



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:23 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 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

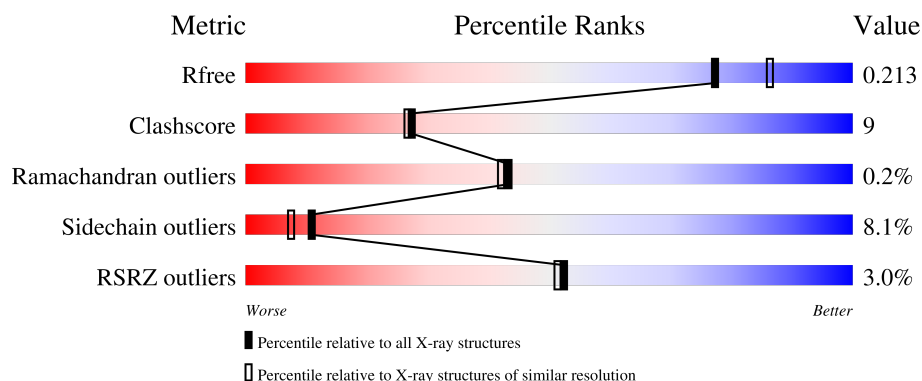
1 Overall quality at a glance

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.



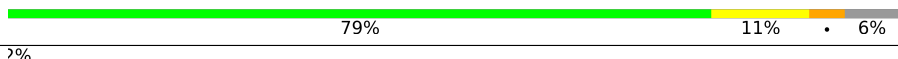
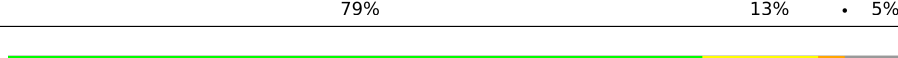
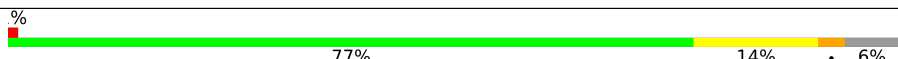
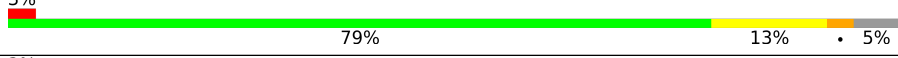
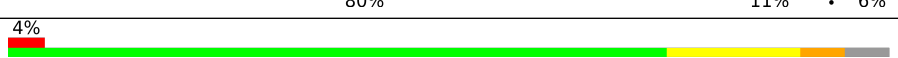
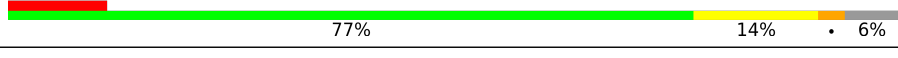
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	0% 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

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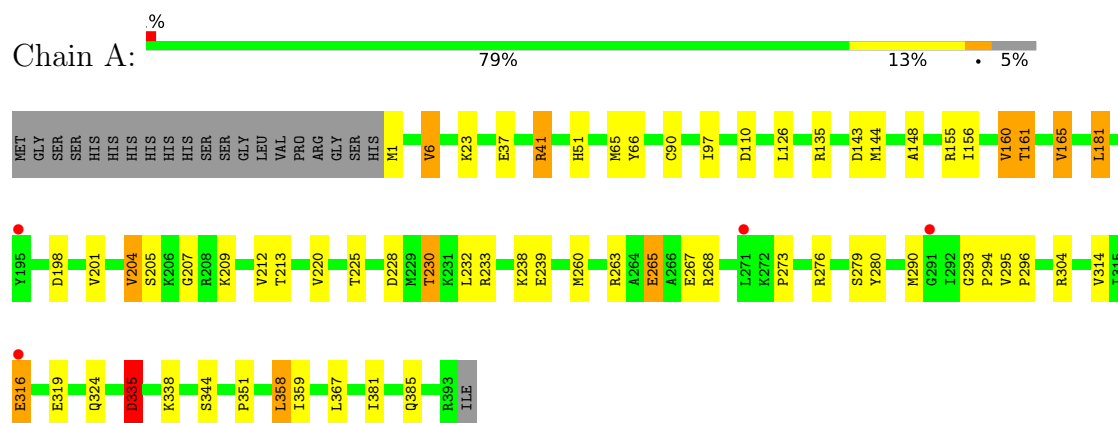
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	66	Total 66	O 66	0	0
2	H	50	Total 51	O 51	0	1
2	I	49	Total 49	O 49	0	0
2	J	30	Total 30	O 30	0	0
2	K	18	Total 18	O 18	0	0
2	L	25	Total 25	O 25	0	0
2	M	36	Total 36	O 36	0	0
2	N	24	Total 24	O 24	0	0
2	O	29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

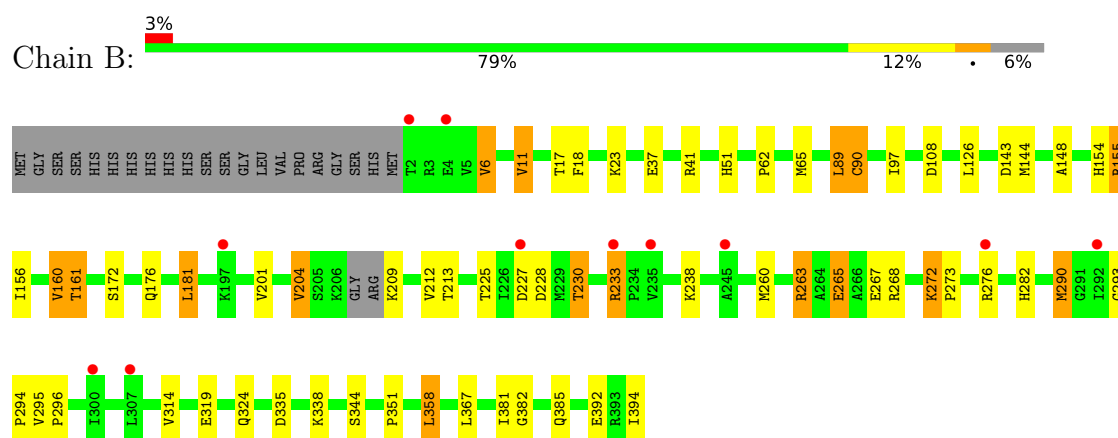
3 Residue-property plots [i](#)

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.

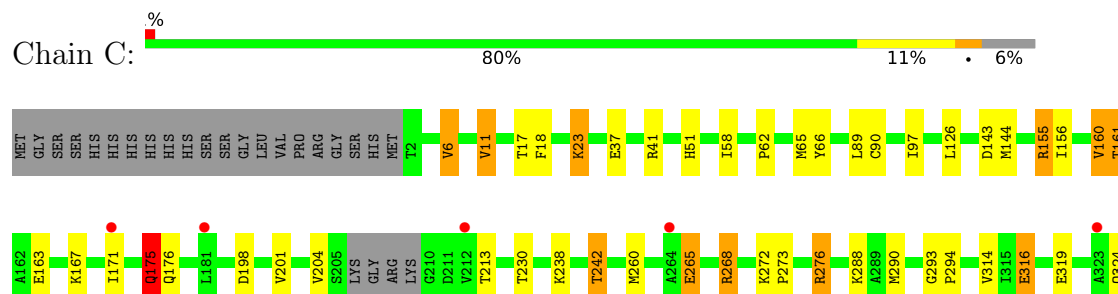
• Molecule 1: Beta-ketothiolase BktB



• Molecule 1: Beta-ketothiolase BktB



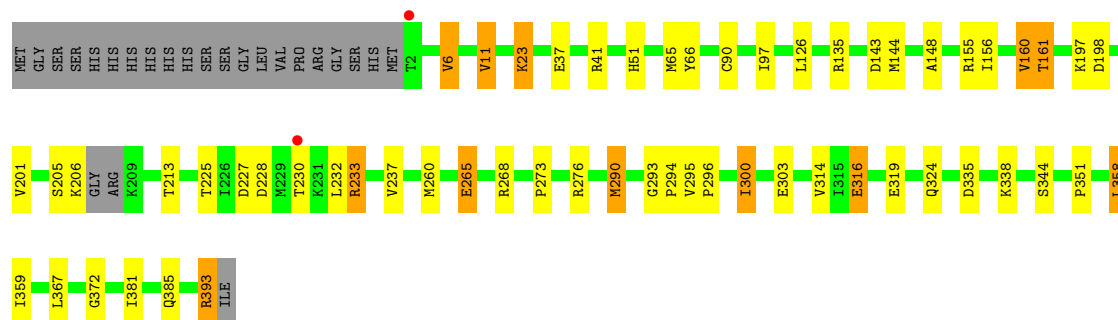
• Molecule 1: Beta-ketothiolase BktB





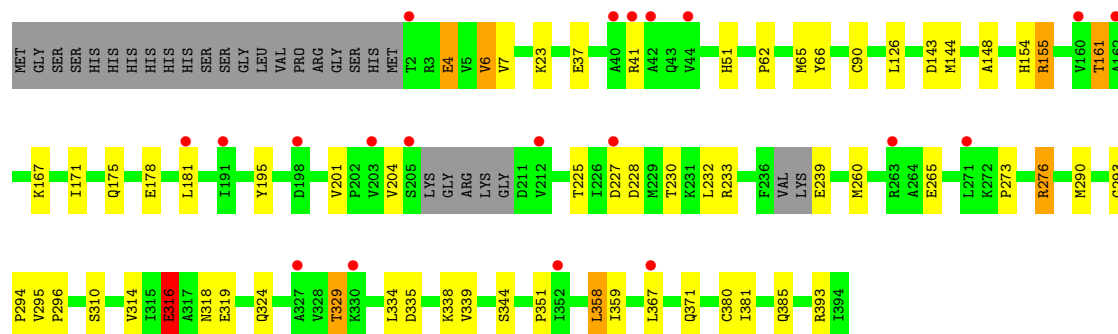
• Molecule 1: Beta-ketothiolase BktB

Chain D: 80% 11% 6%



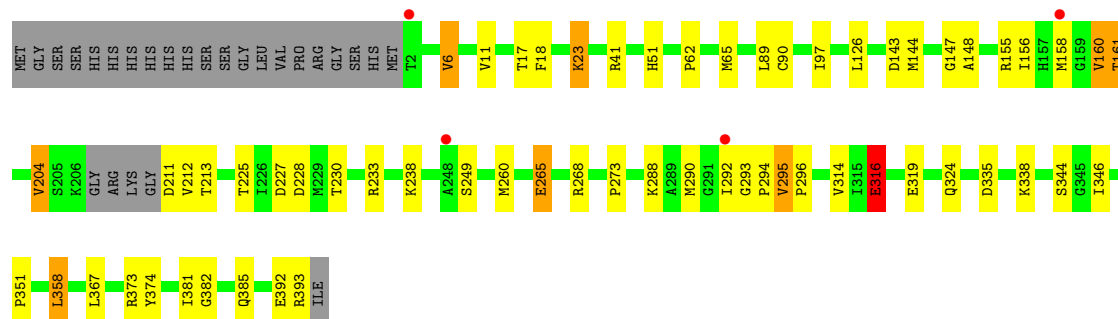
• Molecule 1: Beta-ketothiolase BktB

Chain E: 5% 78% 13% 7%



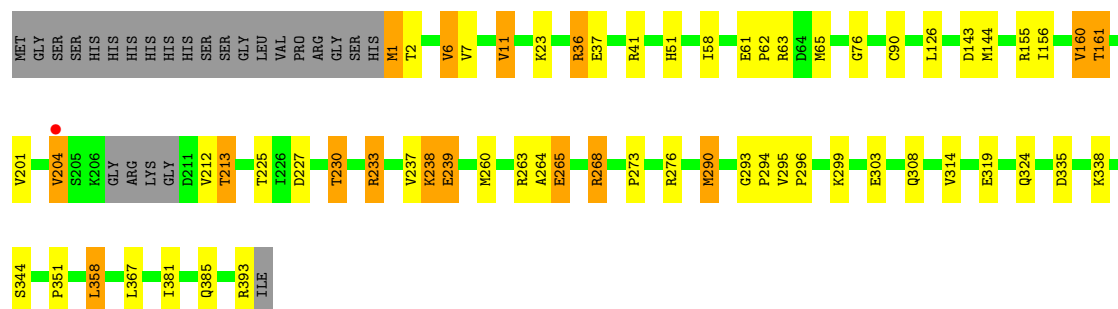
• Molecule 1: Beta-ketothiolase BktB

Chain F: % 79% 13% 6%

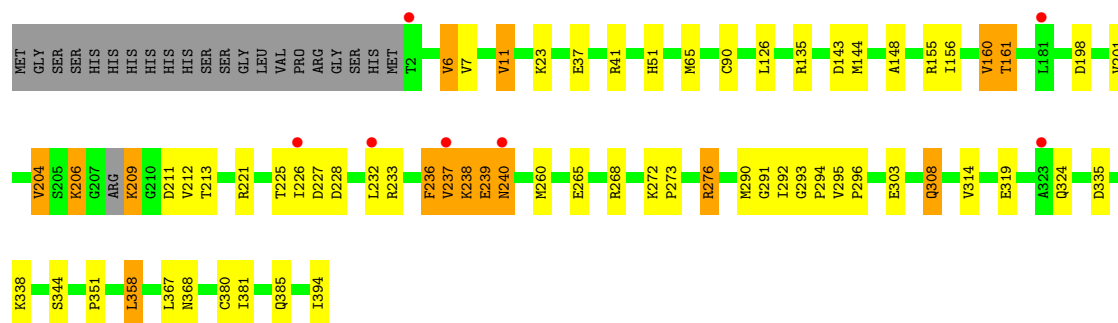
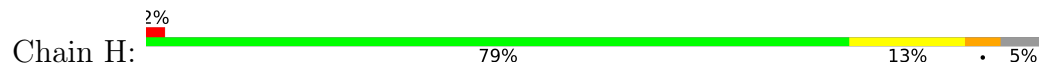


• Molecule 1: Beta-ketothiolase BktB

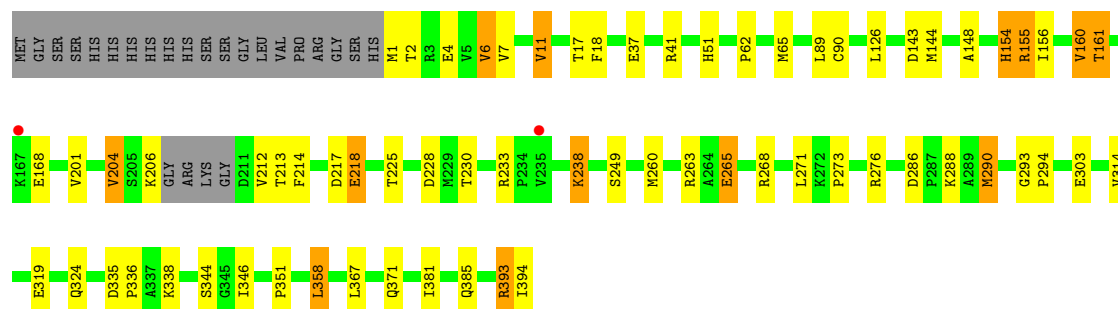
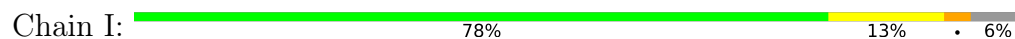
Chain G: 79% 11% 6%



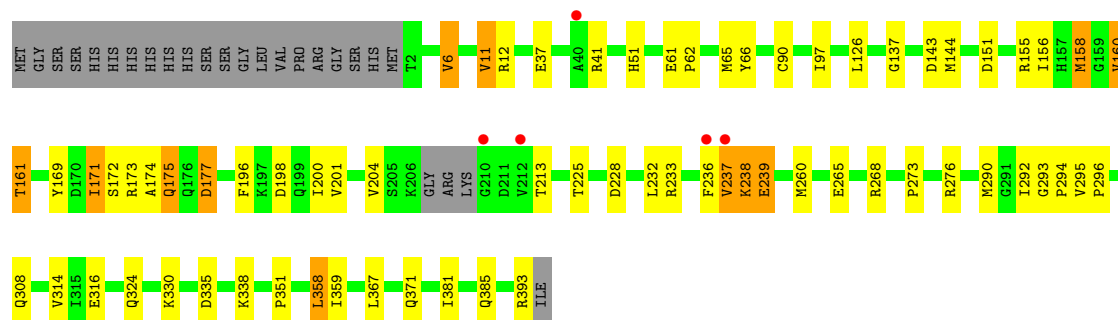
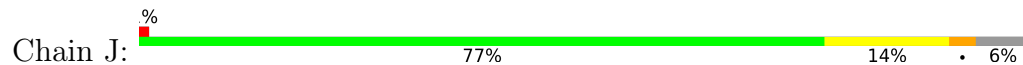
• Molecule 1: Beta-ketothiolase BktB



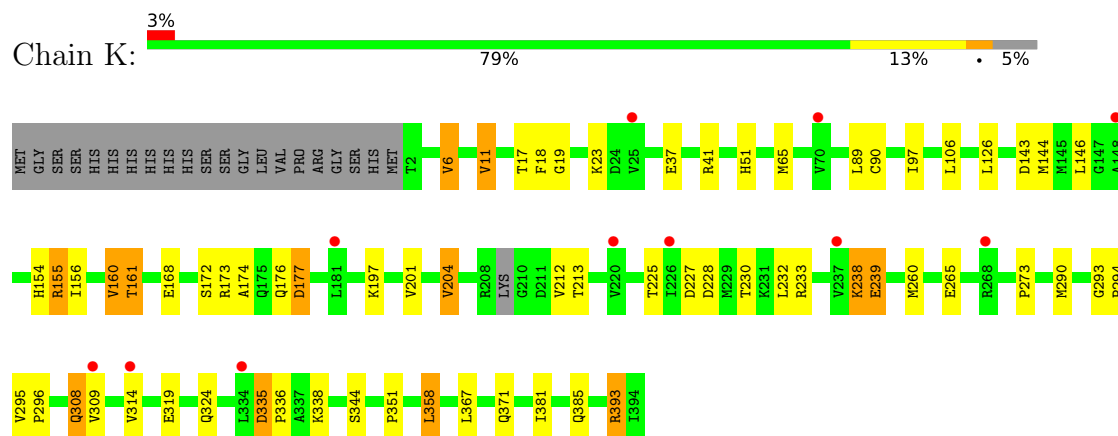
• Molecule 1: Beta-ketothiolase BktB



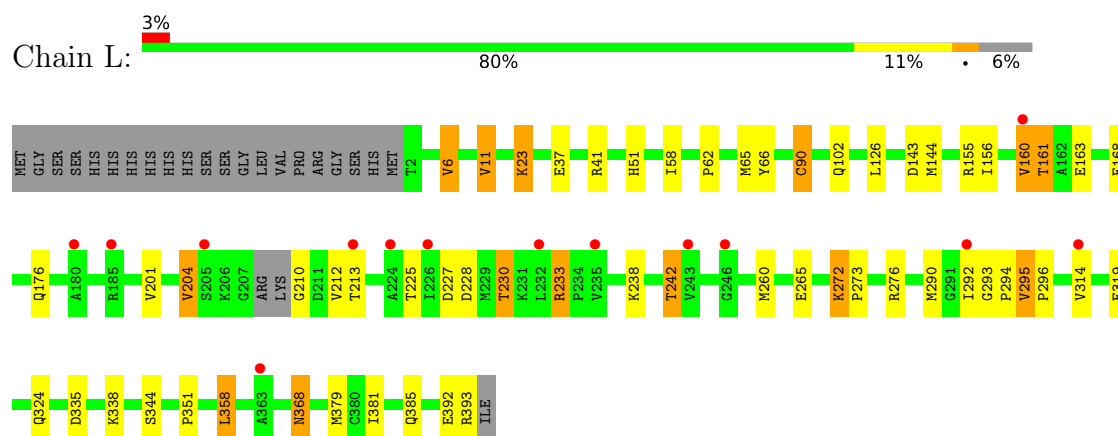
• Molecule 1: Beta-ketothiolase BktB



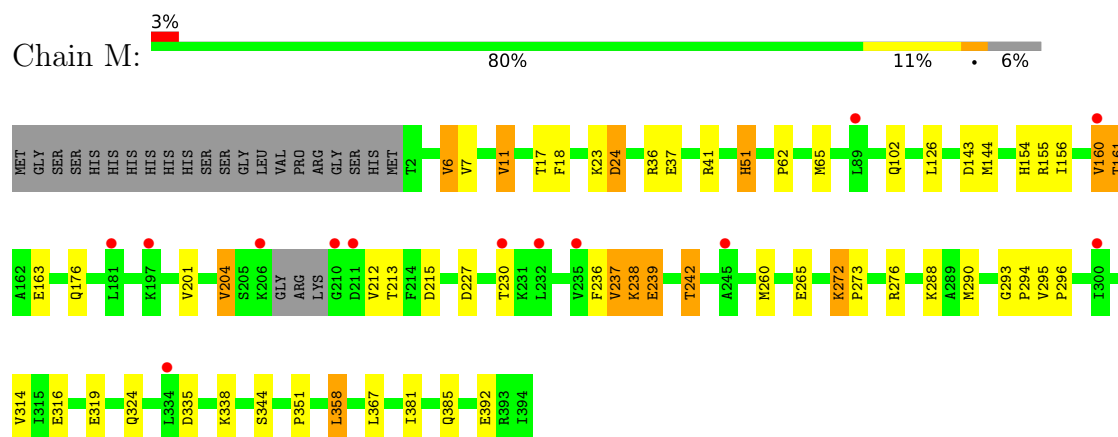
- Molecule 1: Beta-ketothiolase BktB



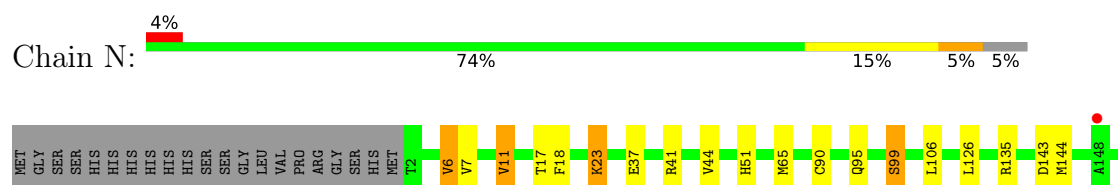
- Molecule 1: Beta-ketothiolase BktB

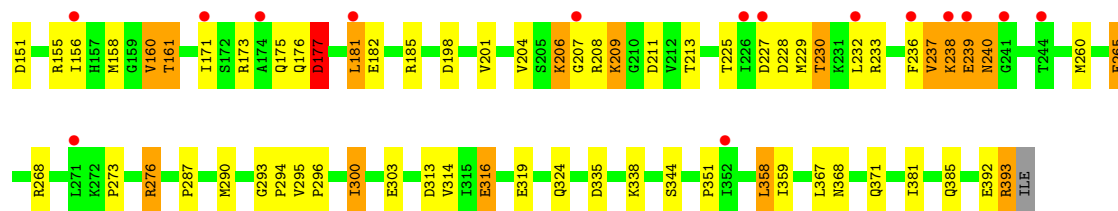


- Molecule 1: Beta-ketothiolase BktB

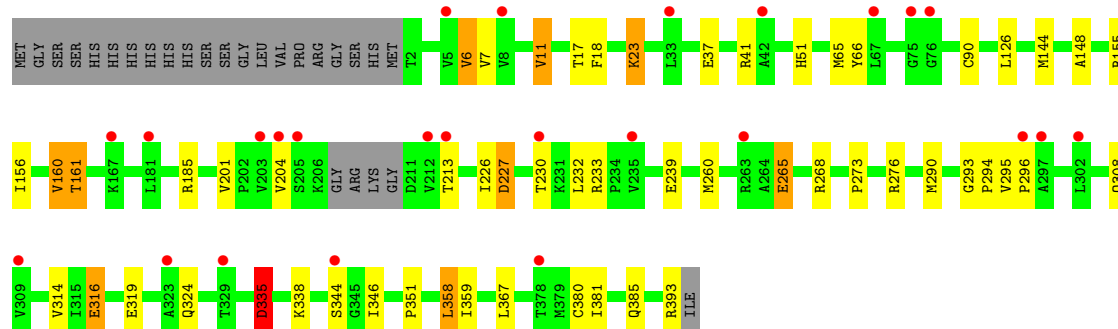
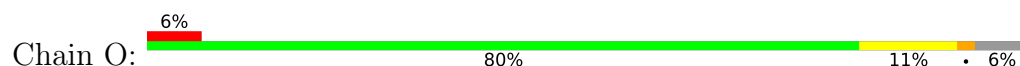


- Molecule 1: Beta-ketothiolase BktB

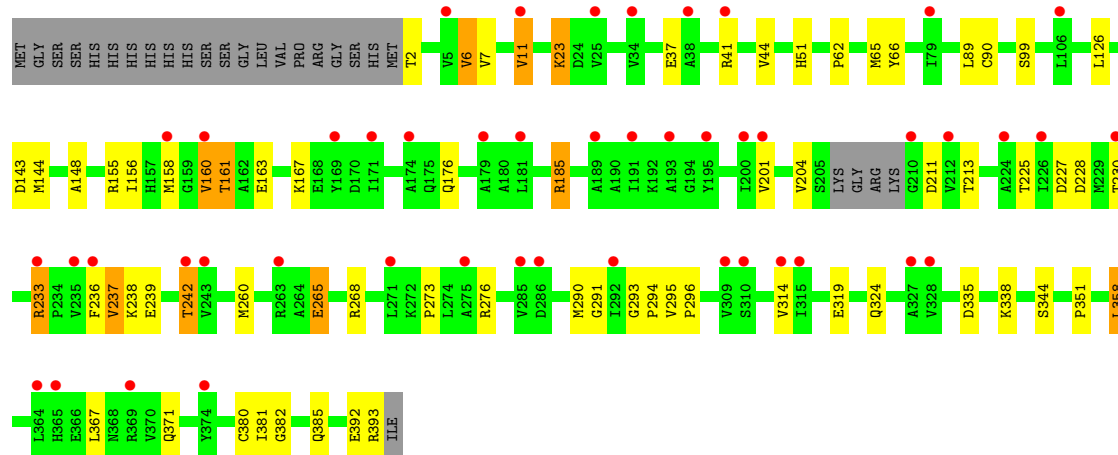




• Molecule 1: Beta-ketothiolase BktB



• 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

All (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
1	D	290	MET	C-O	-5.67	1.17	1.24
1	L	314	VAL	C-O	-5.66	1.18	1.24
1	I	290	MET	C-O	-5.47	1.17	1.24
1	I	154	HIS	CD2-NE2	-5.19	1.32	1.37
1	H	308	GLN	C-O	-5.16	1.17	1.23
1	G	290	MET	C-O	-5.09	1.17	1.24
1	L	260	MET	C-O	-5.04	1.17	1.23
1	J	173	ARG	C-O	-5.01	1.18	1.24
1	J	171	ILE	C-O	-5.01	1.18	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.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	265	GLU	Mainchain
1	A	335	ASP	Sidechain
1	A	351	PRO	Peptide
1	A	41	ARG	Sidechain
1	B	351	PRO	Peptide
1	C	175	GLN	Mainchain
1	C	268	ARG	Sidechain
1	C	276	ARG	Sidechain
1	C	351	PRO	Peptide
1	C	393	ARG	Mainchain
1	D	351	PRO	Peptide
1	E	316	GLU	Sidechain
1	E	351	PRO	Peptide
1	F	316	GLU	Sidechain
1	F	351	PRO	Peptide
1	F	392	GLU	Sidechain
1	F	393	ARG	Sidechain
1	G	1	MET	Peptide
1	G	2	THR	Peptide
1	G	351	PRO	Peptide
1	H	236	PHE	Mainchain
1	H	351	PRO	Peptide
1	I	218	GLU	Mainchain
1	I	351	PRO	Peptide
1	I	393	ARG	Peptide
1	J	151	ASP	Sidechain
1	J	351	PRO	Peptide
1	K	351	PRO	Peptide
1	L	210	GLY	Peptide
1	L	265	GLU	Mainchain
1	L	351	PRO	Peptide
1	M	351	PRO	Peptide
1	N	206	LYS	Peptide
1	N	209	LYS	Peptide
1	N	351	PRO	Peptide
1	N	393	ARG	Sidechain
1	O	335	ASP	Sidechain
1	O	351	PRO	Peptide
1	P	2	THR	Mainchain
1	P	351	PRO	Peptide

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	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.

All (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
1:E:4:GLU:OE1	1:E:276:ARG:NH1	1.94	1.00
1:A:181:LEU:O	1:A:181:LEU:HD23	1.62	0.99
1:K:173:ARG:O	1:K:177:ASP:OD1	1.80	0.99
1:B:181:LEU:HD23	1:B:181:LEU:O	1.63	0.99
1:J:316:GLU:CG	1:J:359:ILE:HB	1.93	0.99
1:J:316:GLU:HG2	1:J:359:ILE:HB	1.43	0.97
1:E:161:THR:HG23	2:E:422:HOH:O	1.66	0.96
1:A:37:GLU:OE2	1:A:41:ARG:NH1	1.98	0.95
1:L:233:ARG:H	1:L:233:ARG:HD2	1.29	0.95
1:H:276:ARG:HD3	1:H:394:ILE:CD1	1.97	0.93
1:B:238:LYS:NZ	1:G:37:GLU:OE1	2.02	0.92
1:F:292:ILE:O	1:F:295:VAL:HG12	1.72	0.90
1:O:65:MET:CE	1:P:144:MET:HE3	2.03	0.89
1:O:126:LEU:CD2	1:P:126:LEU:CD2	2.49	0.89
1:H:238:LYS:O	1:H:239:GLU:HB3	1.71	0.89
1:I:126:LEU:CD2	1:J:126:LEU:CD2	2.50	0.89
1:L:292:ILE:O	1:L:295:VAL:HG12	1.71	0.89
1:P:158:MET:HE1	1:P:382:GLY:HA2	1.54	0.89
1:E:126:LEU:CD2	1:F:126:LEU:CD2	2.50	0.88
1:H:238:LYS:O	1:H:239:GLU:CB	2.20	0.88
1:F:158:MET:HE1	1:F:382:GLY:HA2	1.56	0.88
1:F:155:ARG:NH2	2:F:401:HOH:O	2.06	0.88
1:G:126:LEU:CD2	1:H:126:LEU:CD2	2.51	0.87
1:M:144:MET:HE3	1:N:65:MET:CE	2.04	0.87
1:P:227:ASP:O	1:P:227:ASP:OD2	1.93	0.87
1:K:126:LEU:CD2	1:L:126:LEU:CD2	2.54	0.86
1:A:126:LEU:CD2	1:B:126:LEU:CD2	2.54	0.85
1:C:126:LEU:CD2	1:D:126:LEU:CD2	2.53	0.85
1:D:296:PRO:O	1:D:300:ILE:HD13	1.78	0.84
1:C:288:LYS:HD3	1:G:393:ARG:HH22	1.42	0.83
1:P:236:PHE:O	2:P:401:HOH:O	1.96	0.83
1:A:335:ASP:C	1:A:335:ASP:OD1	2.22	0.83
1:H:290:MET:HE3	1:H:291:GLY:HA2	1.59	0.83
1:N:276:ARG:NH1	1:N:392:GLU:OE1	2.12	0.83
1:K:225:THR:OG1	1:K:227:ASP:OD1	1.97	0.83
1:A:66:TYR:CZ	1:B:89:LEU:HD11	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:295:VAL:HG13	1:L:296:PRO:HD3	1.61	0.83
1:H:225:THR:OG1	1:H:227:ASP:OD1	1.97	0.82
1:O:335:ASP:C	1:O:335:ASP:OD1	2.22	0.82
1:N:296:PRO:O	1:N:300:ILE:HD13	1.78	0.82
1:N:371:GLN:HA	1:N:393:ARG:NH2	1.94	0.82
1:E:225:THR:OG1	1:E:227:ASP:OD1	1.97	0.82
1:N:225:THR:OG1	1:N:227:ASP:OD1	1.97	0.82
1:A:220:VAL:O	2:A:401:HOH:O	1.96	0.82
1:H:290:MET:HE3	1:H:291:GLY:CA	2.09	0.82
1:G:233:ARG:NH2	2:G:401:HOH:O	2.11	0.81
1:E:167:LYS:HG2	1:P:211:ASP:OD1	1.80	0.81
1:I:271:LEU:O	2:I:401:HOH:O	1.98	0.81
1:J:169:TYR:O	1:J:330:LYS:NZ	2.13	0.81
1:H:221:ARG:NH2	2:H:402:HOH:O	2.12	0.81
1:L:225:THR:OG1	1:L:227:ASP:OD1	1.97	0.81
1:N:368:ASN:HA	1:N:393:ARG:NH2	1.95	0.81
1:F:295:VAL:HG13	1:F:296:PRO:HD3	1.62	0.81
1:G:225:THR:OG1	1:G:227:ASP:OD1	1.98	0.81
1:B:181:LEU:HD23	1:B:181:LEU:C	2.07	0.80
1:F:158:MET:HE3	1:F:290:MET:HE2	1.63	0.80
1:O:161:THR:HG21	1:O:290:MET:HG3	1.64	0.80
1:E:161:THR:HG21	1:E:290:MET:HG3	1.64	0.80
1:I:144:MET:HE3	1:J:65:MET:CE	2.10	0.80
1:B:225:THR:OG1	1:B:227:ASP:OD1	1.98	0.80
1:B:282:HIS:O	2:B:401:HOH:O	2.00	0.79
1:K:309:VAL:HG22	2:K:409:HOH:O	1.82	0.79
1:M:24:ASP:OD1	1:M:24:ASP:N	2.15	0.79
1:H:226:ILE:HD12	1:H:226:ILE:H	1.46	0.78
1:A:304:ARG:NH2	2:A:404:HOH:O	2.16	0.78
1:B:276:ARG:NH1	1:B:392:GLU:OE1	2.17	0.78
1:J:158:MET:HE2	1:J:158:MET:CA	2.11	0.78
1:J:177:ASP:HB2	2:J:402:HOH:O	1.84	0.78
1:A:66:TYR:CE2	1:B:89:LEU:CD1	2.67	0.78
1:A:181:LEU:C	1:A:181:LEU:CD2	2.57	0.78
1:E:161:THR:CG2	2:E:422:HOH:O	2.27	0.78
1:L:161:THR:HG21	1:L:290:MET:HG3	1.66	0.78
1:P:276:ARG:NH1	1:P:392:GLU:OE1	2.16	0.78
1:A:181:LEU:HD23	1:A:181:LEU:C	2.06	0.78
1:B:181:LEU:C	1:B:181:LEU:CD2	2.58	0.77
1:M:144:MET:HE3	1:N:65:MET:HE3	1.63	0.77
1:N:161:THR:HG21	1:N:290:MET:HG3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:158:MET:HA	1:J:158:MET:CE	2.11	0.77
1:H:236:PHE:O	1:H:237:VAL:HG12	1.84	0.76
1:D:372:GLY:O	1:D:393:ARG:NE	2.17	0.76
1:J:236:PHE:O	1:J:237:VAL:HG12	1.86	0.76
1:M:276:ARG:NH1	1:M:392:GLU:OE1	2.19	0.76
1:O:65:MET:HE3	1:P:144:MET:CE	2.16	0.76
1:M:161:THR:HG21	1:M:290:MET:HG3	1.69	0.75
1:C:276:ARG:NH2	1:C:392:GLU:OE1	2.19	0.75
1:L:90:CYS:O	1:L:379:MET:HE2	1.85	0.75
1:O:65:MET:HE3	1:P:144:MET:HE3	1.67	0.75
1:D:135:ARG:NE	2:D:401:HOH:O	2.14	0.75
1:N:236:PHE:O	1:N:237:VAL:HG12	1.87	0.75
1:P:236:PHE:O	1:P:237:VAL:HG12	1.85	0.74
1:A:65:MET:CE	1:B:144:MET:HE3	2.18	0.74
1:A:135:ARG:NH1	2:A:403:HOH:O	2.13	0.74
1:J:174:ALA:HA	2:J:402:HOH:O	1.87	0.74
1:B:263:ARG:HD3	1:B:267:GLU:OE2	1.87	0.74
1:M:126:LEU:CD2	1:N:126:LEU:CD2	2.66	0.73
1:J:196:PHE:O	1:J:200:ILE:HG12	1.88	0.72
1:F:158:MET:HE3	1:F:290:MET:CE	2.19	0.72
1:M:238:LYS:O	1:M:239:GLU:HB2	1.88	0.72
1:A:66:TYR:CE2	1:B:89:LEU:HD11	2.25	0.72
1:M:144:MET:CE	1:N:65:MET:HE3	2.19	0.72
1:M:236:PHE:O	1:M:237:VAL:HG12	1.90	0.72
1:C:155:ARG:NH1	2:C:401:HOH:O	2.22	0.71
1:E:329:THR:HG22	1:E:334:LEU:HB2	1.72	0.71
1:N:238:LYS:O	1:N:239:GLU:HB2	1.90	0.71
1:L:295:VAL:HG13	1:L:296:PRO:CD	2.20	0.71
1:I:144:MET:HE3	1:J:65:MET:HE3	1.73	0.71
1:I:161:THR:HG21	1:I:290:MET:HG3	1.73	0.71
1:F:316:GLU:HA	1:F:316:GLU:OE1	1.89	0.71
1:A:66:TYR:CE2	1:B:89:LEU:HD13	2.25	0.71
1:F:295:VAL:HG13	1:F:296:PRO:CD	2.20	0.70
1:L:233:ARG:H	1:L:233:ARG:CD	2.04	0.70
1:G:238:LYS:O	1:G:239:GLU:HB2	1.91	0.69
1:K:65:MET:HE2	1:L:58:ILE:HA	1.74	0.69
1:K:161:THR:HG21	1:K:290:MET:HG3	1.73	0.69
1:H:161:THR:HG21	1:H:290:MET:HG3	1.73	0.69
1:B:276:ARG:HD3	1:B:394:ILE:HD11	1.73	0.69
1:E:329:THR:CG2	1:E:334:LEU:HB2	2.23	0.69
1:G:126:LEU:CD2	1:H:126:LEU:HD23	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:LYS:HG3	2:H:412:HOH:O	1.92	0.69
1:H:290:MET:HE1	1:H:380:CYS:SG	2.33	0.69
1:N:135:ARG:HG3	2:N:405:HOH:O	1.91	0.69
1:C:58:ILE:HA	1:D:65:MET:HE2	1.76	0.68
1:I:144:MET:CE	1:J:65:MET:HE3	2.23	0.68
1:J:238:LYS:O	1:J:239:GLU:HB2	1.91	0.68
1:N:177:ASP:OD1	1:N:229:MET:HB3	1.94	0.68
1:H:276:ARG:HH11	1:H:394:ILE:HD11	1.58	0.68
1:P:44:VAL:O	2:P:402:HOH:O	2.12	0.68
1:J:316:GLU:HG3	1:J:359:ILE:HB	1.75	0.68
1:I:126:LEU:CD2	1:J:126:LEU:HD23	2.24	0.67
1:M:62:PRO:HA	1:M:65:MET:HE2	1.77	0.67
1:B:89:LEU:HD22	1:B:382:GLY:HA3	1.75	0.67
1:A:126:LEU:HD23	1:B:126:LEU:CD2	2.25	0.67
1:E:126:LEU:HD23	1:F:126:LEU:CD2	2.23	0.67
1:F:62:PRO:HA	1:F:65:MET:HE2	1.77	0.67
1:F:161:THR:HG21	1:F:290:MET:HG3	1.76	0.67
1:K:238:LYS:O	1:K:239:GLU:HB2	1.94	0.67
1:K:371:GLN:HA	1:K:393:ARG:NH2	2.09	0.67
1:P:371:GLN:HA	1:P:393:ARG:NH2	2.10	0.67
1:B:238:LYS:HG2	1:G:36:ARG:HD3	1.75	0.67
1:C:288:LYS:CD	1:G:393:ARG:HH22	2.06	0.66
1:L:62:PRO:HA	1:L:65:MET:HE2	1.77	0.66
1:B:89:LEU:HD23	1:B:90:CYS:SG	2.35	0.66
1:G:62:PRO:HA	1:G:65:MET:HE2	1.78	0.66
1:B:181:LEU:O	1:B:181:LEU:CD2	2.43	0.66
1:C:161:THR:HG21	1:C:290:MET:HG3	1.78	0.66
1:N:368:ASN:O	1:N:393:ARG:NH2	2.26	0.65
1:O:126:LEU:HD23	1:P:126:LEU:CD2	2.25	0.65
1:E:126:LEU:CD2	1:F:126:LEU:HD23	2.26	0.65
1:I:126:LEU:HD23	1:J:126:LEU:CD2	2.25	0.65
1:I:62:PRO:HA	1:I:65:MET:HE2	1.78	0.65
1:A:65:MET:HE3	1:B:144:MET:HE3	1.78	0.65
1:M:51:HIS:CE1	2:M:404:HOH:O	2.49	0.65
1:O:126:LEU:CD2	1:P:126:LEU:HD23	2.26	0.65
1:E:62:PRO:HA	1:E:65:MET:HE2	1.79	0.65
1:J:371:GLN:HA	1:J:393:ARG:NH2	2.11	0.65
1:K:126:LEU:HD23	1:L:126:LEU:CD2	2.27	0.64
1:P:62:PRO:HA	1:P:65:MET:HE2	1.79	0.64
1:B:62:PRO:HA	1:B:65:MET:HE2	1.80	0.64
1:P:227:ASP:OD2	1:P:227:ASP:C	2.41	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:THR:HG21	1:D:290:MET:HG3	1.79	0.64
1:C:62:PRO:HA	1:C:65:MET:HE2	1.78	0.64
1:O:185:ARG:NH2	2:O:403:HOH:O	2.30	0.64
1:G:308:GLN:HG2	1:I:371:GLN:O	1.98	0.64
1:C:126:LEU:CD2	1:D:126:LEU:HD23	2.28	0.63
1:L:292:ILE:O	1:L:295:VAL:CG1	2.46	0.63
1:N:44:VAL:HA	2:N:401:HOH:O	1.98	0.63
1:N:393:ARG:NE	2:N:402:HOH:O	2.31	0.63
1:A:181:LEU:O	1:A:181:LEU:CD2	2.42	0.63
1:G:126:LEU:HD23	1:H:126:LEU:CD2	2.26	0.63
1:H:11:VAL:HG22	1:H:201:VAL:HG23	1.80	0.63
1:H:290:MET:HE3	1:H:291:GLY:N	2.14	0.63
1:M:11:VAL:HG22	1:M:201:VAL:HG23	1.80	0.63
1:N:11:VAL:HG22	1:N:201:VAL:HG23	1.80	0.63
1:O:11:VAL:HG22	1:O:201:VAL:HG23	1.80	0.63
1:M:51:HIS:ND1	2:M:404:HOH:O	2.30	0.63
1:C:11:VAL:HG22	1:C:201:VAL:HG23	1.81	0.63
1:K:11:VAL:HG22	1:K:201:VAL:HG23	1.81	0.63
1:I:11:VAL:HG22	1:I:201:VAL:HG23	1.81	0.62
1:O:37:GLU:HG2	1:O:201:VAL:HG22	1.82	0.62
1:P:158:MET:HE1	1:P:290:MET:SD	2.39	0.62
1:G:11:VAL:HG22	1:G:201:VAL:HG23	1.81	0.62
1:P:11:VAL:HG22	1:P:201:VAL:HG23	1.80	0.62
1:C:163:GLU:OE2	1:C:242:THR:HG22	1.99	0.62
1:L:163:GLU:OE2	1:L:242:THR:HG22	1.99	0.62
1:D:372:GLY:O	1:D:393:ARG:CG	2.47	0.62
1:N:37:GLU:HG2	1:N:201:VAL:HG22	1.82	0.62
1:P:163:GLU:OE2	1:P:242:THR:HG22	1.99	0.62
1:C:288:LYS:HE2	1:G:393:ARG:HH22	1.64	0.62
1:G:61:GLU:OE1	2:G:402:HOH:O	2.16	0.62
1:E:37:GLU:HG2	1:E:201:VAL:HG22	1.82	0.62
1:H:37:GLU:HG2	1:H:201:VAL:HG22	1.82	0.62
1:L:11:VAL:HG22	1:L:201:VAL:HG23	1.80	0.62
1:M:163:GLU:OE2	1:M:242:THR:HG22	1.99	0.62
1:N:208:ARG:CG	2:N:403:HOH:O	2.47	0.62
1:N:316:GLU:OE2	1:N:316:GLU:HA	1.99	0.62
1:B:37:GLU:HG2	1:B:201:VAL:HG22	1.82	0.62
1:F:292:ILE:O	1:F:295:VAL:CG1	2.46	0.62
1:J:161:THR:HG21	1:J:290:MET:HG3	1.80	0.62
1:J:11:VAL:HG22	1:J:201:VAL:HG23	1.80	0.61
1:D:11:VAL:HG22	1:D:201:VAL:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:GLU:HG2	1:K:201:VAL:HG22	1.82	0.61
1:L:37:GLU:HG2	1:L:201:VAL:HG22	1.82	0.61
1:M:316:GLU:OE1	2:M:401:HOH:O	2.16	0.61
1:P:158:MET:CE	1:P:290:MET:SD	2.88	0.61
1:I:37:GLU:HG2	1:I:201:VAL:HG22	1.81	0.61
1:J:12:ARG:CZ	1:J:200:ILE:HD11	2.30	0.61
1:P:185:ARG:HA	1:P:185:ARG:NH1	2.16	0.61
1:G:58:ILE:HA	1:H:65:MET:HE2	1.80	0.61
1:G:268:ARG:HD2	1:G:268:ARG:O	1.99	0.61
1:H:239:GLU:HG3	1:H:240:ASN:N	2.16	0.61
1:O:126:LEU:HD23	1:P:126:LEU:HD22	1.83	0.61
1:B:11:VAL:HG22	1:B:201:VAL:HG23	1.81	0.61
1:C:37:GLU:HG2	1:C:201:VAL:HG22	1.81	0.61
1:H:206:LYS:HB3	1:H:211:ASP:OD1	2.01	0.61
1:J:37:GLU:HG2	1:J:201:VAL:HG22	1.82	0.61
1:K:126:LEU:CD2	1:L:126:LEU:HD23	2.31	0.61
1:C:126:LEU:HD23	1:D:126:LEU:CD2	2.31	0.60
1:D:37:GLU:HG2	1:D:201:VAL:HG22	1.82	0.60
1:P:37:GLU:HG2	1:P:201:VAL:HG22	1.82	0.60
1:C:66:TYR:OH	1:D:148:ALA:O	2.18	0.60
1:M:154:HIS:CE1	1:M:288:LYS:HE3	2.36	0.60
1:A:304:ARG:NH1	1:B:108:ASP:OD1	2.33	0.60
1:A:37:GLU:HG2	1:A:201:VAL:HG22	1.84	0.60
1:H:228:ASP:OD2	2:H:402:HOH:O	2.16	0.60
1:I:126:LEU:HD23	1:J:126:LEU:HD22	1.84	0.60
1:M:37:GLU:HG2	1:M:201:VAL:HG22	1.82	0.60
1:A:161:THR:HG21	1:A:290:MET:HG3	1.84	0.60
1:A:126:LEU:CD2	1:B:126:LEU:HD23	2.32	0.60
1:M:176:GLN:CD	1:M:242:THR:HG1	2.09	0.60
1:P:158:MET:HE1	1:P:382:GLY:CA	2.30	0.59
1:C:276:ARG:CZ	1:C:392:GLU:OE1	2.49	0.59
1:A:65:MET:HE3	1:B:144:MET:CE	2.32	0.59
1:I:214:PHE:CE1	1:I:218:GLU:HG3	2.37	0.59
1:N:135:ARG:CD	2:N:405:HOH:O	2.49	0.59
1:E:7:VAL:HG22	1:E:260:MET:HE3	1.84	0.59
1:G:263:ARG:NE	2:G:404:HOH:O	2.33	0.59
1:G:161:THR:HG21	1:G:290:MET:HG3	1.84	0.59
1:E:126:LEU:HD23	1:F:126:LEU:HD22	1.85	0.59
1:K:308:GLN:OE1	1:K:309:VAL:N	2.27	0.59
1:O:126:LEU:HD22	1:P:126:LEU:HD23	1.83	0.59
1:P:161:THR:HG21	1:P:290:MET:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:VAL:HG22	1:G:260:MET:HE3	1.84	0.59
1:G:126:LEU:HD22	1:H:126:LEU:HD23	1.85	0.59
1:K:19:GLY:O	1:K:23:LYS:HE2	2.03	0.59
1:A:207:GLY:C	1:A:209:LYS:H	2.10	0.58
1:H:7:VAL:HG22	1:H:260:MET:HE3	1.84	0.58
1:N:158:MET:SD	1:N:290:MET:HE2	2.43	0.58
1:N:7:VAL:HG22	1:N:260:MET:HE3	1.84	0.58
1:C:316:GLU:HA	1:C:316:GLU:OE2	2.04	0.58
1:F:158:MET:HE1	1:F:382:GLY:CA	2.31	0.58
1:M:7:VAL:HG22	1:M:260:MET:HE3	1.84	0.58
1:O:7:VAL:HG22	1:O:260:MET:HE3	1.85	0.58
1:D:206:LYS:NZ	1:G:264:ALA:C	2.61	0.58
1:A:181:LEU:HD22	2:A:417:HOH:O	2.02	0.58
1:I:7:VAL:HG22	1:I:260:MET:HE3	1.84	0.58
1:E:126:LEU:HD22	1:F:126:LEU:HD23	1.85	0.58
1:C:288:LYS:CE	1:G:393:ARG:HH22	2.17	0.58
1:H:135:ARG:NH1	2:H:401:HOH:O	2.08	0.58
1:K:126:LEU:HD23	1:L:126:LEU:HD22	1.86	0.58
1:C:167:LYS:HE3	2:C:456:HOH:O	2.04	0.57
1:N:95:GLN:O	1:N:99:SER:OG	2.22	0.57
1:N:316:GLU:HG3	1:N:359:ILE:HB	1.86	0.57
1:C:265:GLU:OE2	1:C:268:ARG:NH1	2.37	0.57
1:P:7:VAL:HG22	1:P:260:MET:HE3	1.85	0.57
1:C:126:LEU:HD23	1:D:126:LEU:HD22	1.87	0.57
1:C:288:LYS:HD3	1:G:393:ARG:NH2	2.16	0.57
1:B:89:LEU:HD22	1:B:382:GLY:CA	2.35	0.57
1:K:173:ARG:O	1:K:177:ASP:CG	2.48	0.57
1:L:233:ARG:O	1:L:233:ARG:HD3	2.04	0.57
1:G:126:LEU:HD23	1:H:126:LEU:HD22	1.87	0.57
1:I:126:LEU:HD22	1:J:126:LEU:HD23	1.86	0.57
1:O:335:ASP:OD1	1:O:335:ASP:O	2.22	0.56
1:D:265:GLU:OE1	1:D:268:ARG:NH1	2.38	0.56
1:C:288:LYS:HE2	1:G:393:ARG:NH2	2.20	0.56
1:K:177:ASP:OD1	1:K:177:ASP:N	2.32	0.56
1:B:161:THR:HG21	1:B:290:MET:HG3	1.88	0.56
1:D:372:GLY:O	1:D:393:ARG:CD	2.53	0.56
1:P:158:MET:CE	1:P:382:GLY:HA2	2.31	0.56
1:A:335:ASP:OD1	1:A:335:ASP:O	2.23	0.56
1:D:206:LYS:NZ	1:G:265:GLU:HA	2.21	0.56
1:B:276:ARG:HD3	1:B:394:ILE:CD1	2.35	0.56
1:A:126:LEU:HD23	1:B:126:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD22	1:D:126:LEU:HD23	1.87	0.56
1:D:205:SER:C	1:D:206:LYS:HG3	2.30	0.56
1:O:65:MET:HE2	1:P:144:MET:HE3	1.84	0.55
1:I:206:LYS:NZ	2:I:402:HOH:O	2.35	0.55
1:N:161:THR:HG21	1:N:290:MET:CG	2.35	0.55
1:F:158:MET:CE	1:F:382:GLY:HA2	2.33	0.55
1:A:156:ILE:HD12	1:A:160:VAL:CG2	2.37	0.55
1:P:185:ARG:HA	1:P:185:ARG:CZ	2.36	0.55
1:C:156:ILE:HD12	1:C:160:VAL:CG2	2.36	0.55
1:O:161:THR:HG21	1:O:290:MET:CG	2.34	0.55
1:K:174:ALA:C	1:K:177:ASP:OD1	2.50	0.55
1:N:156:ILE:HD12	1:N:160:VAL:CG2	2.37	0.55
1:P:265:GLU:OE2	1:P:268:ARG:NH2	2.38	0.55
1:E:161:THR:HG21	1:E:290:MET:CG	2.35	0.54
1:H:156:ILE:HD12	1:H:160:VAL:CG2	2.37	0.54
1:G:156:ILE:HD12	1:G:160:VAL:CG2	2.37	0.54
1:M:156:ILE:HD12	1:M:160:VAL:CG2	2.37	0.54
1:K:156:ILE:HD12	1:K:160:VAL:CG2	2.38	0.54
1:O:156:ILE:HD12	1:O:160:VAL:CG2	2.37	0.54
1:D:156:ILE:HD12	1:D:160:VAL:CG2	2.37	0.54
1:B:265:GLU:HA	1:B:268[B]:ARG:HG2	1.89	0.54
1:J:156:ILE:HD12	1:J:160:VAL:CG2	2.37	0.54
1:I:156:ILE:HD12	1:I:160:VAL:CG2	2.37	0.54
1:C:23:LYS:HG2	2:C:414:HOH:O	2.07	0.54
1:F:156:ILE:HD12	1:F:160:VAL:CG2	2.37	0.54
1:L:156:ILE:HD12	1:L:160:VAL:CG2	2.37	0.54
1:B:156:ILE:HD12	1:B:160:VAL:CG2	2.37	0.54
1:C:163:GLU:OE2	1:C:242:THR:CG2	2.56	0.53
1:A:279:SER:HA	2:A:404:HOH:O	2.07	0.53
1:G:6:VAL:HG22	1:G:273:PRO:HB3	1.91	0.53
1:M:126:LEU:CD2	1:N:126:LEU:HD23	2.38	0.53
1:P:156:ILE:HD12	1:P:160:VAL:CG2	2.37	0.53
1:B:154:HIS:C	1:B:155:ARG:HG2	2.32	0.53
1:M:6:VAL:HG22	1:M:273:PRO:HB3	1.91	0.53
1:C:265:GLU:HA	1:C:268:ARG:HH11	1.74	0.53
1:K:126:LEU:HD22	1:L:126:LEU:HD23	1.89	0.53
1:M:215:ASP:OD2	2:M:402:HOH:O	2.18	0.53
1:D:206:LYS:HZ3	1:G:264:ALA:C	2.17	0.53
1:F:335:ASP:C	1:F:335:ASP:OD1	2.52	0.53
1:K:6:VAL:HG22	1:K:273:PRO:HB3	1.91	0.53
1:P:163:GLU:OE2	1:P:242:THR:CG2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:ILE:O	1:J:260:MET:HE1	2.09	0.53
1:M:163:GLU:OE2	1:M:242:THR:CG2	2.57	0.53
1:C:381:ILE:HB	1:C:385:GLN:HB2	1.91	0.53
1:K:97:ILE:O	1:K:260:MET:HE1	2.09	0.53
1:A:126:LEU:HD22	1:B:126:LEU:HD23	1.91	0.53
1:L:163:GLU:OE2	1:L:242:THR:CG2	2.56	0.53
1:N:207:GLY:O	1:N:208:ARG:HB2	2.09	0.53
1:E:6:VAL:HG22	1:E:273:PRO:HB3	1.91	0.52
1:H:381:ILE:HB	1:H:385:GLN:HB2	1.91	0.52
1:N:6:VAL:HG22	1:N:273:PRO:HB3	1.92	0.52
1:D:97:ILE:O	1:D:260:MET:HE1	2.09	0.52
1:H:6:VAL:HG22	1:H:273:PRO:HB3	1.92	0.52
1:K:381:ILE:HB	1:K:385:GLN:HB2	1.92	0.52
1:O:6:VAL:HG22	1:O:273:PRO:HB3	1.92	0.52
1:I:144:MET:HE3	1:J:65:MET:HE2	1.90	0.52
1:A:97:ILE:O	1:A:260:MET:HE1	2.10	0.52
1:F:97:ILE:O	1:F:260:MET:HE1	2.09	0.52
1:I:214:PHE:HE1	1:I:218:GLU:HG3	1.73	0.52
1:O:66:TYR:OH	1:P:148:ALA:O	2.27	0.52
1:L:6:VAL:HG22	1:L:273:PRO:HB3	1.91	0.52
1:A:6:VAL:HG22	1:A:273:PRO:HB3	1.92	0.52
1:A:279:SER:CA	2:A:404:HOH:O	2.57	0.52
1:L:381:ILE:HB	1:L:385:GLN:HB2	1.92	0.52
1:N:208:ARG:HG3	2:N:403:HOH:O	2.07	0.52
1:P:335:ASP:OD1	1:P:335:ASP:C	2.53	0.52
1:C:6:VAL:HG22	1:C:273:PRO:HB3	1.92	0.52
1:C:97:ILE:O	1:C:260:MET:HE1	2.10	0.52
1:D:381:ILE:HB	1:D:385:GLN:HB2	1.92	0.52
1:I:6:VAL:HG22	1:I:273:PRO:HB3	1.92	0.52
1:M:381:ILE:HB	1:M:385:GLN:HB2	1.92	0.52
1:C:335:ASP:C	1:C:335:ASP:OD1	2.53	0.52
1:J:335:ASP:C	1:J:335:ASP:OD1	2.52	0.52
1:N:335:ASP:OD1	1:N:335:ASP:C	2.53	0.52
1:O:381:ILE:HB	1:O:385:GLN:HB2	1.92	0.52
1:A:381:ILE:HB	1:A:385:GLN:HB2	1.93	0.51
1:J:6:VAL:HG22	1:J:273:PRO:HB3	1.93	0.51
1:B:6:VAL:HG22	1:B:273:PRO:HB3	1.92	0.51
1:B:97:ILE:O	1:B:260:MET:HE1	2.10	0.51
1:B:381:ILE:HB	1:B:385:GLN:HB2	1.92	0.51
1:E:335:ASP:OD1	1:E:335:ASP:C	2.52	0.51
1:J:381:ILE:HB	1:J:385:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:VAL:HG22	1:D:273:PRO:HB3	1.93	0.51
1:I:286:ASP:OD2	1:I:288:LYS:HD3	2.10	0.51
1:P:99:SER:CB	2:P:403:HOH:O	2.58	0.51
1:A:161:THR:O	1:A:165:VAL:HG22	2.10	0.51
1:F:6:VAL:HG22	1:F:273:PRO:HB3	1.92	0.51
1:F:158:MET:CE	1:F:290:MET:SD	2.99	0.51
1:G:314:VAL:HG12	1:G:367:LEU:HD13	1.93	0.51
1:G:381:ILE:HB	1:G:385:GLN:HB2	1.93	0.51
1:L:335:ASP:OD1	1:L:335:ASP:C	2.52	0.51
1:N:381:ILE:HB	1:N:385:GLN:HB2	1.92	0.51
1:P:381:ILE:HB	1:P:385:GLN:HB2	1.92	0.51
1:C:23:LYS:CG	2:C:414:HOH:O	2.59	0.51
1:E:381:ILE:HB	1:E:385:GLN:HB2	1.93	0.51
1:N:293:GLY:N	1:N:294:PRO:CD	2.74	0.51
1:I:381:ILE:HB	1:I:385:GLN:HB2	1.93	0.50
1:P:6:VAL:HG22	1:P:273:PRO:HB3	1.92	0.50
1:E:239:GLU:N	2:E:405:HOH:O	2.43	0.50
1:E:314:VAL:HG12	1:E:367:LEU:HD13	1.93	0.50
1:G:358:LEU:C	1:G:358:LEU:HD12	2.36	0.50
1:K:358:LEU:HD12	1:K:358:LEU:C	2.37	0.50
1:M:335:ASP:C	1:M:335:ASP:OD1	2.54	0.50
1:I:314:VAL:HG12	1:I:367:LEU:HD13	1.94	0.50
1:O:346:ILE:O	2:O:401:HOH:O	2.19	0.50
1:C:171:ILE:HG23	1:C:175:GLN:OE1	2.11	0.50
1:D:335:ASP:OD1	1:D:335:ASP:C	2.53	0.50
1:M:314:VAL:HG12	1:M:367:LEU:HD13	1.93	0.50
1:B:314:VAL:HG12	1:B:367:LEU:HD13	1.93	0.50
1:E:195:TYR:OH	2:E:401:HOH:O	2.18	0.50
1:F:158:MET:HE1	1:F:290:MET:SD	2.52	0.50
1:F:381:ILE:HB	1:F:385:GLN:HB2	1.93	0.50
1:G:263:ARG:CD	2:G:404:HOH:O	2.59	0.50
1:H:238:LYS:O	1:H:239:GLU:HB2	2.08	0.50
1:I:335:ASP:OD1	1:I:335:ASP:C	2.53	0.50
1:B:265:GLU:CD	1:B:268[B]:ARG:HE	2.20	0.50
1:H:293:GLY:N	1:H:294:PRO:CD	2.75	0.50
1:C:176:GLN:CD	1:C:242:THR:HG1	2.18	0.50
1:I:126:LEU:HD21	1:J:126:LEU:CD2	2.40	0.50
1:P:290:MET:HE1	1:P:380:CYS:SG	2.51	0.50
1:B:358:LEU:C	1:B:358:LEU:HD12	2.36	0.50
1:C:358:LEU:HD12	1:C:358:LEU:C	2.37	0.50
1:L:176:GLN:CD	1:L:242:THR:HG1	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:126:LEU:HG	1:N:144:MET:CG	2.42	0.50
1:N:206:LYS:HG2	1:N:211:ASP:OD1	2.12	0.50
1:B:263:ARG:NH2	1:B:267:GLU:OE2	2.45	0.49
1:L:11:VAL:CG2	1:L:201:VAL:CG2	2.90	0.49
1:C:293:GLY:N	1:C:294:PRO:CD	2.75	0.49
1:E:371:GLN:HG3	1:E:393:ARG:NH1	2.27	0.49
1:H:126:LEU:HG	1:H:144:MET:CG	2.43	0.49
1:J:172:SER:OG	1:J:175:GLN:HG3	2.12	0.49
1:N:208:ARG:NE	2:N:403:HOH:O	2.45	0.49
1:A:314:VAL:HG12	1:A:367:LEU:HD13	1.93	0.49
1:K:126:LEU:HG	1:K:144:MET:CG	2.42	0.49
1:L:233:ARG:HD2	1:L:233:ARG:N	2.10	0.49
1:A:126:LEU:CD2	1:B:126:LEU:HD21	2.40	0.49
1:D:314:VAL:HG12	1:D:367:LEU:HD13	1.92	0.49
1:F:358:LEU:HD12	1:F:358:LEU:C	2.38	0.49
1:G:11:VAL:HG21	1:G:201:VAL:CG2	2.43	0.49
1:H:358:LEU:HD12	1:H:358:LEU:C	2.37	0.49
1:J:11:VAL:CG2	1:J:201:VAL:CG2	2.90	0.49
1:K:11:VAL:HG21	1:K:201:VAL:CG2	2.43	0.49
1:K:314:VAL:HG12	1:K:367:LEU:HD13	1.93	0.49
1:L:11:VAL:CG2	1:L:201:VAL:HG23	2.43	0.49
1:N:314:VAL:HG12	1:N:367:LEU:HD13	1.94	0.49
1:O:11:VAL:CG2	1:O:201:VAL:CG2	2.91	0.49
1:P:314:VAL:HG12	1:P:367:LEU:HD13	1.94	0.49
1:G:58:ILE:HG12	1:H:65:MET:HE1	1.94	0.49
1:K:367:LEU:HG	1:K:393:ARG:HG2	1.94	0.49
1:L:126:LEU:HG	1:L:144:MET:CG	2.43	0.49
1:M:144:MET:HE3	1:N:65:MET:HE2	1.89	0.49
1:O:314:VAL:HG12	1:O:367:LEU:HD13	1.94	0.49
1:O:358:LEU:HD12	1:O:358:LEU:C	2.37	0.49
1:P:11:VAL:CG2	1:P:201:VAL:CG2	2.91	0.49
1:D:37:GLU:HG2	1:D:201:VAL:CG2	2.43	0.49
1:H:314:VAL:HG12	1:H:367:LEU:HD13	1.94	0.49
1:J:37:GLU:HG2	1:J:201:VAL:CG2	2.43	0.49
1:M:126:LEU:HG	1:M:144:MET:CG	2.43	0.49
1:P:158:MET:HE3	1:P:290:MET:SD	2.52	0.49
1:P:358:LEU:C	1:P:358:LEU:HD12	2.37	0.49
1:B:263:ARG:HD3	1:B:267:GLU:CD	2.38	0.49
1:I:11:VAL:CG2	1:I:201:VAL:CG2	2.91	0.49
1:J:11:VAL:HG21	1:J:201:VAL:CG2	2.43	0.49
1:K:11:VAL:CG2	1:K:201:VAL:CG2	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HB	1:A:160:VAL:HG21	1.95	0.49
1:C:37:GLU:HG2	1:C:201:VAL:CG2	2.43	0.49
1:C:314:VAL:HG12	1:C:367:LEU:HD13	1.95	0.49
1:D:11:VAL:CG2	1:D:201:VAL:CG2	2.91	0.49
1:H:276:ARG:CD	1:H:394:ILE:CD1	2.83	0.49
1:I:126:LEU:HG	1:I:144:MET:CG	2.43	0.49
1:O:11:VAL:CG2	1:O:201:VAL:HG23	2.43	0.49
1:P:11:VAL:CG2	1:P:201:VAL:HG23	2.43	0.49
1:A:358:LEU:HD12	1:A:358:LEU:C	2.38	0.49
1:B:126:LEU:HG	1:B:144:MET:CG	2.43	0.49
1:G:11:VAL:CG2	1:G:201:VAL:HG23	2.42	0.49
1:H:11:VAL:HG21	1:H:201:VAL:CG2	2.43	0.49
1:J:11:VAL:CG2	1:J:201:VAL:HG23	2.42	0.49
1:B:11:VAL:CG2	1:B:201:VAL:CG2	2.91	0.48
1:F:373:ARG:NH1	1:F:374:TYR:OH	2.45	0.48
1:M:156:ILE:HB	1:M:160:VAL:HG21	1.95	0.48
1:A:126:LEU:HG	1:A:144:MET:CG	2.43	0.48
1:A:293:GLY:N	1:A:294:PRO:CD	2.75	0.48
1:B:11:VAL:CG2	1:B:201:VAL:HG23	2.43	0.48
1:B:335:ASP:OD1	1:B:335:ASP:C	2.55	0.48
1:C:126:LEU:HG	1:C:144:MET:CG	2.43	0.48
1:F:314:VAL:HG12	1:F:367:LEU:HD13	1.94	0.48
1:G:126:LEU:HG	1:G:144:MET:CG	2.44	0.48
1:K:156:ILE:HB	1:K:160:VAL:HG21	1.96	0.48
1:L:11:VAL:HG21	1:L:201:VAL:CG2	2.43	0.48
1:O:293:GLY:N	1:O:294:PRO:CD	2.77	0.48
1:F:126:LEU:HG	1:F:144:MET:CG	2.43	0.48
1:I:156:ILE:HB	1:I:160:VAL:HG21	1.95	0.48
1:J:358:LEU:HD12	1:J:358:LEU:C	2.38	0.48
1:M:358:LEU:HD12	1:M:358:LEU:C	2.37	0.48
1:P:126:LEU:HG	1:P:144:MET:CG	2.43	0.48
1:H:11:VAL:CG2	1:H:201:VAL:HG23	2.42	0.48
1:K:293:GLY:N	1:K:294:PRO:CD	2.75	0.48
1:D:156:ILE:HB	1:D:160:VAL:HG21	1.95	0.48
1:H:11:VAL:CG2	1:H:201:VAL:CG2	2.90	0.48
1:H:156:ILE:HB	1:H:160:VAL:HG21	1.95	0.48
1:I:11:VAL:CG2	1:I:201:VAL:HG23	2.43	0.48
1:K:37:GLU:HG2	1:K:201:VAL:CG2	2.43	0.48
1:L:156:ILE:HB	1:L:160:VAL:HG21	1.96	0.48
1:M:11:VAL:HG21	1:M:201:VAL:CG2	2.44	0.48
1:M:293:GLY:N	1:M:294:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:VAL:CG2	1:C:201:VAL:HG23	2.43	0.48
1:D:11:VAL:HG21	1:D:201:VAL:CG2	2.44	0.48
1:K:11:VAL:CG2	1:K:201:VAL:HG23	2.43	0.48
1:M:11:VAL:CG2	1:M:201:VAL:CG2	2.90	0.48
1:N:11:VAL:CG2	1:N:201:VAL:HG23	2.43	0.48
1:P:37:GLU:HG2	1:P:201:VAL:CG2	2.43	0.48
1:C:11:VAL:CG2	1:C:201:VAL:CG2	2.91	0.48
1:G:11:VAL:CG2	1:G:201:VAL:CG2	2.90	0.48
1:G:293:GLY:N	1:G:294:PRO:CD	2.77	0.48
1:J:156:ILE:HB	1:J:160:VAL:HG21	1.95	0.48
1:J:393:ARG:O	1:J:393:ARG:HG3	2.13	0.48
1:K:65:MET:HE1	1:L:58:ILE:HG12	1.96	0.48
1:N:11:VAL:CG2	1:N:201:VAL:CG2	2.91	0.48
1:N:11:VAL:HG21	1:N:201:VAL:CG2	2.44	0.48
1:N:135:ARG:CG	2:N:405:HOH:O	2.56	0.48
1:A:37:GLU:CD	1:A:41:ARG:NH1	2.71	0.48
1:B:11:VAL:HG21	1:B:201:VAL:CG2	2.44	0.48
1:G:37:GLU:HG2	1:G:201:VAL:HG22	1.96	0.48
1:G:156:ILE:HB	1:G:160:VAL:HG21	1.96	0.48
1:J:126:LEU:HG	1:J:144:MET:CG	2.44	0.48
1:N:156:ILE:HB	1:N:160:VAL:HG21	1.96	0.48
1:O:11:VAL:HG21	1:O:201:VAL:CG2	2.44	0.48
1:P:11:VAL:HG21	1:P:201:VAL:CG2	2.44	0.48
1:A:280:TYR:N	2:A:404:HOH:O	2.28	0.48
1:B:156:ILE:HB	1:B:160:VAL:HG21	1.96	0.48
1:G:319:GLU:CD	1:G:344:SER:HB3	2.39	0.48
1:M:126:LEU:HD23	1:N:126:LEU:CD2	2.42	0.48
1:O:126:LEU:HG	1:O:144:MET:CG	2.44	0.48
1:E:126:LEU:HG	1:E:144:MET:CG	2.44	0.48
1:I:148:ALA:O	1:J:66:TYR:OH	2.29	0.48
1:L:37:GLU:HG2	1:L:201:VAL:CG2	2.43	0.48
1:M:37:GLU:HG2	1:M:201:VAL:CG2	2.44	0.48
1:E:293:GLY:N	1:E:294:PRO:CD	2.77	0.47
1:L:176:GLN:OE1	1:L:242:THR:OG1	2.26	0.47
1:B:37:GLU:HG2	1:B:201:VAL:CG2	2.43	0.47
1:D:11:VAL:CG2	1:D:201:VAL:HG23	2.43	0.47
1:D:358:LEU:C	1:D:358:LEU:HD12	2.39	0.47
1:E:37:GLU:HG2	1:E:201:VAL:CG2	2.43	0.47
1:G:335:ASP:OD1	1:G:335:ASP:C	2.56	0.47
1:J:314:VAL:HG12	1:J:367:LEU:HD13	1.94	0.47
1:M:176:GLN:CD	1:M:242:THR:OG1	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:GLU:HG2	1:N:201:VAL:CG2	2.44	0.47
1:O:156:ILE:HB	1:O:160:VAL:HG21	1.96	0.47
1:C:156:ILE:HB	1:C:160:VAL:HG21	1.96	0.47
1:H:37:GLU:HG2	1:H:201:VAL:CG2	2.44	0.47
1:I:11:VAL:HG21	1:I:201:VAL:CG2	2.43	0.47
1:K:126:LEU:CD2	1:L:126:LEU:HD21	2.43	0.47
1:M:11:VAL:CG2	1:M:201:VAL:HG23	2.43	0.47
1:N:208:ARG:CD	2:N:403:HOH:O	2.62	0.47
1:O:148:ALA:O	1:P:66:TYR:OH	2.31	0.47
1:O:185:ARG:CZ	2:O:403:HOH:O	2.62	0.47
1:P:156:ILE:HB	1:P:160:VAL:HG21	1.95	0.47
1:D:126:LEU:HG	1:D:144:MET:CG	2.45	0.47
1:K:19:GLY:C	1:K:23:LYS:HE2	2.40	0.47
1:N:368:ASN:CA	1:N:393:ARG:NH2	2.72	0.47
1:O:37:GLU:HG2	1:O:201:VAL:CG2	2.43	0.47
1:D:206:LYS:NZ	1:G:265:GLU:N	2.62	0.47
1:P:233:ARG:NH2	2:P:408:HOH:O	2.47	0.47
1:N:358:LEU:C	1:N:358:LEU:HD12	2.39	0.47
1:C:126:LEU:HD21	1:D:126:LEU:CD2	2.43	0.47
1:O:126:LEU:CD2	1:P:126:LEU:HD21	2.39	0.47
1:I:154:HIS:C	1:I:155:ARG:CG	2.87	0.47
1:I:358:LEU:C	1:I:358:LEU:HD12	2.40	0.47
1:K:174:ALA:CA	1:K:177:ASP:OD1	2.63	0.47
1:L:358:LEU:C	1:L:358:LEU:HD12	2.39	0.47
1:A:37:GLU:HG2	1:A:201:VAL:CG2	2.45	0.47
1:F:293:GLY:N	1:F:294:PRO:CD	2.77	0.47
1:I:37:GLU:HG2	1:I:201:VAL:CG2	2.43	0.47
1:F:156:ILE:HB	1:F:160:VAL:HG21	1.96	0.46
1:H:209:LYS:HB2	1:H:209:LYS:HE2	1.74	0.46
1:C:11:VAL:HG21	1:C:201:VAL:CG2	2.44	0.46
1:C:89:LEU:HD11	1:D:66:TYR:CD1	2.50	0.46
1:C:176:GLN:OE1	1:C:242:THR:OG1	2.27	0.46
1:L:176:GLN:CD	1:L:242:THR:OG1	2.59	0.46
1:N:198:ASP:HB2	2:N:411:HOH:O	2.15	0.46
1:F:227:ASP:OD1	1:F:227:ASP:O	2.34	0.46
1:J:137:GLY:HA2	1:K:146:LEU:HD12	1.97	0.46
1:K:19:GLY:O	1:K:23:LYS:CE	2.63	0.46
1:C:394:ILE:HA	1:C:394:ILE:HD12	1.71	0.46
1:E:23:LYS:HD2	2:E:410:HOH:O	2.15	0.46
1:E:358:LEU:C	1:E:358:LEU:HD12	2.40	0.46
1:F:265:GLU:OE2	1:F:268:ARG:NH1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:LEU:HD22	1:J:66:TYR:CZ	2.51	0.46
1:A:207:GLY:O	1:A:209:LYS:N	2.48	0.46
1:B:293:GLY:N	1:B:294:PRO:CD	2.77	0.46
1:I:286:ASP:OD2	1:I:288:LYS:CE	2.64	0.46
1:L:319:GLU:CD	1:L:344:SER:HB3	2.40	0.46
1:C:58:ILE:HG12	1:D:65:MET:HE1	1.97	0.46
1:L:293:GLY:N	1:L:294:PRO:CD	2.77	0.46
1:H:276:ARG:NH1	1:H:394:ILE:HD11	2.29	0.46
1:I:393:ARG:HG2	1:I:394:ILE:HA	1.97	0.46
1:P:176:GLN:CD	1:P:242:THR:OG1	2.58	0.46
1:B:233:ARG:NH2	1:G:76:GLY:HA2	2.31	0.46
1:L:368:ASN:HA	1:L:393:ARG:HD3	1.98	0.46
1:O:226:ILE:HG23	1:O:227:ASP:OD1	2.16	0.46
1:F:143:ASP:OD1	1:F:143:ASP:C	2.58	0.46
1:K:309:VAL:CG2	2:K:409:HOH:O	2.50	0.46
1:O:290:MET:HE1	1:O:380:CYS:SG	2.56	0.46
1:E:329:THR:HG23	1:E:339:VAL:HG21	1.97	0.45
1:G:126:LEU:HD21	1:H:126:LEU:CD2	2.40	0.45
1:M:126:LEU:HD22	1:N:126:LEU:HD23	1.98	0.45
1:C:23:LYS:HB2	1:C:23:LYS:HE3	1.85	0.45
1:E:171:ILE:HA	1:E:175:GLN:OE1	2.17	0.45
1:I:126:LEU:HD21	1:J:126:LEU:HD21	1.98	0.45
1:I:265:GLU:OE2	1:I:268:ARG:NH1	2.43	0.45
1:N:143:ASP:C	1:N:143:ASP:OD1	2.60	0.45
1:I:293:GLY:N	1:I:294:PRO:CD	2.79	0.45
1:A:143:ASP:OD1	1:A:143:ASP:C	2.59	0.45
1:P:293:GLY:N	1:P:294:PRO:CD	2.78	0.45
1:E:290:MET:HE1	1:E:380:CYS:SG	2.57	0.45
1:N:173:ARG:HA	1:N:176:GLN:HG2	1.99	0.45
1:G:263:ARG:HD3	2:G:404:HOH:O	2.17	0.45
1:L:233:ARG:CD	1:L:233:ARG:N	2.73	0.45
1:E:126:LEU:HD21	1:F:126:LEU:HD21	1.98	0.45
1:I:238:LYS:HA	1:I:238:LYS:HD2	1.70	0.45
1:A:279:SER:HB2	2:A:404:HOH:O	2.16	0.45
1:B:204:VAL:HA	1:B:212:VAL:O	2.17	0.45
1:I:126:LEU:CD2	1:J:126:LEU:HD21	2.43	0.44
1:J:158:MET:CA	1:J:158:MET:CE	2.85	0.44
1:C:89:LEU:HD22	1:D:66:TYR:CE1	2.52	0.44
1:E:126:LEU:CD2	1:F:126:LEU:HD21	2.40	0.44
1:F:17:THR:HG22	1:F:18:PHE:N	2.32	0.44
1:F:158:MET:CE	1:F:382:GLY:CA	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:286:ASP:OD2	1:I:288:LYS:HE2	2.17	0.44
1:J:238:LYS:HD2	1:J:238:LYS:HA	1.87	0.44
1:A:37:GLU:CG	1:A:41:ARG:NH1	2.80	0.44
1:G:143:ASP:C	1:G:143:ASP:OD1	2.61	0.44
1:N:126:LEU:HG	1:N:144:MET:HG2	1.99	0.44
1:N:135:ARG:NE	2:N:405:HOH:O	2.50	0.44
1:N:182:GLU:OE1	1:N:185:ARG:NH2	2.49	0.44
1:O:66:TYR:CZ	1:P:89:LEU:HD22	2.52	0.44
1:C:175:GLN:HG3	2:C:436:HOH:O	2.17	0.44
1:E:143:ASP:C	1:E:143:ASP:OD1	2.61	0.44
1:H:126:LEU:HG	1:H:144:MET:HG2	1.99	0.44
1:O:126:LEU:HD21	1:P:126:LEU:HD21	1.98	0.44
1:A:65:MET:HE2	1:B:144:MET:HE3	1.99	0.44
1:A:230:THR:O	1:A:230:THR:CG2	2.66	0.44
1:B:295:VAL:HB	1:B:296:PRO:CD	2.48	0.44
1:J:171:ILE:HA	1:J:175:GLN:OE1	2.17	0.44
1:J:293:GLY:N	1:J:294:PRO:CD	2.80	0.44
1:M:102:GLN:HG2	1:N:106:LEU:CD1	2.48	0.44
1:A:148:ALA:N	1:B:65:MET:HE1	2.33	0.44
1:G:268:ARG:HD2	1:G:268:ARG:C	2.42	0.44
1:K:154:HIS:C	1:K:155:ARG:HG3	2.42	0.44
1:N:161:THR:CG2	1:N:290:MET:HG3	2.44	0.44
1:O:23:LYS:HB2	1:O:23:LYS:HE3	1.84	0.44
1:P:290:MET:HE3	1:P:291:GLY:HA2	2.00	0.44
1:K:319:GLU:CD	1:K:344:SER:HB3	2.42	0.44
1:L:143:ASP:C	1:L:143:ASP:OD1	2.61	0.44
1:G:204:VAL:HA	1:G:212:VAL:O	2.18	0.44
1:J:143:ASP:C	1:J:143:ASP:OD1	2.61	0.44
1:M:36:ARG:NE	2:M:403:HOH:O	2.25	0.44
1:M:319:GLU:CD	1:M:344:SER:HB3	2.43	0.44
1:O:319:GLU:CD	1:O:344:SER:HB3	2.42	0.44
1:P:319:GLU:CD	1:P:344:SER:HB3	2.43	0.44
1:D:233:ARG:CZ	2:D:428:HOH:O	2.66	0.43
1:F:126:LEU:HG	1:F:144:MET:HG2	2.00	0.43
1:I:126:LEU:CD2	1:J:126:LEU:HD22	2.42	0.43
1:I:319:GLU:CD	1:I:344:SER:HB3	2.43	0.43
1:K:89:LEU:HD22	1:L:66:TYR:CZ	2.53	0.43
1:P:176:GLN:NE2	1:P:242:THR:OG1	2.51	0.43
1:B:272:LYS:H	1:B:272:LYS:HG3	1.63	0.43
1:C:176:GLN:CD	1:C:242:THR:OG1	2.60	0.43
1:D:293:GLY:N	1:D:294:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:GLU:CD	1:E:344:SER:HB3	2.42	0.43
1:G:126:LEU:HD21	1:H:126:LEU:HD21	2.00	0.43
1:H:290:MET:CE	1:H:291:GLY:HA2	2.39	0.43
1:A:41:ARG:NH2	1:A:198:ASP:O	2.52	0.43
1:D:319:GLU:CD	1:D:344:SER:HB3	2.44	0.43
1:E:148:ALA:N	1:F:65:MET:HE1	2.33	0.43
1:F:319:GLU:CD	1:F:344:SER:HB3	2.43	0.43
1:K:295:VAL:HB	1:K:296:PRO:CD	2.48	0.43
1:M:295:VAL:HB	1:M:296:PRO:CD	2.48	0.43
1:I:126:LEU:HG	1:I:144:MET:HG2	2.00	0.43
1:C:265:GLU:OE2	1:C:268:ARG:NE	2.49	0.43
1:I:143:ASP:OD1	1:I:143:ASP:C	2.60	0.43
1:A:37:GLU:O	1:A:41:ARG:HG2	2.17	0.43
1:B:319:GLU:CD	1:B:344:SER:HB3	2.43	0.43
1:E:161:THR:CG2	1:E:290:MET:HG3	2.44	0.43
1:E:318:ASN:HB3	2:E:402:HOH:O	2.19	0.43
1:K:17:THR:HG22	1:K:18:PHE:N	2.34	0.43
1:K:65:MET:CE	1:L:58:ILE:HA	2.46	0.43
1:K:126:LEU:HG	1:K:144:MET:HG2	2.00	0.43
1:A:66:TYR:CD2	1:B:89:LEU:HD13	2.53	0.43
1:C:319:GLU:CD	1:C:344:SER:HB3	2.43	0.43
1:D:206:LYS:NZ	1:G:265:GLU:CA	2.82	0.43
1:G:295:VAL:HB	1:G:296:PRO:CD	2.49	0.43
1:M:204:VAL:HA	1:M:212:VAL:O	2.19	0.43
1:N:236:PHE:O	1:N:237:VAL:O	2.37	0.43
1:N:238:LYS:HD2	1:N:238:LYS:HA	1.85	0.43
1:O:295:VAL:HB	1:O:296:PRO:CD	2.49	0.43
1:A:66:TYR:OH	1:B:148:ALA:O	2.32	0.43
1:G:299:LYS:HE2	1:I:394:ILE:HD11	2.01	0.43
1:L:11:VAL:HG21	1:L:201:VAL:HG22	2.01	0.43
1:L:276:ARG:NH2	1:L:392:GLU:OE1	2.49	0.43
1:M:126:LEU:HD23	1:N:126:LEU:HD22	2.01	0.43
1:N:151:ASP:OD2	1:N:287:PRO:HB3	2.19	0.43
1:P:126:LEU:HG	1:P:144:MET:HG2	2.00	0.43
1:N:319:GLU:CD	1:N:344:SER:HB3	2.44	0.42
1:A:126:LEU:HG	1:A:144:MET:HG2	2.00	0.42
1:C:126:LEU:CD2	1:D:126:LEU:HD22	2.42	0.42
1:D:23:LYS:HB2	1:D:23:LYS:HE3	1.84	0.42
1:E:295:VAL:HB	1:E:296:PRO:CD	2.49	0.42
1:G:11:VAL:HG21	1:G:201:VAL:HG22	2.01	0.42
1:L:126:LEU:HG	1:L:144:MET:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:TYR:CE2	1:P:89:LEU:HD22	2.54	0.42
1:P:265:GLU:OE2	1:P:268:ARG:NE	2.52	0.42
1:O:161:THR:CG2	1:O:290:MET:HG3	2.43	0.42
1:O:316:GLU:HG3	1:O:359:ILE:HB	1.99	0.42
1:A:295:VAL:HB	1:A:296:PRO:CD	2.49	0.42
1:I:11:VAL:HG21	1:I:201:VAL:HG22	2.01	0.42
1:J:11:VAL:HG21	1:J:201:VAL:HG22	2.01	0.42
1:K:174:ALA:HA	1:K:177:ASP:OD1	2.19	0.42
1:P:23:LYS:HB2	1:P:23:LYS:HE3	1.85	0.42
1:K:174:ALA:O	1:K:177:ASP:OD1	2.36	0.42
1:O:11:VAL:HG21	1:O:201:VAL:HG22	2.02	0.42
1:E:66:TYR:CZ	1:F:89:LEU:HD22	2.53	0.42
1:H:295:VAL:HB	1:H:296:PRO:CD	2.49	0.42
1:K:89:LEU:HD11	1:L:66:TYR:CD2	2.54	0.42
1:M:238:LYS:HD2	1:M:238:LYS:HA	1.61	0.42
1:J:126:LEU:HG	1:J:144:MET:HG2	2.01	0.42
1:N:7:VAL:CG2	1:N:260:MET:HE3	2.50	0.42
1:B:11:VAL:HG21	1:B:201:VAL:HG22	2.02	0.42
1:C:126:LEU:HG	1:C:144:MET:HG2	2.01	0.42
1:D:295:VAL:HB	1:D:296:PRO:CD	2.50	0.42
1:G:227:ASP:HA	1:G:230:THR:OG1	2.20	0.42
1:H:204:VAL:HA	1:H:212:VAL:O	2.19	0.42
1:L:23:LYS:HB2	1:L:23:LYS:HE3	1.84	0.42
1:M:11:VAL:HG21	1:M:201:VAL:HG22	2.02	0.42
1:N:236:PHE:O	1:N:237:VAL:CG1	2.64	0.42
1:N:295:VAL:HB	1:N:296:PRO:CD	2.49	0.42
1:O:265:GLU:OE2	1:O:268:ARG:NH1	2.53	0.42
1:B:17:THR:HG22	1:B:18:PHE:N	2.34	0.42
1:B:126:LEU:HG	1:B:144:MET:HG2	2.01	0.42
1:C:11:VAL:HG21	1:C:201:VAL:HG22	2.02	0.42
1:C:167:LYS:HE3	2:C:450:HOH:O	2.20	0.42
1:E:126:LEU:HG	1:E:144:MET:HG2	2.01	0.42
1:J:295:VAL:HB	1:J:296:PRO:CD	2.50	0.42
1:M:143:ASP:OD1	1:M:143:ASP:C	2.63	0.42
1:P:143:ASP:OD1	1:P:143:ASP:C	2.62	0.42
1:A:204:VAL:HA	1:A:212:VAL:O	2.20	0.42
1:J:161:THR:HG21	1:J:290:MET:CG	2.49	0.42
1:N:23:LYS:HB2	1:N:23:LYS:HE3	1.84	0.42
1:N:181:LEU:HD13	1:N:181:LEU:O	2.20	0.42
1:N:368:ASN:HA	1:N:393:ARG:HH21	1.79	0.41
1:O:126:LEU:HG	1:O:144:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLU:OE2	1:D:268:ARG:NH1	2.53	0.41
1:H:143:ASP:OD1	1:H:143:ASP:C	2.63	0.41
1:I:204:VAL:HA	1:I:212:VAL:O	2.21	0.41
1:K:143:ASP:OD1	1:K:143:ASP:C	2.62	0.41
1:K:168:GLU:OE1	2:K:401:HOH:O	2.22	0.41
1:M:126:LEU:HG	1:M:144:MET:HG2	2.01	0.41
1:D:11:VAL:HG21	1:D:201:VAL:HG22	2.02	0.41
1:F:23:LYS:HB2	1:F:23:LYS:HE3	1.84	0.41
1:H:11:VAL:HG21	1:H:201:VAL:HG22	2.02	0.41
1:K:154:HIS:C	1:K:155:ARG:CG	2.93	0.41
1:K:335:ASP:HA	1:K:336:PRO:HD3	1.90	0.41
1:O:227:ASP:OD1	1:O:227:ASP:N	2.53	0.41
1:M:17:THR:HG22	1:M:18:PHE:N	2.34	0.41
1:C:126:LEU:CD2	1:D:126:LEU:HD21	2.48	0.41
1:N:227:ASP:HA	1:N:230:THR:OG1	2.21	0.41
1:O:17:THR:HG22	1:O:18:PHE:N	2.36	0.41
1:P:290:MET:HE3	1:P:291:GLY:CA	2.50	0.41
1:C:17:THR:HG22	1:C:18:PHE:N	2.36	0.41
1:E:167:LYS:HG2	1:P:211:ASP:CG	2.44	0.41
1:G:65:MET:HE1	1:H:148:ALA:N	2.35	0.41
1:J:316:GLU:HG3	1:J:359:ILE:HD12	2.02	0.41
1:A:265:GLU:OE2	1:A:268:ARG:NH1	2.53	0.41
1:A:319:GLU:CD	1:A:344:SER:HB3	2.45	0.41
1:C:126:LEU:HD21	1:D:126:LEU:HD21	2.03	0.41
1:D:225:THR:O	1:D:228:ASP:HB2	2.21	0.41
1:E:7:VAL:CG2	1:E:260:MET:HE3	2.50	0.41
1:G:126:LEU:HG	1:G:144:MET:HG2	2.02	0.41
1:H:319:GLU:CD	1:H:344:SER:HB3	2.45	0.41
1:H:335:ASP:OD2	1:H:335:ASP:C	2.63	0.41
1:I:249:SER:HA	1:I:346:ILE:HA	2.03	0.41
1:N:171:ILE:HA	1:N:175:GLN:OE1	2.21	0.41
1:C:89:LEU:HD22	1:D:66:TYR:CZ	2.55	0.41
1:E:65:MET:HE1	1:F:147:GLY:C	2.46	0.41
1:F:158:MET:HE3	1:F:290:MET:SD	2.60	0.41
1:I:17:THR:HG22	1:I:18:PHE:N	2.35	0.41
1:J:292:ILE:H	1:J:292:ILE:HG13	1.73	0.41
1:K:11:VAL:HG21	1:K:201:VAL:HG22	2.01	0.41
1:K:204:VAL:HA	1:K:212:VAL:O	2.20	0.41
1:B:172:SER:O	1:B:176:GLN:HG3	2.21	0.41
1:D:206:LYS:HZ2	1:G:265:GLU:HA	1.85	0.41
1:D:316:GLU:HG3	1:D:359:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:MET:HE1	1:F:148:ALA:N	2.36	0.41
1:F:225:THR:O	1:F:228:ASP:HB2	2.21	0.41
1:G:63:ARG:NH2	2:G:406:HOH:O	2.34	0.41
1:G:204:VAL:HG12	1:G:213:THR:HB	2.02	0.41
1:I:4:GLU:OE1	1:I:263:ARG:HD3	2.20	0.41
1:K:106:LEU:CD1	1:L:102:GLN:HG2	2.51	0.41
1:L:272:LYS:H	1:L:272:LYS:HG3	1.66	0.41
1:M:272:LYS:H	1:M:272:LYS:HG3	1.58	0.41
1:B:227:ASP:HA	1:B:230:THR:OG1	2.21	0.41
1:H:225:THR:O	1:H:228:ASP:HB2	2.21	0.41
1:H:276:ARG:HH11	1:H:394:ILE:CD1	2.30	0.41
1:I:286:ASP:OD2	1:I:288:LYS:CD	2.68	0.41
1:I:335:ASP:HA	1:I:336:PRO:HD3	1.93	0.41
1:N:11:VAL:HG21	1:N:201:VAL:HG22	2.02	0.41
1:N:17:THR:HG22	1:N:18:PHE:N	2.36	0.41
1:B:143:ASP:C	1:B:143:ASP:OD1	2.64	0.40
1:D:126:LEU:HG	1:D:144:MET:HG2	2.02	0.40
1:F:249:SER:HA	1:F:346:ILE:HA	2.04	0.40
1:I:225:THR:O	1:I:228:ASP:HB2	2.21	0.40
1:J:225:THR:O	1:J:228:ASP:HB2	2.21	0.40
1:K:225:THR:O	1:K:228:ASP:HB2	2.21	0.40
1:L:204:VAL:HA	1:L:212:VAL:O	2.21	0.40
1:E:154:HIS:C	1:E:155:ARG:CG	2.94	0.40
1:F:204:VAL:HA	1:F:212:VAL:O	2.21	0.40
1:H:276:ARG:HD3	1:H:394:ILE:HD12	1.94	0.40
1:H:292:ILE:H	1:H:292:ILE:HG13	1.75	0.40
1:N:225:THR:O	1:N:228:ASP:HB2	2.21	0.40
1:P:225:THR:O	1:P:228:ASP:HB2	2.21	0.40
1:D:367:LEU:HG	1:D:393:ARG:HG2	2.02	0.40
1:I:7:VAL:CG2	1:I:260:MET:HE3	2.50	0.40
1:P:7:VAL:CG2	1:P:260:MET:HE3	2.51	0.40
1:P:158:MET:CE	1:P:382:GLY:CA	2.94	0.40
1:A:225:THR:O	1:A:228:ASP:HB2	2.21	0.40
1:B:225:THR:O	1:B:228:ASP:HB2	2.21	0.40
1:B:265:GLU:OE2	1:B:268[A]:ARG:NH1	2.53	0.40
1:C:143:ASP:OD1	1:C:143:ASP:C	2.63	0.40
1:E:225:THR:O	1:E:228:ASP:HB2	2.20	0.40
1:I:161:THR:HG21	1:I:290:MET:CG	2.46	0.40
1:J:61:GLU:HB2	1:J:62:PRO:HD2	2.04	0.40
1:N:265:GLU:OE2	1:N:268:ARG:NH1	2.52	0.40
1:N:368:ASN:C	1:N:393:ARG:NH2	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:VAL:CG2	1:O:260:MET:HE3	2.51	0.40
1:P:295:VAL:HB	1:P:296:PRO:CD	2.51	0.40
1:B:295:VAL:HB	1:B:296:PRO:HD3	2.04	0.40
1:D:143:ASP:OD1	1:D:143:ASP:C	2.64	0.40
1:K:172:SER:O	1:K:176:GLN:HG3	2.22	0.40
1:L:225:THR:O	1:L:228:ASP:HB2	2.21	0.40
1:L:227:ASP:HA	1:L:230:THR:OG1	2.21	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	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

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

All (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
1	M	237	VAL
1	G	239	GLU
1	M	239	GLU
1	N	239	GLU
1	J	239	GLU
1	K	239	GLU

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

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

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	VAL
1	A	23	LYS
1	A	51	HIS
1	A	90	CYS
1	A	110	ASP
1	A	155	ARG
1	A	160	VAL
1	A	161	THR
1	A	165	VAL
1	A	181	LEU
1	A	204	VAL
1	A	213	THR
1	A	230	THR
1	A	232	LEU
1	A	233	ARG
1	A	238	LYS
1	A	239	GLU
1	A	276	ARG
1	A	316	GLU
1	A	324	GLN
1	A	335	ASP
1	A	338	LYS
1	A	358	LEU
1	B	6	VAL
1	B	11	VAL
1	B	23	LYS
1	B	41	ARG

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Mol	Chain	Res	Type
1	B	51	HIS
1	B	89	LEU
1	B	90	CYS
1	B	155	ARG
1	B	160	VAL
1	B	161	THR
1	B	181	LEU
1	B	204	VAL
1	B	209	LYS
1	B	213	THR
1	B	230	THR
1	B	233	ARG
1	B	263	ARG
1	B	265	GLU
1	B	272	LYS
1	B	324	GLN
1	B	338	LYS
1	B	358	LEU
1	C	6	VAL
1	C	11	VAL
1	C	23	LYS
1	C	41	ARG
1	C	51	HIS
1	C	90	CYS
1	C	155	ARG
1	C	160	VAL
1	C	161	THR
1	C	175	GLN
1	C	198	ASP
1	C	204	VAL
1	C	213	THR
1	C	230	THR
1	C	238	LYS
1	C	242	THR
1	C	265	GLU
1	C	272	LYS
1	C	316	GLU
1	C	324	GLN
1	C	338	LYS
1	C	358	LEU
1	C	394	ILE
1	D	6	VAL

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Mol	Chain	Res	Type
1	D	11	VAL
1	D	23	LYS
1	D	41	ARG
1	D	51	HIS
1	D	90	CYS
1	D	155	ARG
1	D	160	VAL
1	D	161	THR
1	D	197	LYS
1	D	198	ASP
1	D	213	THR
1	D	227	ASP
1	D	230	THR
1	D	232	LEU
1	D	233	ARG
1	D	237	VAL
1	D	265	GLU
1	D	276	ARG
1	D	300	ILE
1	D	303	GLU
1	D	316	GLU
1	D	324	GLN
1	D	338	LYS
1	D	358	LEU
1	D	393	ARG
1	E	4	GLU
1	E	6	VAL
1	E	41	ARG
1	E	51	HIS
1	E	90	CYS
1	E	155	ARG
1	E	161	THR
1	E	178	GLU
1	E	181	LEU
1	E	204	VAL
1	E	230	THR
1	E	232	LEU
1	E	233	ARG
1	E	265	GLU
1	E	276	ARG
1	E	310	SER
1	E	316	GLU

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Mol	Chain	Res	Type
1	E	324	GLN
1	E	329	THR
1	E	338	LYS
1	E	358	LEU
1	F	6	VAL
1	F	11	VAL
1	F	23	LYS
1	F	41	ARG
1	F	51	HIS
1	F	90	CYS
1	F	160	VAL
1	F	161	THR
1	F	204	VAL
1	F	211	ASP
1	F	213	THR
1	F	230	THR
1	F	233	ARG
1	F	238	LYS
1	F	265	GLU
1	F	288	LYS
1	F	295	VAL
1	F	316	GLU
1	F	324	GLN
1	F	338	LYS
1	F	358	LEU
1	G	1	MET
1	G	6	VAL
1	G	11	VAL
1	G	23	LYS
1	G	41	ARG
1	G	51	HIS
1	G	90	CYS
1	G	155	ARG
1	G	160	VAL
1	G	161	THR
1	G	204	VAL
1	G	213	THR
1	G	230	THR
1	G	233	ARG
1	G	237	VAL
1	G	238	LYS
1	G	265	GLU

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Mol	Chain	Res	Type
1	G	268	ARG
1	G	303	GLU
1	G	324	GLN
1	G	338	LYS
1	G	358	LEU
1	H	6	VAL
1	H	11	VAL
1	H	23	LYS
1	H	41	ARG
1	H	51	HIS
1	H	90	CYS
1	H	155	ARG
1	H	160	VAL
1	H	161	THR
1	H	198	ASP
1	H	204	VAL
1	H	206	LYS
1	H	209	LYS
1	H	213	THR
1	H	232	LEU
1	H	233	ARG
1	H	238	LYS
1	H	240	ASN
1	H	265	GLU
1	H	268	ARG
1	H	276	ARG
1	H	303	GLU
1	H	308	GLN
1	H	324	GLN
1	H	338	LYS
1	H	358	LEU
1	H	368	ASN
1	I	1	MET
1	I	2	THR
1	I	6	VAL
1	I	11	VAL
1	I	41	ARG
1	I	51	HIS
1	I	90	CYS
1	I	155	ARG
1	I	160	VAL
1	I	161	THR

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Mol	Chain	Res	Type
1	I	168	GLU
1	I	204	VAL
1	I	213	THR
1	I	230	THR
1	I	233	ARG
1	I	238	LYS
1	I	265	GLU
1	I	276	ARG
1	I	303	GLU
1	I	324	GLN
1	I	338	LYS
1	I	358	LEU
1	J	6	VAL
1	J	11	VAL
1	J	41	ARG
1	J	51	HIS
1	J	90	CYS
1	J	155	ARG
1	J	158	MET
1	J	160	VAL
1	J	161	THR
1	J	198	ASP
1	J	204	VAL
1	J	213	THR
1	J	232	LEU
1	J	233	ARG
1	J	238	LYS
1	J	265	GLU
1	J	268	ARG
1	J	276	ARG
1	J	308	GLN
1	J	324	GLN
1	J	338	LYS
1	J	358	LEU
1	K	6	VAL
1	K	11	VAL
1	K	41	ARG
1	K	51	HIS
1	K	90	CYS
1	K	155	ARG
1	K	160	VAL
1	K	161	THR

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Mol	Chain	Res	Type
1	K	177	ASP
1	K	197	LYS
1	K	204	VAL
1	K	213	THR
1	K	230	THR
1	K	232	LEU
1	K	233	ARG
1	K	238	LYS
1	K	265	GLU
1	K	308	GLN
1	K	324	GLN
1	K	335	ASP
1	K	338	LYS
1	K	358	LEU
1	K	393	ARG
1	L	6	VAL
1	L	11	VAL
1	L	23	LYS
1	L	41	ARG
1	L	51	HIS
1	L	90	CYS
1	L	155	ARG
1	L	160	VAL
1	L	161	THR
1	L	168	GLU
1	L	204	VAL
1	L	213	THR
1	L	230	THR
1	L	233	ARG
1	L	238	LYS
1	L	242	THR
1	L	272	LYS
1	L	295	VAL
1	L	324	GLN
1	L	338	LYS
1	L	358	LEU
1	L	368	ASN
1	M	6	VAL
1	M	11	VAL
1	M	23	LYS
1	M	24	ASP
1	M	41	ARG

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Mol	Chain	Res	Type
1	M	51	HIS
1	M	155	ARG
1	M	160	VAL
1	M	161	THR
1	M	204	VAL
1	M	213	THR
1	M	227	ASP
1	M	230	THR
1	M	238	LYS
1	M	242	THR
1	M	265	GLU
1	M	272	LYS
1	M	324	GLN
1	M	338	LYS
1	M	358	LEU
1	N	6	VAL
1	N	11	VAL
1	N	23	LYS
1	N	41	ARG
1	N	51	HIS
1	N	90	CYS
1	N	99	SER
1	N	155	ARG
1	N	160	VAL
1	N	161	THR
1	N	177	ASP
1	N	181	LEU
1	N	204	VAL
1	N	209	LYS
1	N	213	THR
1	N	230	THR
1	N	232	LEU
1	N	233	ARG
1	N	238	LYS
1	N	240	ASN
1	N	265	GLU
1	N	276	ARG
1	N	300	ILE
1	N	303	GLU
1	N	313	ASP
1	N	316	GLU
1	N	324	GLN

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Mol	Chain	Res	Type
1	N	338	LYS
1	N	358	LEU
1	O	6	VAL
1	O	11	VAL
1	O	23	LYS
1	O	41	ARG
1	O	51	HIS
1	O	90	CYS
1	O	155	ARG
1	O	160	VAL
1	O	161	THR
1	O	204	VAL
1	O	213	THR
1	O	227	ASP
1	O	230	THR
1	O	232	LEU
1	O	233	ARG
1	O	239	GLU
1	O	265	GLU
1	O	276	ARG
1	O	308	GLN
1	O	316	GLU
1	O	324	GLN
1	O	335	ASP
1	O	338	LYS
1	O	358	LEU
1	O	393	ARG
1	P	6	VAL
1	P	11	VAL
1	P	23	LYS
1	P	41	ARG
1	P	51	HIS
1	P	90	CYS
1	P	155	ARG
1	P	160	VAL
1	P	161	THR
1	P	167	LYS
1	P	185	ARG
1	P	204	VAL
1	P	213	THR
1	P	230	THR
1	P	233	ARG

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Mol	Chain	Res	Type
1	P	238	LYS
1	P	239	GLU
1	P	242	THR
1	P	265	GLU
1	P	324	GLN
1	P	338	LYS
1	P	358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	B	308	GLN
1	B	318	ASN
1	C	318	ASN
1	C	368	ASN
1	D	59	GLN
1	D	219	HIS
1	D	368	ASN
1	E	59	GLN
1	E	154	HIS
1	E	318	ASN
1	F	175	GLN
1	F	318	ASN
1	F	368	ASN
1	G	154	HIS
1	G	175	GLN
1	G	219	HIS
1	G	318	ASN
1	H	56	ASN
1	H	318	ASN
1	I	56	ASN
1	J	368	ASN
1	K	368	ASN
1	L	175	GLN
1	L	318	ASN
1	M	154	HIS
1	M	175	GLN
1	M	318	ASN
1	N	318	ASN
1	O	318	ASN

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 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 ⓘ

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%)

All (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

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Mol	Chain	Res	Type	RSRZ
1	J	237	VAL	3.7
1	P	364	LEU	3.6
1	B	235	VAL	3.6
1	P	212	VAL	3.6
1	E	42	ALA	3.5
1	N	271	LEU	3.5
1	O	76	GLY	3.5
1	E	44	VAL	3.4
1	O	329	THR	3.4
1	N	236	PHE	3.4
1	P	181	LEU	3.4
1	M	210	GLY	3.3
1	K	226	ILE	3.3
1	E	205	SER	3.2
1	E	160	VAL	3.2
1	P	171	ILE	3.2
1	P	226	ILE	3.1
1	P	201	VAL	3.0
1	B	233	ARG	2.9
1	H	181	LEU	2.9
1	O	230	THR	2.9
1	P	242	THR	2.9
1	B	245	ALA	2.9
1	L	363	ALA	2.9
1	E	212	VAL	2.9
1	P	309	VAL	2.9
1	F	2	THR	2.9
1	N	148	ALA	2.9
1	P	174	ALA	2.9
1	O	263	ARG	2.8
1	I	167	LYS	2.8
1	K	268	ARG	2.8
1	P	286	ASP	2.8
1	B	307	LEU	2.8
1	L	180	ALA	2.8
1	K	334	LEU	2.8
1	N	241	GLY	2.7
1	M	245	ALA	2.7
1	P	275	ALA	2.7
1	O	344	SER	2.7
1	H	323	ALA	2.7
1	O	323	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	243	VAL	2.7
1	E	2	THR	2.7
1	E	271	LEU	2.7
1	O	67	LEU	2.7
1	C	212	VAL	2.7
1	E	191	ILE	2.7
1	E	203	VAL	2.7
1	H	237	VAL	2.7
1	P	200	ILE	2.7
1	P	189	ALA	2.6
1	M	232	LEU	2.6
1	P	230	THR	2.6
1	P	160	VAL	2.6
1	P	224	ALA	2.6
1	K	314	VAL	2.6
1	P	328	VAL	2.6
1	D	230	THR	2.6
1	K	148	ALA	2.6
1	N	244	THR	2.6
1	C	171	ILE	2.6
1	O	5	VAL	2.6
1	P	285	VAL	2.6
1	L	226	ILE	2.5
1	P	11	VAL	2.5
1	O	75	GLY	2.5
1	P	38	ALA	2.5
1	L	232	LEU	2.5
1	M	334	LEU	2.5
1	P	210	GLY	2.5
1	O	204	VAL	2.4
1	O	212	VAL	2.4
1	P	25	VAL	2.4
1	P	315	ILE	2.5
1	C	323	ALA	2.4
1	P	179	ALA	2.4
1	B	292	ILE	2.4
1	L	160	VAL	2.4
1	D	2	THR	2.4
1	L	185[A]	ARG	2.4
1	N	239	GLU	2.4
1	N	227	ASP	2.4
1	E	327	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	232	LEU	2.4
1	O	302	LEU	2.4
1	P	236	PHE	2.4
1	P	191	ILE	2.4
1	P	41	ARG	2.4
1	C	181	LEU	2.3
1	H	226	ILE	2.3
1	O	203	VAL	2.3
1	O	205	SER	2.3
1	E	40	ALA	2.3
1	O	42	ALA	2.3
1	L	246	GLY	2.3
1	B	276	ARG	2.3
1	L	292	ILE	2.3
1	O	213	THR	2.3
1	J	40	ALA	2.3
1	M	211	ASP	2.3
1	N	226	ILE	2.3
1	P	292	ILE	2.3
1	G	204	VAL	2.3
1	K	70	VAL	2.3
1	F	248	ALA	2.3
1	A	291	GLY	2.3
1	F	158	MET	2.3
1	P	271	LEU	2.3
1	B	300	ILE	2.2
1	L	243	VAL	2.2
1	M	197	LYS	2.2
1	E	198	ASP	2.2
1	N	207	GLY	2.2
1	P	365	HIS	2.2
1	B	2	THR	2.2
1	F	292	ILE	2.2
1	H	240	ASN	2.2
1	O	378	THR	2.2
1	A	271	LEU	2.2
1	O	181	LEU	2.2
1	P	169	TYR	2.2
1	J	212	VAL	2.2
1	K	25	VAL	2.2
1	O	309	VAL	2.2
1	H	232	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	33	LEU	2.2
1	O	167	LYS	2.2
1	P	158	MET	2.2
1	L	213	THR	2.2
1	J	236	PHE	2.1
1	M	300	ILE	2.1
1	K	220	VAL	2.1
1	N	181	LEU	2.1
1	L	205	SER	2.1
1	P	195	TYR	2.1
1	B	4	GLU	2.1
1	H	2	THR	2.1
1	N	171	ILE	2.1
1	P	79	ILE	2.1
1	L	314	VAL	2.1
1	O	235	VAL	2.1
1	E	330	LYS	2.1
1	K	181	LEU	2.1
1	M	206	LYS	2.1
1	P	310	SER	2.1
1	A	316	GLU	2.1
1	B	227	ASP	2.1
1	E	263	ARG	2.1
1	E	352	ILE	2.1
1	P	233	ARG	2.1
1	K	237	VAL	2.1
1	O	8	VAL	2.1
1	P	5	VAL	2.1
1	N	238	LYS	2.1
1	E	162	ALA	2.1
1	O	297	ALA	2.1
1	P	193	ALA	2.1
1	E	367	LEU	2.1
1	M	181	LEU	2.1
1	E	41	ARG	2.1
1	N	156	ILE	2.1
1	M	160	VAL	2.1
1	C	264	ALA	2.1
1	M	89	LEU	2.0
1	P	263	ARG	2.0
1	M	230	THR	2.0
1	O	296	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	197	LYS	2.0
1	N	352	ILE	2.0
1	I	235	VAL	2.0
1	K	309	VAL	2.0
1	L	235	VAL	2.0
1	P	34	VAL	2.0
1	P	314	VAL	2.0
1	N	174	ALA	2.0
1	E	181	LEU	2.0
1	P	106	LEU	2.0
1	E	227	ASP	2.0
1	P	369	ARG	2.0
1	A	195	TYR	2.0
1	P	374	TYR	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.