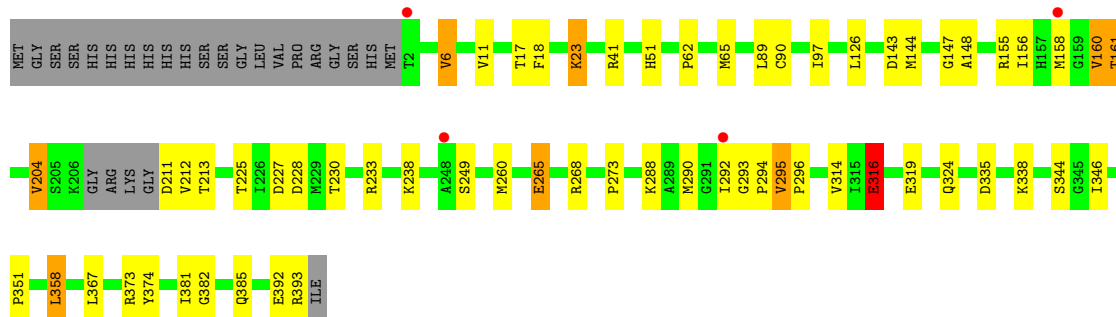
• Molecule 1: Beta-ketothiolase BktB

Chain E: 5% 78% 13% 7%



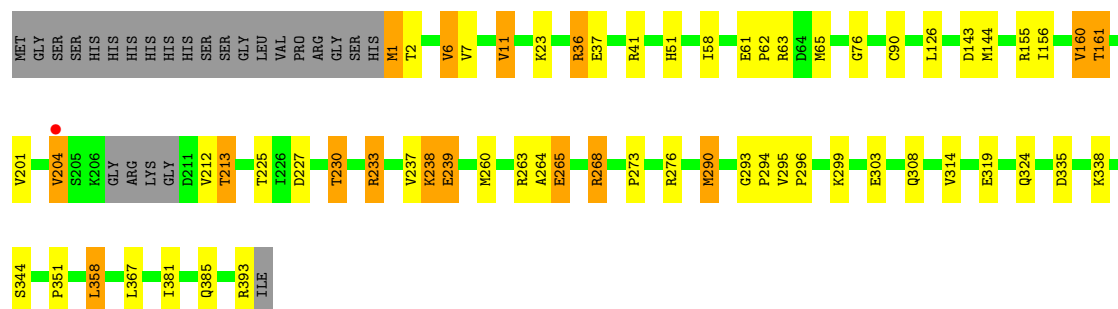
• Molecule 1: Beta-ketothiolase BktB

Chain F: % 79% 13% 6%

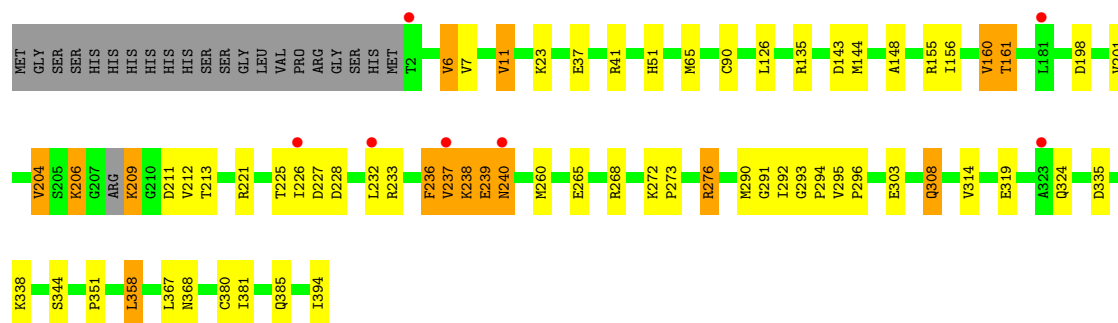
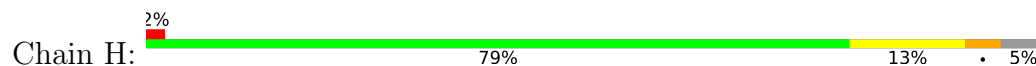


• Molecule 1: Beta-ketothiolase BktB

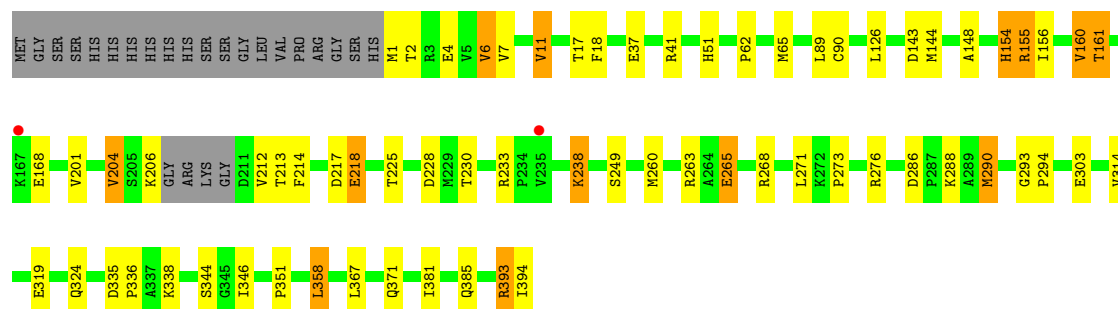
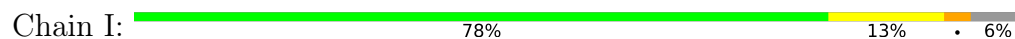
Chain G: 79% 11% 6%



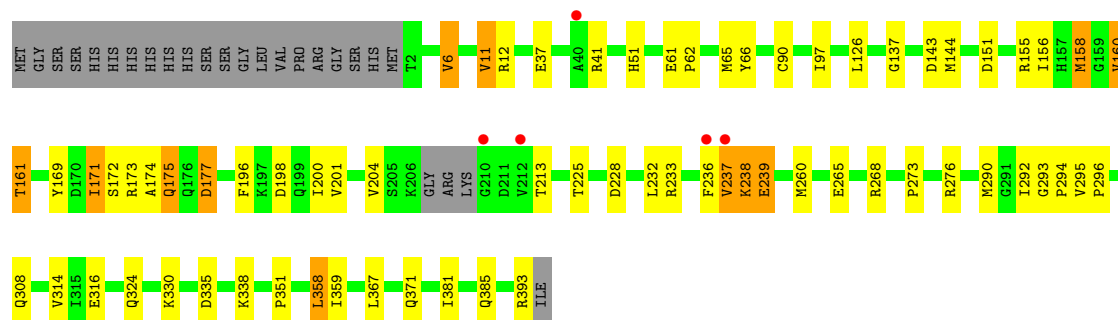
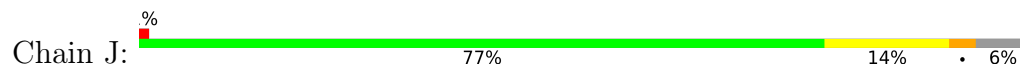
• Molecule 1: Beta-ketothiolase BktB



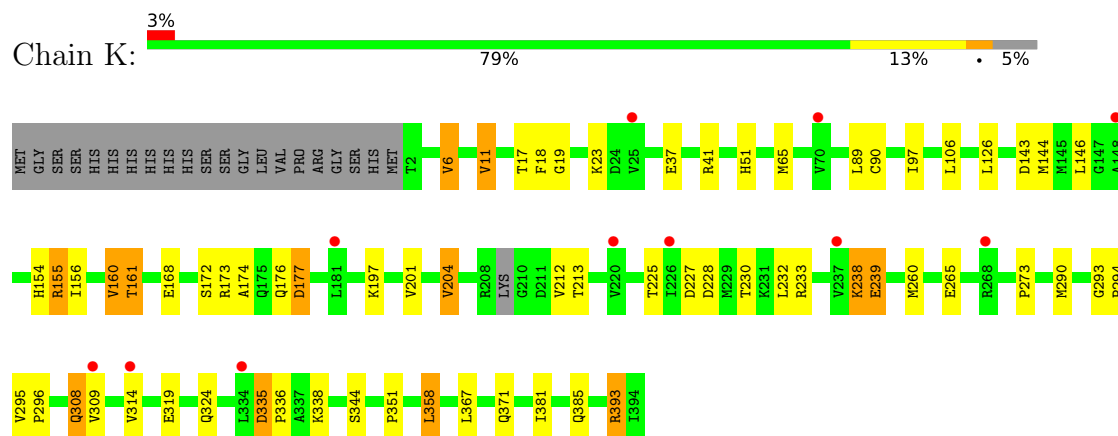
• Molecule 1: Beta-ketothiolase BktB



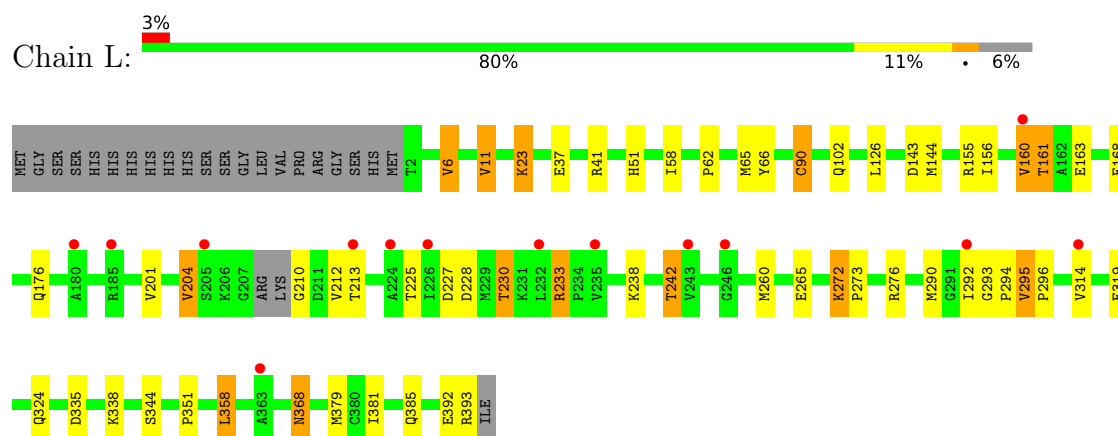
• Molecule 1: Beta-ketothiolase BktB



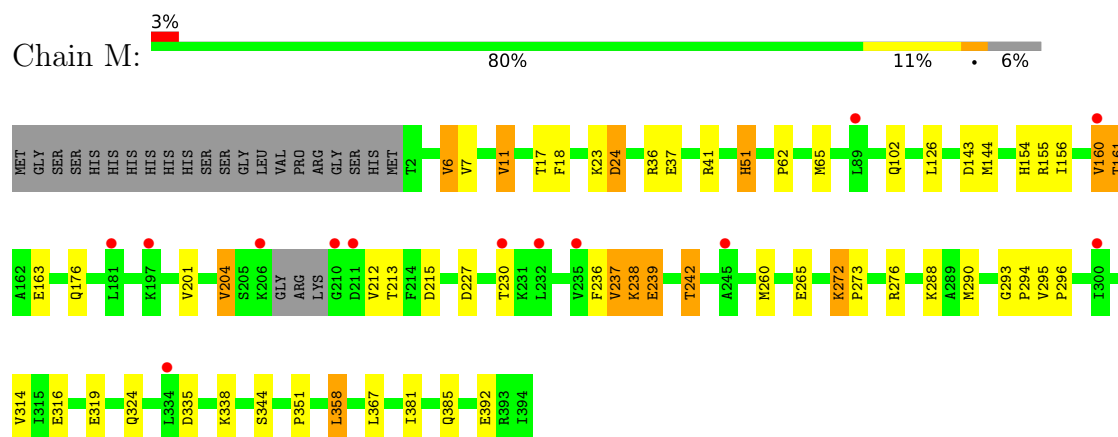
- Molecule 1: Beta-ketothiolase BktB



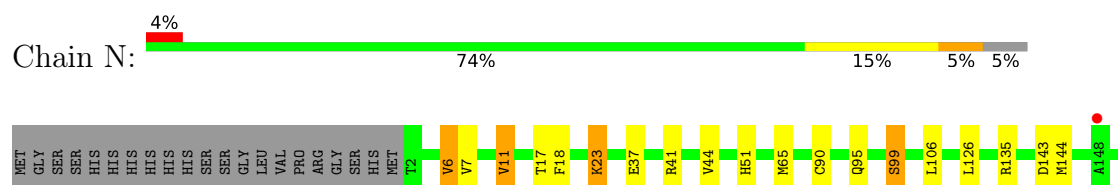
- Molecule 1: Beta-ketothiolase BktB

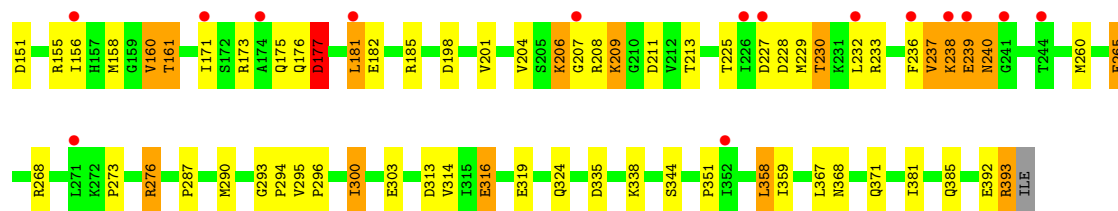


- Molecule 1: Beta-ketothiolase BktB

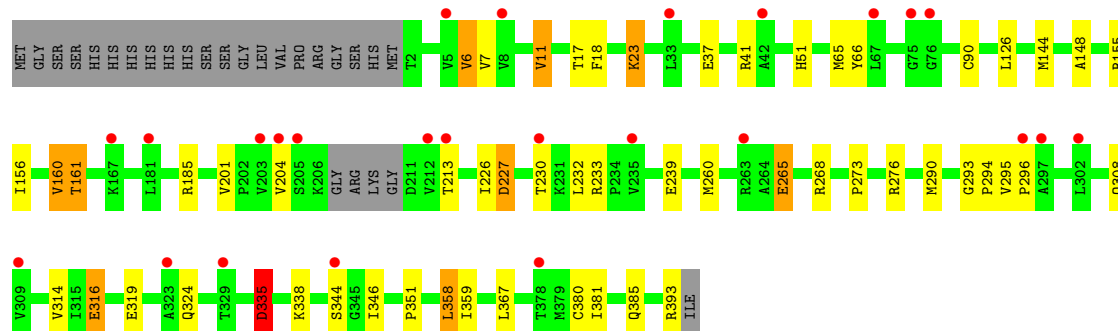
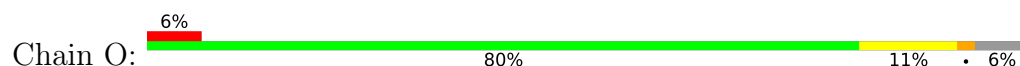


- Molecule 1: Beta-ketothiolase BktB

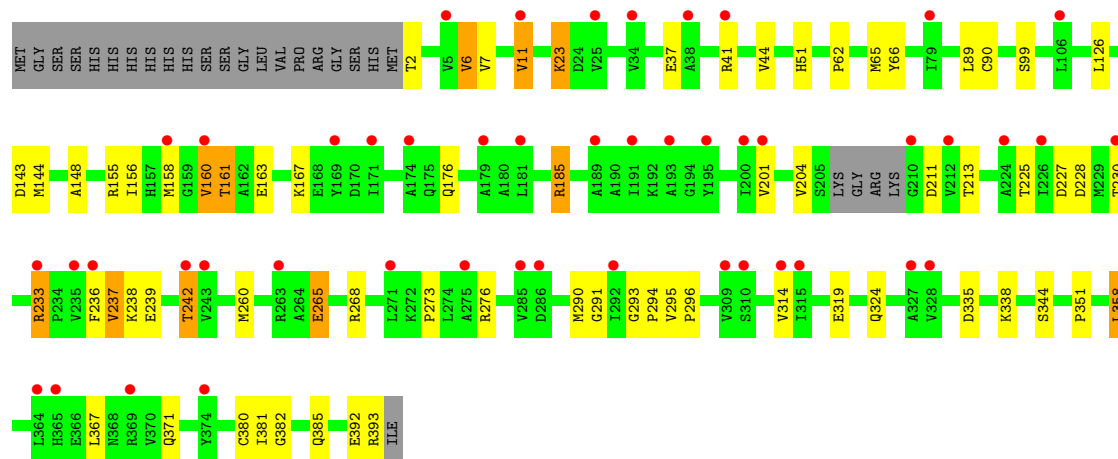




● Molecule 1: Beta-ketothiolase BktB



● Molecule 1: Beta-ketothiolase BktB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.05Å 105.99Å 201.14Å 89.97° 89.98° 89.93°	Depositor
Resolution (Å)	41.79 – 2.01 41.79 – 2.01	Depositor EDS
% Data completeness (in resolution range)	92.9 (41.79-2.01) 99.6 (41.79-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.176 , 0.208 0.184 , 0.213	Depositor DCC
R_{free} test set	19991 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.106 for h,-k,-l 0.125 for -h,k,-l 0.289 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	46062	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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	0.40	0/2899	0.71	0/3929
1	B	0.45	1/2894 (0.0%)	0.68	0/3922
1	C	0.45	0/2876	0.70	0/3900
1	D	0.42	1/2875 (0.0%)	0.68	0/3897
1	E	0.42	0/2844	0.70	0/3857
1	F	0.44	0/2862	0.69	0/3881
1	G	0.52	3/2870 (0.1%)	0.70	0/3891
1	H	0.45	1/2887 (0.0%)	0.71	0/3913
1	I	0.51	3/2886 (0.1%)	0.71	2/3913 (0.1%)
1	J	0.53	3/2866 (0.1%)	0.72	1/3886 (0.0%)
1	K	0.42	0/2889	0.67	0/3916
1	L	0.44	2/2881 (0.1%)	0.68	0/3905
1	M	0.43	0/2874	0.68	0/3897
1	N	0.39	0/2891	0.69	2/3919 (0.1%)
1	O	0.36	0/2862	0.66	0/3881
1	P	0.41	0/2857	0.68	0/3875
All	All	0.44	14/46013 (0.0%)	0.69	5/62382 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	1
1	C	0	5
1	D	0	1
1	E	0	2
1	F	0	4
1	G	0	3
1	H	0	2
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	K	0	1
1	L	0	3
1	M	0	1
1	N	0	4
1	O	0	2
1	P	0	2
All	All	0	41

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	36	ARG	C-O	-6.43	1.16	1.24
1	G	276	ARG	C-O	-5.99	1.16	1.23
1	I	154	HIS	CG-ND1	-5.94	1.31	1.38
1	J	177	ASP	C-O	-5.86	1.16	1.24
1	B	290	MET	C-O	-5.67	1.16	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	175	GLN	N-CA-C	-6.14	104.14	111.69
1	N	240	ASN	CB-CA-C	-6.13	107.80	115.89
1	I	217	ASP	CA-C-N	5.61	128.83	120.31
1	I	217	ASP	C-N-CA	5.61	128.83	120.31
1	N	177	ASP	N-CA-C	-5.36	106.06	113.18

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	SER	Mainchain
1	A	265	GLU	Mainchain
1	A	335	ASP	Sidechain
1	A	351	PRO	Peptide
1	A	41	ARG	Sidechain

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	2859	0	2897	62	0
1	B	2855	0	2891	70	0
1	C	2837	0	2865	64	0
1	D	2836	0	2868	56	0
1	E	2806	0	2827	49	0
1	F	2823	0	2852	49	0
1	G	2831	0	2864	62	0
1	H	2848	0	2882	60	0
1	I	2847	0	2880	59	0
1	J	2827	0	2855	61	0
1	K	2850	0	2882	59	0
1	L	2842	0	2870	55	0
1	M	2835	0	2866	51	0
1	N	2851	0	2885	77	0
1	O	2823	0	2852	50	0
1	P	2818	0	2842	69	0
2	A	63	0	0	8	0
2	B	59	0	0	1	0
2	C	60	0	0	6	0
2	D	53	0	0	2	0
2	E	44	0	0	6	0
2	F	32	0	0	1	0
2	G	66	0	0	6	0
2	H	51	0	0	4	0
2	I	49	0	0	2	0
2	J	30	0	0	2	0
2	K	18	0	0	3	0
2	L	25	0	0	0	0
2	M	36	0	0	5	0
2	N	24	0	0	11	0
2	O	29	0	0	3	0
2	P	35	0	0	4	0
All	All	46062	0	45878	827	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 9.

The worst 5 of 827 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:J:158:MET:HA	1:J:158:MET:HE2	1.25	1.16
1:A:263:ARG:NH2	1:A:267:GLU:OE2	1.80	1.13
1:A:316:GLU:HG3	1:A:359:ILE:HB	1.32	1.10
1:E:316:GLU:HG3	1:E:359:ILE:HB	1.35	1.03
1:H:276:ARG:HD3	1:H:394:ILE:HD11	1.40	1.01

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	391/414 (94%)	382 (98%)	9 (2%)	0	100	100
1	B	388/414 (94%)	380 (98%)	8 (2%)	0	100	100
1	C	386/414 (93%)	378 (98%)	8 (2%)	0	100	100
1	D	386/414 (93%)	377 (98%)	9 (2%)	0	100	100
1	E	380/414 (92%)	371 (98%)	9 (2%)	0	100	100
1	F	384/414 (93%)	377 (98%)	7 (2%)	0	100	100
1	G	385/414 (93%)	375 (97%)	9 (2%)	1 (0%)	36	35
1	H	388/414 (94%)	375 (97%)	11 (3%)	2 (0%)	24	21
1	I	387/414 (94%)	374 (97%)	13 (3%)	0	100	100
1	J	385/414 (93%)	372 (97%)	11 (3%)	2 (0%)	24	21
1	K	388/414 (94%)	377 (97%)	10 (3%)	1 (0%)	36	35
1	L	387/414 (94%)	377 (97%)	10 (3%)	0	100	100
1	M	386/414 (93%)	374 (97%)	10 (3%)	2 (0%)	24	21
1	N	390/414 (94%)	375 (96%)	13 (3%)	2 (0%)	24	21
1	O	384/414 (93%)	375 (98%)	9 (2%)	0	100	100
1	P	384/414 (93%)	371 (97%)	12 (3%)	1 (0%)	36	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6179/6624 (93%)	6010 (97%)	158 (3%)	11 (0%)	43	42

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	237	VAL
1	H	239	GLU
1	J	237	VAL
1	N	237	VAL
1	P	237	VAL

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	287/305 (94%)	263 (92%)	24 (8%)	10	7
1	B	287/305 (94%)	265 (92%)	22 (8%)	12	8
1	C	285/305 (93%)	262 (92%)	23 (8%)	11	7
1	D	285/305 (93%)	259 (91%)	26 (9%)	9	6
1	E	282/305 (92%)	261 (93%)	21 (7%)	13	9
1	F	284/305 (93%)	263 (93%)	21 (7%)	13	9
1	G	285/305 (93%)	263 (92%)	22 (8%)	12	8
1	H	286/305 (94%)	259 (91%)	27 (9%)	8	5
1	I	287/305 (94%)	265 (92%)	22 (8%)	12	8
1	J	284/305 (93%)	262 (92%)	22 (8%)	12	8
1	K	286/305 (94%)	263 (92%)	23 (8%)	11	8
1	L	285/305 (93%)	263 (92%)	22 (8%)	12	8
1	M	285/305 (93%)	265 (93%)	20 (7%)	14	10
1	N	286/305 (94%)	257 (90%)	29 (10%)	7	4
1	O	284/305 (93%)	259 (91%)	25 (9%)	9	6
1	P	283/305 (93%)	261 (92%)	22 (8%)	11	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4561/4880 (94%)	4190 (92%)	371 (8%)	11 7

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	11	VAL
1	M	227	ASP
1	K	177	ASP
1	L	160	VAL
1	N	90	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	154	HIS
1	M	318	ASN
1	G	318	ASN
1	O	318	ASN
1	L	318	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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, 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	393/414 (94%)	0.30	4 (1%)	79 79	19, 35, 53, 75	0
1	B	391/414 (94%)	0.33	11 (2%)	55 54	17, 35, 57, 93	1 (0%)
1	C	389/414 (93%)	0.23	5 (1%)	75 74	16, 32, 54, 87	1 (0%)
1	D	390/414 (94%)	0.10	2 (0%)	87 87	15, 29, 53, 89	0
1	E	386/414 (93%)	0.61	20 (5%)	33 31	19, 39, 68, 104	0
1	F	388/414 (93%)	0.47	4 (1%)	79 79	19, 38, 61, 84	0
1	G	389/414 (93%)	0.14	1 (0%)	90 89	15, 31, 51, 75	0
1	H	392/414 (94%)	0.24	7 (1%)	67 67	17, 33, 59, 93	0
1	I	390/414 (94%)	0.03	2 (0%)	87 87	15, 28, 53, 81	1 (0%)
1	J	389/414 (93%)	0.26	5 (1%)	75 74	18, 33, 57, 98	0
1	K	392/414 (94%)	0.49	11 (2%)	55 54	22, 39, 60, 81	0
1	L	390/414 (94%)	0.49	14 (3%)	46 45	20, 37, 60, 98	1 (0%)
1	M	390/414 (94%)	0.51	13 (3%)	49 48	24, 38, 60, 95	0
1	N	392/414 (94%)	0.57	16 (4%)	41 40	22, 39, 64, 117	0
1	O	388/414 (93%)	0.78	25 (6%)	25 24	25, 44, 69, 99	0
1	P	388/414 (93%)	0.88	47 (12%)	8 8	23, 44, 73, 97	0
All	All	6237/6624 (94%)	0.40	187 (2%)	52 51	15, 36, 61, 117	4 (0%)

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	235	VAL	4.4
1	P	235	VAL	4.0
1	P	327	ALA	4.0
1	J	210	GLY	3.9
1	L	224	ALA	3.8

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.