



Full wwPDB X-ray Structure Validation Report i

Apr 22, 2025 – 12:38 AM EDT

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 i 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

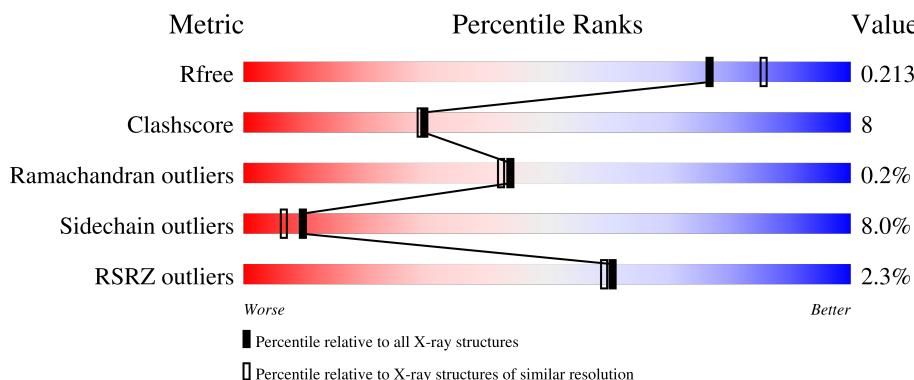
1 Overall quality at a glance

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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.



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

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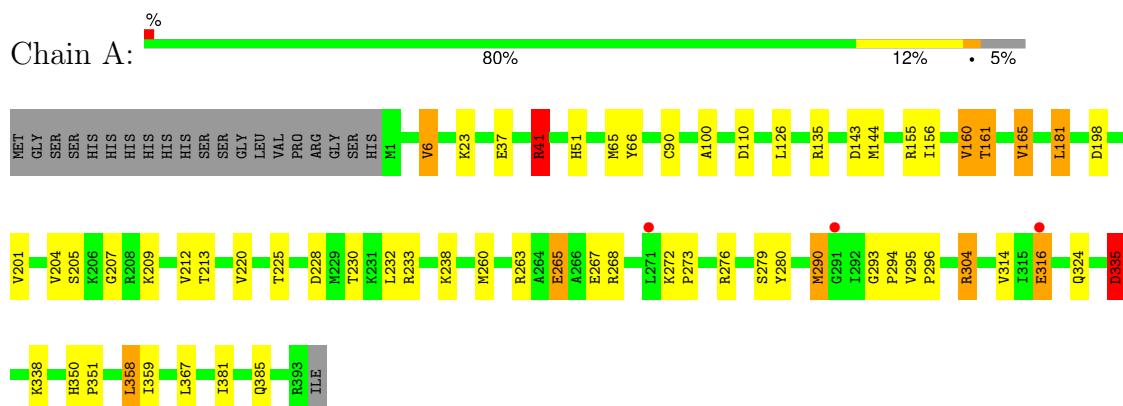
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	66	Total O 66 66	0	0
2	H	50	Total O 51 51	0	1
2	I	49	Total O 49 49	0	0
2	J	30	Total O 30 30	0	0
2	K	18	Total O 18 18	0	0
2	L	25	Total O 25 25	0	0
2	M	36	Total O 36 36	0	0
2	N	24	Total O 24 24	0	0
2	O	29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

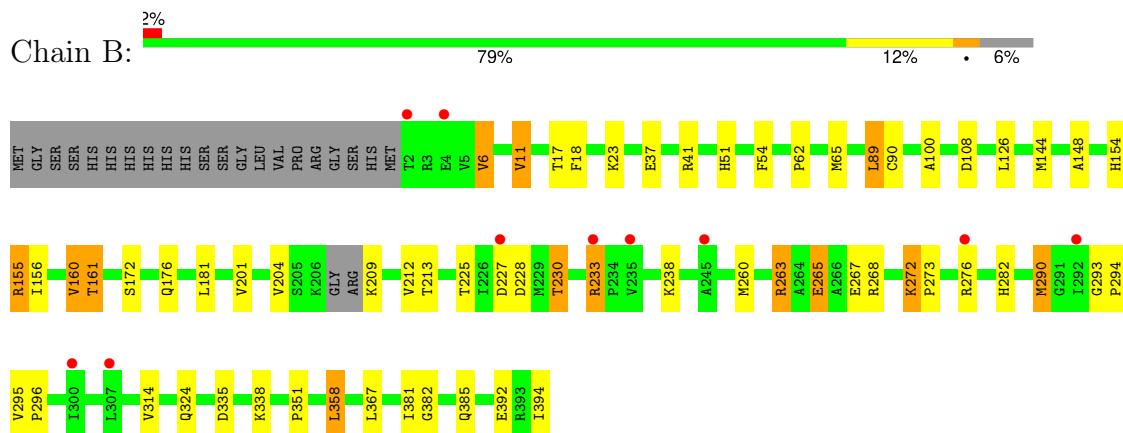
3 Residue-property plots

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.

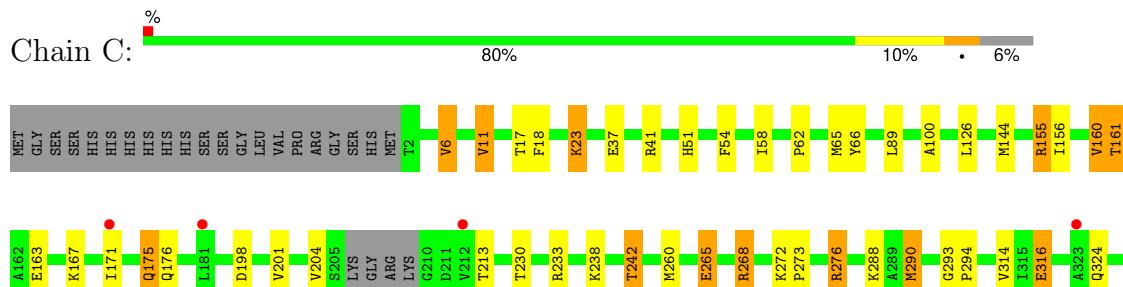
- Molecule 1: Beta-ketothiolase BktB



- Molecule 1: Beta-ketothiolase BktB



- Molecule 1: Beta-ketothiolase BktB





- Molecule 1: Beta-ketothiolase BktB

Chain D:

- Molecule 1: Beta-ketothiolase BktB

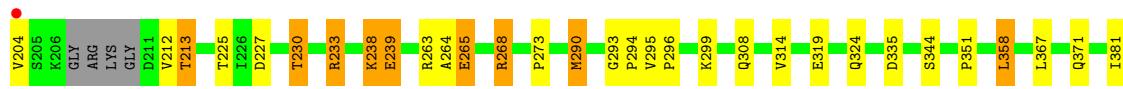
Chain E:

- Molecule 1: Beta-ketothiolase BktB

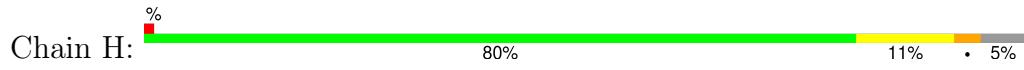
Chain F:

- Molecule 1: Beta-ketothiolase BktB

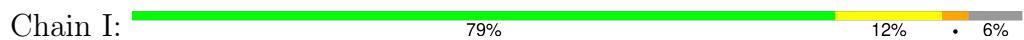
Chain G:



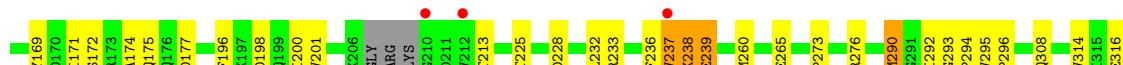
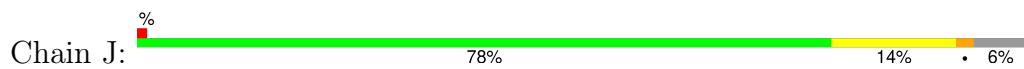
- Molecule 1: Beta-ketothiolase BktB



- Molecule 1: Beta-ketothiolase BktB



- Molecule 1: Beta-ketothiolase BktB



• Molecule 1: Beta-ketothiolase BktB



I156 V160 T161 E168 S172 R173 A174 Q175 Q176 D177 K197 V201 V204 F208 LYS G210 D211 V212 T213 V220 T225 I226 D227 D228 N229 T230 K231 L232 R233 K238 E239 M260 E265 R268 P273 M290 Q308 V309

- Molecule 1: Beta-ketothiolase BktB



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	T2	V6	V11	K23	E37	R41	H51	F54	I58	P62	M65	Y66	Q102	L126	M144	R155	I156	V160	T161	A162	E163	E168
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------

The diagram shows the protein backbone with various mutations indicated by colored bars above the backbone. The mutations are: K338 (yellow), S344 (yellow), P351 (yellow), L358 (orange), A365 (green, marked with a red dot), N368 (orange), I381 (yellow), Q385 (yellow), E392 (green), R393 (green), and ILE (grey).

- Molecule 1: Beta-ketothiolase BktB



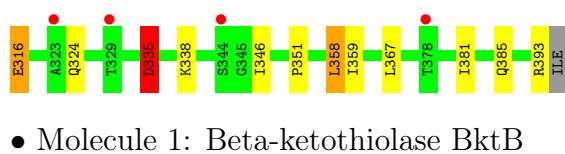
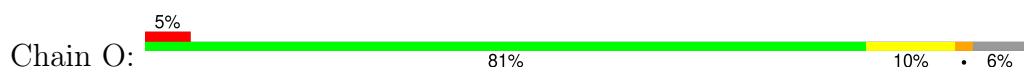
Q176	K197	V201	V204	S205	K206	GLY	ARG	LYS	D211	V212	T213	F214	D215	D227	T230	K231	L232	V235	F236	V237	K238	E239	T242	A245	E295	K272	P273	R226	K288	A289	M290	G293	P294	V295	P296	I300	V314	I315	E316	Q324
------	------	------	------	------	------	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 1: Beta-ketothiolase BktB

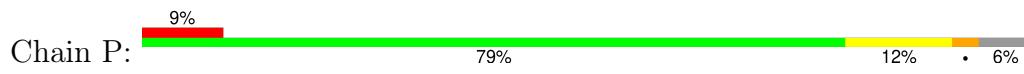




- Molecule 1: Beta-ketothiolase BktB



- Molecule 1: Beta-ketothiolase BktB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.05 Å 105.99 Å 201.14 Å 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 2.01 Å)	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	19985 reflections (5.06%)	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	0.28	0/2899	0.48	1/3929 (0.0%)
1	B	0.30	0/2894	0.44	0/3922
1	C	0.31	0/2876	0.44	0/3900
1	D	0.29	0/2875	0.44	0/3897
1	E	0.30	0/2844	0.45	0/3857
1	F	0.31	0/2862	0.44	0/3881
1	G	0.37	0/2870	0.44	0/3891
1	H	0.31	0/2887	0.46	1/3913 (0.0%)
1	I	0.34	0/2886	0.46	0/3913
1	J	0.36	0/2866	0.45	0/3886
1	K	0.28	0/2889	0.42	0/3916
1	L	0.30	0/2881	0.43	0/3905
1	M	0.30	0/2874	0.43	0/3897
1	N	0.27	0/2891	0.43	0/3919
1	O	0.25	0/2862	0.42	1/3881 (0.0%)
1	P	0.29	0/2857	0.43	0/3875
All	All	0.31	0/46013	0.44	3/62382 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ASP	CB-CG-OD1	-8.28	110.84	118.30
1	O	335	ASP	CB-CG-OD1	-7.94	111.16	118.30
1	H	268	ARG	NE-CZ-NH2	5.06	122.83	120.30

There are no chirality outliers.

All (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
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

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Mol	Chain	Res	Type	Group
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 [\(i\)](#)

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	57	0
1	B	2855	0	2891	64	0
1	C	2837	0	2865	60	0
1	D	2836	0	2868	53	0
1	E	2806	0	2827	40	0
1	F	2823	0	2852	43	0
1	G	2831	0	2864	57	0
1	H	2848	0	2882	52	0
1	I	2847	0	2880	55	0
1	J	2827	0	2855	61	0
1	K	2850	0	2882	54	0
1	L	2842	0	2870	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2835	0	2866	50	0
1	N	2851	0	2885	74	0
1	O	2823	0	2852	50	0
1	P	2818	0	2842	64	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	767	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 8.

All (767) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:ARG:HD3	1:H:394:ILE:CD1	1.97	0.93
1:H:290:MET:HE3	1:H:291:GLY:HA2	1.51	0.92
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: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: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: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: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: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
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: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: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:O:161:THR:HG21	1:O:290:MET:HG3	1.64	0.80
1:P:158:MET:HE1	1:P:382:GLY:HA2	1.64	0.80
1:E:161:THR:HG21	1:E:290:MET:HG3	1.64	0.80

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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	0.80
1:B:225:THR:OG1	1:B:227:ASP:OD1	1.98	0.80
1:A:335:ASP:C	1:A:335:ASP:OD1	2.22	0.79
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:177:ASP:HB2	2:J:402:HOH:O	1.84	0.78
1:O:335:ASP:C	1:O:335:ASP:OD1	2.22	0.78
1:A:66:TYR:CE2	1:B:89:LEU:CD1	2.67	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:F:158:MET:HE1	1:F:290:MET:SD	2.24	0.77
1:N:161:THR:HG21	1:N:290:MET:HG3	1.66	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:B:181:LEU:HD23	1:B:181:LEU:C	2.07	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: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: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:A:181:LEU:C	1:A:181:LEU:CD2	2.57	0.73
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:P:158:MET:HE1	1:P:290:MET:SD	2.30	0.72
1:B:181:LEU:C	1:B:181:LEU:CD2	2.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:MET:HE2	1:L:58:ILE:HA	1.71	0.71
1:L:295:VAL:HG13	1:L:296:PRO:CD	2.20	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:A:181:LEU:HD23	1:A:181:LEU:C	2.06	0.71
1:J:158:MET:HA	1:J:158:MET:HE2	1.71	0.70
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: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:C:58:ILE:HA	1:D:65:MET:HE2	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
1:H:272:LYS:HG3	2:H:412:HOH:O	1.92	0.69
1:N:135:ARG:HG3	2:N:405:HOH:O	1.91	0.69
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: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: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:M:62:PRO:HA	1:M:65:MET:HE2	1.77	0.66
1:B:89:LEU:HD23	1:B:90:CYS:SG	2.35	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:L:62:PRO:HA	1:L:65:MET:HE2	1.78	0.66
1:E:62:PRO:HA	1:E:65:MET:HE2	1.79	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:62:PRO:HA	1:F:65:MET:HE2	1.79	0.65
1:I:62:PRO:HA	1:I:65:MET:HE2	1.78	0.65
1:C:62:PRO:HA	1:C:65:MET:HE2	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:J:371:GLN:HA	1:J:393:ARG:NH2	2.11	0.65
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:K:126:LEU:HD23	1:L:126:LEU:CD2	2.27	0.64
1:D:161:THR:HG21	1:D:290:MET:HG3	1.79	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: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:G:62:PRO:HA	1:G:65:MET:HE2	1.81	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:G:58:ILE:HA	1:H:65:MET:HE2	1.80	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:290:MET:HE3	1:H:291:GLY:CA	2.28	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:P:158:MET:CE	1:P:382:GLY:HA2	2.31	0.61
1:D:11:VAL:HG22	1:D:201:VAL:HG23	1.81	0.61
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: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: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:P:158:MET:CE	1:P:290:MET:SD	2.88	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:C:276:ARG:CZ	1:C:392:GLU:OE1	2.49	0.59
1:F:158:MET:CE	1:F:382:GLY:HA2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:227:ASP:OD2	1:P:227:ASP:C	2.41	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:G:263:ARG:NE	2:G:404:HOH:O	2.33	0.59
1:O:65:MET:CE	1:P:144:MET:CE	2.80	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
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:P:290:MET:HE3	1:P:291:GLY:HA2	1.85	0.58
1:C:316:GLU:HA	1:C:316:GLU:OE2	2.04	0.58
1:A:181:LEU:HD22	2:A:417:HOH:O	2.02	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: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: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: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:F:158:MET:HE1	1:F:382:GLY:HA2	1.87	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: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
1:C:126:LEU:HD22	1:D:126:LEU:HD23	1.87	0.56
1:N:161:THR:HG21	1:N:290:MET:CG	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:176:GLN:CD	1:L:242:THR:HG1	2.09	0.55
1:M:176:GLN:CD	1:M:242:THR:HG1	2.09	0.55
1:A:156:ILE:HD12	1:A:160:VAL:CG2	2.37	0.55
1:M:144:MET:CE	1:N:65:MET:CE	2.85	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:D:206:LYS:NZ	1:G:264:ALA:C	2.61	0.55
1:O:161:THR:HG21	1:O:290:MET:CG	2.34	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:A:207:GLY:C	1:A:209:LYS:H	2.10	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:O:65:MET:CE	1:P:144:MET:HE3	2.38	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:I:206:LYS:NZ	2:I:402:HOH:O	2.35	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: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:O:65:MET:HE3	1:P:144:MET:CE	2.39	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
1:J:158:MET:CE	1:J:158:MET:CA	2.85	0.53
1:M:163:GLU:OE2	1:M:242:THR:CG2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ILE:HB	1:C:385:GLN:HB2	1.91	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: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:CE	1:J:65:MET:CE	2.87	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:D:206:LYS:HZ2	1:G:265:GLU:HA	1.74	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:C:6:VAL:HG22	1:C:273:PRO:HB3	1.92	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: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:381:ILE:HB	1:B:385:GLN:HB2	1.92	0.51
1:J:381:ILE:HB	1:J:385:GLN:HB2	1.92	0.51
1:D:6:VAL:HG22	1:D:273:PRO:HB3	1.93	0.51
1:D:100:ALA:HB3	1:D:260:MET:HE1	1.93	0.51
1:D:205:SER:C	1:D:206:LYS:HG3	2.30	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:100:ALA:HB3	1:C:260:MET:HE1	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: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: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:A:100:ALA:HB3	1:A:260:MET:HE1	1.93	0.50
1:E:195:TYR:OH	2:E:401:HOH:O	2.18	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:K:174:ALA:C	1:K:177:ASP:OD1	2.50	0.50
1:H:293:GLY:N	1:H:294:PRO:CD	2.75	0.50
1:I:126:LEU:HD21	1:J:126:LEU:CD2	2.40	0.50
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:G:11:VAL:HG21	1:G:201:VAL:CG2	2.43	0.49
1:J:11:VAL:CG2	1:J:201:VAL:CG2	2.90	0.49
1:J:100:ALA:HB3	1:J:260:MET:HE1	1.95	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:95:GLN:O	1:N:99:SER:OG	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:100:ALA:HB3	1:B:260:MET:HE1	1.95	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:O:314:VAL:HG12	1:O:367:LEU:HD13	1.94	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:K:100:ALA:HB3	1:K:260:MET:HE1	1.94	0.49
1:M:126:LEU:HG	1:M:144:MET:CG	2.43	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
1:O:65:MET:HE2	1:P:144:MET:HE3	1.93	0.49
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:B:126:LEU:HG	1:B:144:MET:CG	2.43	0.49
1:B:154:HIS:C	1:B:155:ARG:HG2	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:335:ASP:C	1:F:335:ASP:OD1	2.52	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:I:144:MET:CE	1:J:65:MET:HE2	2.44	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
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: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: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:K:173:ARG:O	1:K:177:ASP:CG	2.48	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:M:126:LEU:HD23	1:N:126:LEU:CD2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:37:GLU:HG2	1:E:201:VAL:CG2	2.43	0.47
1:J:314:VAL:HG12	1:J:367:LEU:HD13	1.94	0.47
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: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:P:335:ASP:OD1	1:P:335:ASP:C	2.53	0.47
1:C:126:LEU:HD21	1:D:126:LEU:CD2	2.43	0.47
1:C:335:ASP:C	1:C:335:ASP:OD1	2.53	0.47
1:I:144:MET:HE3	1:J:65:MET:HE2	1.97	0.47
1:J:335:ASP:C	1:J:335:ASP:OD1	2.52	0.47
1:N:335:ASP:OD1	1:N:335:ASP:C	2.53	0.47
1:O:126:LEU:CD2	1:P:126:LEU:HD21	2.39	0.47
1:K:174:ALA:CA	1:K:177:ASP:OD1	2.63	0.47
1:A:37:GLU:HG2	1:A:201:VAL:CG2	2.45	0.47
1:E:335:ASP:OD1	1:E:335:ASP:C	2.52	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:M:144:MET:CE	1:N:65:MET:HE2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:198:ASP:HB2	2:N:411:HOH:O	2.15	0.46
1:O:65:MET:HE2	1:P:144:MET:CE	2.45	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:F:265:GLU:OE2	1:F:268:ARG:NH1	2.47	0.46
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:G:358:LEU:C	1:G:358:LEU:HD12	2.36	0.46
1:I:286:ASP:OD2	1:I:288:LYS:CE	2.64	0.46
1:L:335:ASP:OD1	1:L:335:ASP:C	2.52	0.46
1:D:206:LYS:HZ1	1:G:264:ALA:C	2.18	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:B:233:ARG:NH2	1:G:76:GLY:HA2	2.31	0.46
1:K:358:LEU:HD12	1:K:358:LEU:C	2.37	0.46
1:L:368:ASN:HA	1:L:393:ARG:HD3	1.98	0.46
1:M:335:ASP:C	1:M:335:ASP:OD1	2.54	0.46
1:O:226:ILE:HG23	1:O:227:ASP:OD1	2.16	0.46
1:F:158:MET:CE	1:F:290:MET:SD	2.99	0.46
1:K:309:VAL:CG2	2:K:409:HOH:O	2.50	0.46
1:O:290:MET:HE3	1:O:291:GLY:HA2	1.98	0.46
1:P:158:MET:CE	1:P:382:GLY:CA	2.94	0.46
1:D:335:ASP:OD1	1:D:335:ASP:C	2.53	0.45
1:B:265:GLU:CD	1:B:268[B]:ARG:HE	2.20	0.45
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:E:290:MET:HE3	1:E:291:GLY:HA2	1.98	0.45
1:I:126:LEU:HD21	1:J:126:LEU:HD21	1.98	0.45
1:I:335:ASP:OD1	1:I:335:ASP:C	2.53	0.45
1:I:265:GLU:OE2	1:I:268:ARG:NH1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:MET:HE3	1:J:65:MET:CE	2.47	0.45
1:I:293:GLY:N	1:I:294:PRO:CD	2.79	0.45
1:B:358:LEU:C	1:B:358:LEU:HD12	2.36	0.45
1:C:176:GLN:CD	1:C:242:THR:HG1	2.18	0.45
1:P:293:GLY:N	1:P:294:PRO:CD	2.78	0.45
1:C:358:LEU:HD12	1:C:358:LEU:C	2.37	0.45
1:L:176:GLN:OE1	1:L:242:THR:OG1	2.26	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:F:100:ALA:HB3	1:F:260:MET:HE1	1.98	0.45
1:F:358:LEU:HD12	1:F:358:LEU:C	2.38	0.44
1:H:358:LEU:HD12	1:H:358:LEU:C	2.37	0.44
1:I:126:LEU:CD2	1:J:126:LEU:HD21	2.43	0.44
1:O:358:LEU:HD12	1:O:358:LEU:C	2.37	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
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:P:358:LEU:C	1:P:358:LEU:HD12	2.37	0.44
1:A:37:GLU:CG	1:A:41:ARG:NH1	2.80	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:B:263:ARG:HD3	1:B:267:GLU:CD	2.38	0.44
1:C:175:GLN:HG3	2:C:436:HOH:O	2.17	0.44
1:H:126:LEU:HG	1:H:144:MET:HG2	1.99	0.44
1:M:358:LEU:HD12	1:M:358:LEU:C	2.37	0.44
1:O:126:LEU:HD21	1:P:126:LEU:HD21	1.98	0.44
1:A:230:THR:O	1:A:230:THR:CG2	2.66	0.44
1:A:358:LEU:HD12	1:A:358:LEU:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:102:GLN:HG2	1:N:106:LEU:CD1	2.48	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:B:335:ASP:OD1	1:B:335:ASP:C	2.55	0.44
1:F:158:MET:HE3	1:F:290:MET:CE	2.48	0.44
1:J:358:LEU:HD12	1:J:358:LEU:C	2.38	0.44
1:G:204:VAL:HA	1:G:212:VAL:O	2.18	0.44
1:M:36:ARG:NE	2:M:403:HOH:O	2.25	0.44
1:A:65:MET:CE	1:B:144:MET:CE	2.96	0.43
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:G:319:GLU:CD	1:G:344:SER:HB3	2.39	0.43
1:I:126:LEU:CD2	1:J:126:LEU:HD22	2.42	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:D:293:GLY:N	1:D:294:PRO:CD	2.81	0.43
1:G:126:LEU:HD21	1:H:126:LEU:HD21	2.00	0.43
1:M:144:MET:HE1	1:N:65:MET:CE	2.48	0.43
1:M:144:MET:HE3	1:N:65:MET:CE	2.48	0.43
1:A:41:ARG:NH2	1:A:198:ASP:O	2.52	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:A:37:GLU:CD	1:A:41:ARG:NH1	2.71	0.43
1:I:126:LEU:HG	1:I:144:MET:HG2	2.00	0.43
1:M:176:GLN:CD	1:M:242:THR:OG1	2.56	0.43
1:C:265:GLU:OE2	1:C:268:ARG:NE	2.49	0.43
1:A:37:GLU:O	1:A:41:ARG:HG2	2.17	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: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:65:MET:HE3	1:P:144:MET:HE1	2.01	0.43
1:O:295:VAL:HB	1:O:296:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:335:ASP:OD1	1:G:335:ASP:C	2.56	0.43
1:L:11:VAL:HG21	1:L:201:VAL:HG22	2.01	0.43
1:H:290:MET:HE3	1:H:380:CYS:SG	2.59	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:K:19:GLY:C	1:K:23:LYS:HE2	2.40	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
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:D:358:LEU:C	1:D:358:LEU:HD12	2.39	0.42
1:M:144:MET:HE3	1:N:65:MET:HE2	2.01	0.42
1:N:358:LEU:C	1:N:358:LEU:HD12	2.39	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:F:158:MET:HE2	1:F:382:GLY:CA	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:I:17:THR:HG22	1:I:18:PHE:N	2.35	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:I:358:LEU:C	1:I:358:LEU:HD12	2.40	0.42
1:J:126:LEU:HG	1:J:144:MET:HG2	2.01	0.42
1:L:358:LEU:C	1:L:358:LEU:HD12	2.39	0.42
1:B:11:VAL:HG21	1:B:201:VAL:HG22	2.02	0.42
1:B:17:THR:HG22	1:B:18:PHE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:M:144:MET:CE	1:N:65:MET:HE3	2.49	0.41
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
1:D:265:GLU:OE2	1:D:268:ARG:NH1	2.53	0.41
1:I:204:VAL:HA	1:I:212:VAL:O	2.21	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:E:358:LEU:C	1:E:358:LEU:HD12	2.40	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: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:L:176:GLN:CD	1:L:242:THR:OG1	2.59	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:I:154:HIS:C	1:I:155:ARG:CG	2.87	0.41
1:J:158:MET:HA	1:J:158:MET:HE3	1.99	0.41
1:L:319:GLU:CD	1:L:344:SER:HB3	2.40	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:C:17:THR:HG22	1:C:18:PHE:N	2.36	0.41
1:J:316:GLU:HG3	1:J:359:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:176:GLN:CD	1:P:242:THR:OG1	2.58	0.41
1:A:265:GLU:OE2	1:A:268:ARG:NH1	2.53	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:G:126:LEU:HG	1:G:144:MET:HG2	2.02	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: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:316:GLU:HG3	1:D:359:ILE:HB	2.02	0.41
1:F:143:ASP:OD1	1:F:143:ASP:C	2.58	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:J:158:MET:CA	1:J:158:MET:HE3	2.50	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: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:N:143:ASP:OD1	1:N:143:ASP:C	2.60	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:O:65:MET:CE	1:P:144:MET:HE1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:225:THR:O	1:P:228:ASP:HB2	2.21	0.40
1:A:143:ASP:OD1	1:A:143:ASP:C	2.59	0.40
1:D:367:LEU:HG	1:D:393:ARG:HG2	2.02	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: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: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: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
1:P:158:MET:HE1	1:P:382:GLY:CA	2.42	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%)	37 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	388/414 (94%)	375 (97%)	11 (3%)	2 (0%)	25 21
1	I	387/414 (94%)	374 (97%)	13 (3%)	0	100 100
1	J	385/414 (93%)	372 (97%)	11 (3%)	2 (0%)	25 21
1	K	388/414 (94%)	377 (97%)	10 (3%)	1 (0%)	37 35
1	L	387/414 (94%)	377 (97%)	10 (3%)	0	100 100
1	M	386/414 (93%)	374 (97%)	10 (3%)	2 (0%)	25 21
1	N	390/414 (94%)	375 (96%)	13 (3%)	2 (0%)	25 21
1	O	384/414 (93%)	375 (98%)	9 (2%)	0	100 100
1	P	384/414 (93%)	371 (97%)	12 (3%)	1 (0%)	37 35
All	All	6179/6624 (93%)	6010 (97%)	158 (3%)	11 (0%)	44 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 [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	287/305 (94%)	262 (91%)	25 (9%)	8 5
1	B	287/305 (94%)	266 (93%)	21 (7%)	11 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	285/305 (93%)	260 (91%)	25 (9%)	8	5
1	D	285/305 (93%)	262 (92%)	23 (8%)	9	6
1	E	282/305 (92%)	262 (93%)	20 (7%)	12	9
1	F	284/305 (93%)	262 (92%)	22 (8%)	10	7
1	G	285/305 (93%)	265 (93%)	20 (7%)	12	9
1	H	286/305 (94%)	260 (91%)	26 (9%)	7	5
1	I	287/305 (94%)	264 (92%)	23 (8%)	10	6
1	J	284/305 (93%)	264 (93%)	20 (7%)	12	9
1	K	286/305 (94%)	264 (92%)	22 (8%)	10	7
1	L	285/305 (93%)	262 (92%)	23 (8%)	9	6
1	M	285/305 (93%)	264 (93%)	21 (7%)	11	8
1	N	286/305 (94%)	259 (91%)	27 (9%)	7	4
1	O	284/305 (93%)	258 (91%)	26 (9%)	7	4
1	P	283/305 (93%)	262 (93%)	21 (7%)	11	8
All	All	4561/4880 (94%)	4196 (92%)	365 (8%)	10	6

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	23	LYS
1	A	41	ARG
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	213	THR
1	A	232	LEU
1	A	233	ARG
1	A	238	LYS
1	A	272	LYS
1	A	276	ARG
1	A	290	MET

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Mol	Chain	Res	Type
1	A	304	ARG
1	A	316	GLU
1	A	324	GLN
1	A	335	ASP
1	A	338	LYS
1	A	350	HIS
1	A	358	LEU
1	B	6	VAL
1	B	11	VAL
1	B	23	LYS
1	B	41	ARG
1	B	51	HIS
1	B	54	PHE
1	B	89	LEU
1	B	155	ARG
1	B	160	VAL
1	B	161	THR
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	290	MET
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	54	PHE
1	C	155	ARG
1	C	160	VAL
1	C	161	THR
1	C	198	ASP
1	C	204	VAL
1	C	213	THR
1	C	230	THR
1	C	233	ARG

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Mol	Chain	Res	Type
1	C	238	LYS
1	C	242	THR
1	C	265	GLU
1	C	272	LYS
1	C	290	MET
1	C	316	GLU
1	C	324	GLN
1	C	338	LYS
1	C	350	HIS
1	C	358	LEU
1	C	394	ILE
1	D	6	VAL
1	D	11	VAL
1	D	23	LYS
1	D	41	ARG
1	D	51	HIS
1	D	155	ARG
1	D	160	VAL
1	D	161	THR
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	265	GLU
1	D	276	ARG
1	D	290	MET
1	D	300	ILE
1	D	316	GLU
1	D	324	GLN
1	D	338	LYS
1	D	358	LEU
1	D	393	ARG
1	E	6	VAL
1	E	41	ARG
1	E	51	HIS
1	E	54	PHE
1	E	155	ARG
1	E	161	THR
1	E	178	GLU
1	E	181	LEU

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Mol	Chain	Res	Type
1	E	230	THR
1	E	232	LEU
1	E	233	ARG
1	E	265	GLU
1	E	276	ARG
1	E	290	MET
1	E	310	SER
1	E	316	GLU
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	54	PHE
1	F	160	VAL
1	F	161	THR
1	F	198	ASP
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	290	MET
1	F	295	VAL
1	F	324	GLN
1	F	338	LYS
1	F	350	HIS
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	54	PHE
1	G	155	ARG

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Mol	Chain	Res	Type
1	G	160	VAL
1	G	161	THR
1	G	213	THR
1	G	230	THR
1	G	233	ARG
1	G	238	LYS
1	G	265	GLU
1	G	268	ARG
1	G	290	MET
1	G	324	GLN
1	G	358	LEU
1	G	371	GLN
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	206	LYS
1	H	209	LYS
1	H	213	THR
1	H	232	LEU
1	H	233	ARG
1	H	238	LYS
1	H	265	GLU
1	H	268	ARG
1	H	276	ARG
1	H	290	MET
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

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Mol	Chain	Res	Type
1	I	41	ARG
1	I	51	HIS
1	I	54	PHE
1	I	155	ARG
1	I	160	VAL
1	I	161	THR
1	I	168	GLU
1	I	213	THR
1	I	230	THR
1	I	233	ARG
1	I	238	LYS
1	I	263	ARG
1	I	265	GLU
1	I	276	ARG
1	I	290	MET
1	I	324	GLN
1	I	338	LYS
1	I	350	HIS
1	I	358	LEU
1	J	6	VAL
1	J	11	VAL
1	J	41	ARG
1	J	51	HIS
1	J	54	PHE
1	J	155	ARG
1	J	160	VAL
1	J	161	THR
1	J	198	ASP
1	J	213	THR
1	J	232	LEU
1	J	233	ARG
1	J	238	LYS
1	J	265	GLU
1	J	276	ARG
1	J	290	MET
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

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Mol	Chain	Res	Type
1	K	51	HIS
1	K	155	ARG
1	K	160	VAL
1	K	161	THR
1	K	177	ASP
1	K	197	LYS
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	290	MET
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	54	PHE
1	L	155	ARG
1	L	160	VAL
1	L	161	THR
1	L	168	GLU
1	L	198	ASP
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	290	MET
1	L	295	VAL
1	L	324	GLN
1	L	338	LYS
1	L	358	LEU
1	L	368	ASN

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Mol	Chain	Res	Type
1	M	6	VAL
1	M	11	VAL
1	M	23	LYS
1	M	24	ASP
1	M	41	ARG
1	M	51	HIS
1	M	54	PHE
1	M	155	ARG
1	M	160	VAL
1	M	161	THR
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	290	MET
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	99	SER
1	N	155	ARG
1	N	160	VAL
1	N	161	THR
1	N	177	ASP
1	N	181	LEU
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	290	MET

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Mol	Chain	Res	Type
1	N	300	ILE
1	N	313	ASP
1	N	316	GLU
1	N	324	GLN
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	54	PHE
1	O	155	ARG
1	O	160	VAL
1	O	161	THR
1	O	198	ASP
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	290	MET
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	54	PHE
1	P	155	ARG
1	P	160	VAL
1	P	161	THR
1	P	185	ARG

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Mol	Chain	Res	Type
1	P	213	THR
1	P	230	THR
1	P	233	ARG
1	P	238	LYS
1	P	239	GLU
1	P	242	THR
1	P	265	GLU
1	P	290	MET
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	G	318	ASN
1	M	154	HIS
1	M	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	393/414 (94%)	0.20	3 (0%)	82	82	0
1	B	391/414 (94%)	0.23	10 (2%)	57	55	1 (0%)
1	C	389/414 (93%)	0.12	4 (1%)	79	78	1 (0%)
1	D	390/414 (94%)	-0.01	2 (0%)	87	86	0
1	E	386/414 (93%)	0.50	14 (3%)	46	44	0
1	F	388/414 (93%)	0.36	4 (1%)	79	78	0
1	G	389/414 (93%)	0.04	1 (0%)	90	89	0
1	H	392/414 (94%)	0.13	6 (1%)	71	70	0
1	I	390/414 (94%)	-0.07	1 (0%)	90	89	1 (0%)
1	J	389/414 (93%)	0.15	4 (1%)	79	78	0
1	K	392/414 (94%)	0.38	8 (2%)	64	63	0
1	L	390/414 (94%)	0.38	12 (3%)	51	49	1 (0%)
1	M	390/414 (94%)	0.40	9 (2%)	61	59	0
1	N	392/414 (94%)	0.46	11 (2%)	55	53	0
1	O	388/414 (93%)	0.66	21 (5%)	32	30	0
1	P	388/414 (93%)	0.77	36 (9%)	16	14	0
All	All	6237/6624 (94%)	0.29	146 (2%)	61	59	4 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	235	VAL	4.2
1	P	235	VAL	3.8
1	P	327	ALA	3.8
1	J	210	GLY	3.7
1	L	224	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	237	VAL	3.6
1	P	364	LEU	3.5
1	B	235	VAL	3.4
1	P	212	VAL	3.4
1	E	42	ALA	3.4
1	N	271	LEU	3.3
1	O	76	GLY	3.3
1	O	329	THR	3.3
1	E	44	VAL	3.3
1	N	236	PHE	3.2
1	P	181	LEU	3.2
1	K	226	ILE	3.2
1	M	210	GLY	3.2
1	E	205	SER	3.1
1	P	171	ILE	3.0
1	E	160	VAL	3.0
1	P	226	ILE	3.0
1	B	233	ARG	2.9
1	P	201	VAL	2.8
1	O	263	ARG	2.8
1	O	230	THR	2.8
1	P	242	THR	2.8
1	H	181	LEU	2.8
1	I	167	LYS	2.7
1	F	2	THR	2.7
1	K	268	ARG	2.7
1	E	212	VAL	2.7
1	P	309	VAL	2.7
1	B	245	ALA	2.7
1	L	363	ALA	2.7
1	P	286	ASP	2.7
1	N	148	ALA	2.7
1	P	174	ALA	2.7
1	B	307	LEU	2.6
1	O	344	SER	2.6
1	K	334	LEU	2.6
1	L	180	ALA	2.6
1	N	241	GLY	2.6
1	M	245	ALA	2.6
1	P	275	ALA	2.6
1	H	323	ALA	2.5
1	O	323	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	243	VAL	2.5
1	E	2	THR	2.5
1	E	191	ILE	2.5
1	P	200	ILE	2.5
1	E	271	LEU	2.5
1	O	67	LEU	2.5
1	C	212	VAL	2.5
1	E	203	VAL	2.5
1	H	237	VAL	2.5
1	P	230	THR	2.5
1	M	232	LEU	2.5
1	P	189	ALA	2.5
1	P	160	VAL	2.5
1	P	224	ALA	2.5
1	D	230	THR	2.5
1	K	314	VAL	2.5
1	N	244	THR	2.5
1	P	328	VAL	2.5
1	C	171	ILE	2.4
1	K	148	ALA	2.4
1	O	5	VAL	2.4
1	P	285	VAL	2.4
1	L	226	ILE	2.4
1	P	11	VAL	2.4
1	O	75	GLY	2.4
1	L	232	LEU	2.4
1	M	334	LEU	2.4
1	P	38	ALA	2.4
1	L	185[A]	ARG	2.3
1	P	210	GLY	2.3
1	N	239	GLU	2.3
1	P	315	ILE	2.3
1	O	204	VAL	2.3
1	O	212	VAL	2.3
1	P	25	VAL	2.3
1	N	227	ASP	2.3
1	B	292	ILE	2.3
1	P	41	ARG	2.3
1	C	323	ALA	2.3
1	D	2	THR	2.3
1	P	179	ALA	2.3
1	L	160	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	276	ARG	2.2
1	P	191	ILE	2.2
1	N	232	LEU	2.2
1	O	302	LEU	2.2
1	E	327	ALA	2.2
1	O	205	SER	2.2
1	P	236	PHE	2.2
1	H	226	ILE	2.2
1	C	181	LEU	2.2
1	M	211	ASP	2.2
1	O	203	VAL	2.2
1	L	292	ILE	2.2
1	O	213	THR	2.2
1	E	40	ALA	2.2
1	O	42	ALA	2.2
1	M	197	LYS	2.2
1	L	246	GLY	2.2
1	F	158	MET	2.2
1	N	226	ILE	2.1
1	P	292	ILE	2.1
1	E	198	ASP	2.1
1	J	40	ALA	2.1
1	G	204	VAL	2.1
1	K	70	VAL	2.1
1	B	300	ILE	2.1
1	P	271	LEU	2.1
1	F	248	ALA	2.1
1	P	365	HIS	2.1
1	A	291	GLY	2.1
1	H	240	ASN	2.1
1	L	243	VAL	2.1
1	O	167	LYS	2.1
1	B	2	THR	2.1
1	F	292	ILE	2.1
1	O	378	THR	2.1
1	N	207	GLY	2.1
1	A	271	LEU	2.1
1	O	181	LEU	2.1
1	P	158	MET	2.1
1	B	4	GLU	2.0
1	P	169	TYR	2.0
1	E	330	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	206	LYS	2.0
1	J	212	VAL	2.0
1	K	25	VAL	2.0
1	O	309	VAL	2.0
1	L	205	SER	2.0
1	H	232	LEU	2.0
1	L	213	THR	2.0
1	O	33	LEU	2.0
1	M	300	ILE	2.0
1	A	316	GLU	2.0
1	E	263	ARG	2.0
1	N	238	LYS	2.0
1	P	233	ARG	2.0
1	K	220	VAL	2.0
1	B	227	ASP	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 monosaccharides 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.