



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:59 PM GMT

PDB ID : 4W61  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

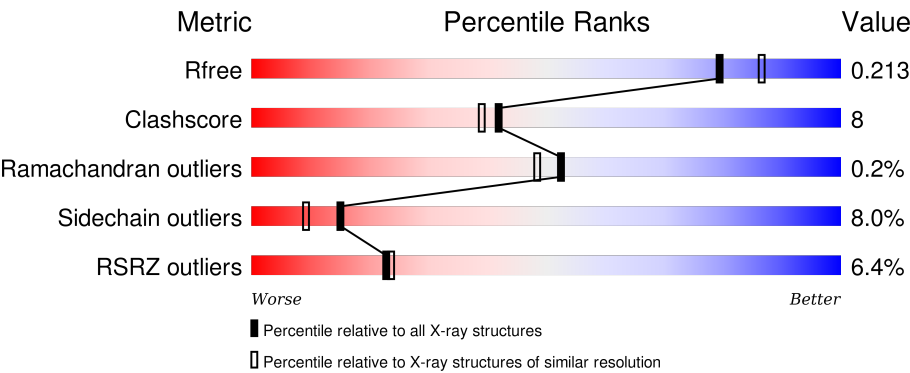
MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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.






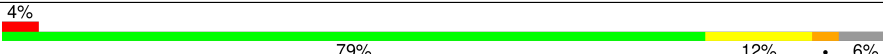
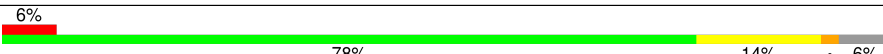
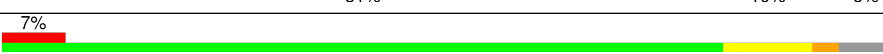

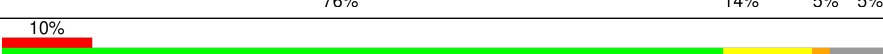
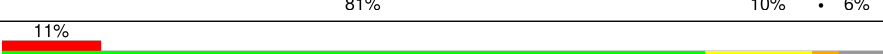
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	<div><div>5%</div><div><div></div><div>80%</div><div>12%</div><div>• 5%</div></div></div>
1	B	414	<div><div>5%</div><div><div></div><div>79%</div><div>12%</div><div>• 6%</div></div></div>
1	C	414	<div><div>2%</div><div><div></div><div>80%</div><div>10%</div><div>• 6%</div></div></div>
1	D	414	<div><div>3%</div><div><div></div><div>82%</div><div>10%</div><div>• 6%</div></div></div>
1	E	414	<div><div>9%</div><div><div></div><div>80%</div><div>12%</div><div>• 7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	414	
1	G	414	
1	H	414	
1	I	414	
1	J	414	
1	K	414	
1	L	414	
1	M	414	
1	N	414	
1	O	414	
1	P	414	

## 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

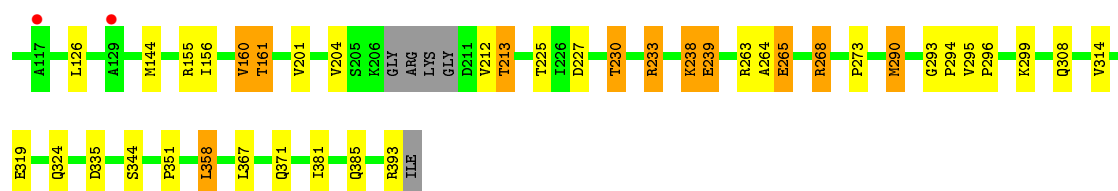
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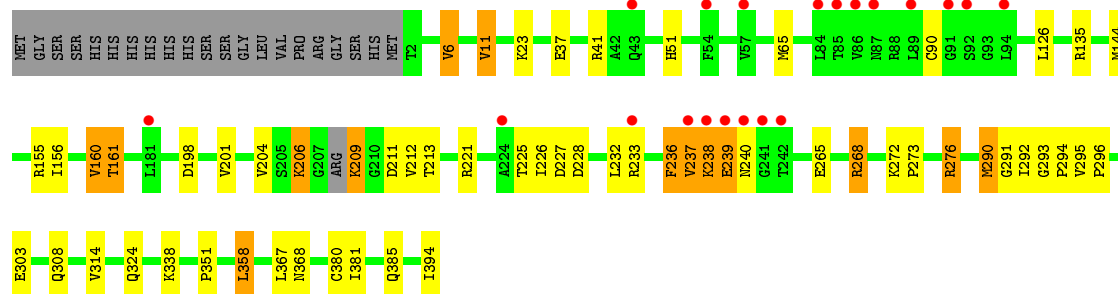
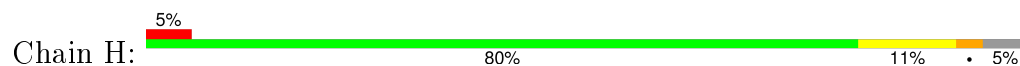
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	66	Total 66	O 66	0	0
2	H	50	Total 51	O 51	0	1
2	I	49	Total 49	O 49	0	0
2	J	30	Total 30	O 30	0	0
2	K	18	Total 18	O 18	0	0
2	L	25	Total 25	O 25	0	0
2	M	36	Total 36	O 36	0	0
2	N	24	Total 24	O 24	0	0
2	O	29	Total 29	O 29	0	0
2	P	35	Total 35	O 35	0	0



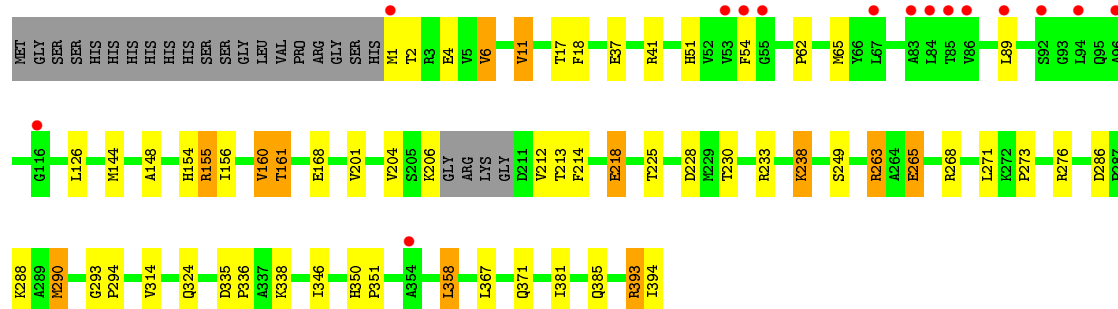
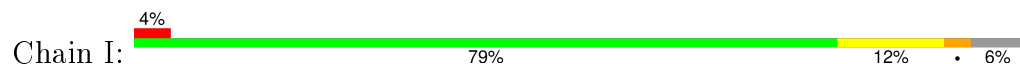




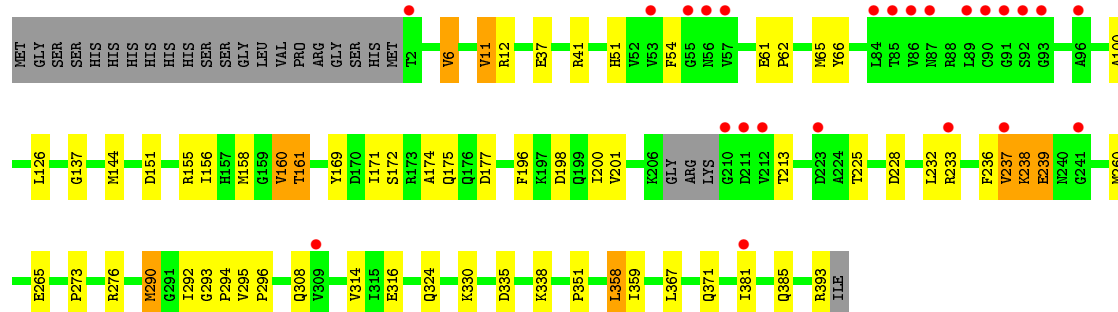
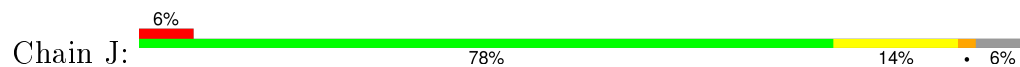
• Molecule 1: Beta-ketothiolase BktB



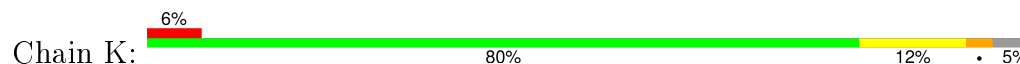
• Molecule 1: Beta-ketothiolase BktB



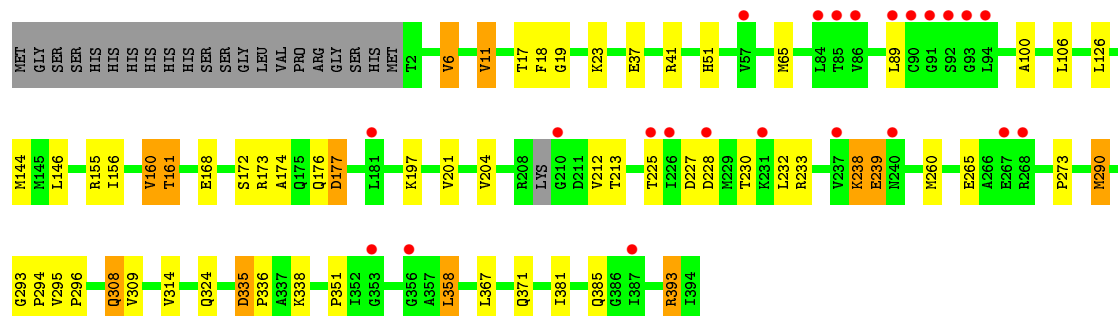
• Molecule 1: Beta-ketothiolase BktB



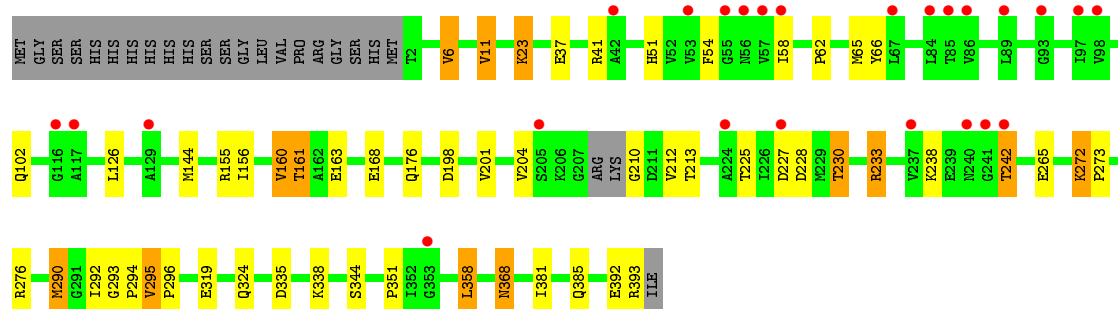
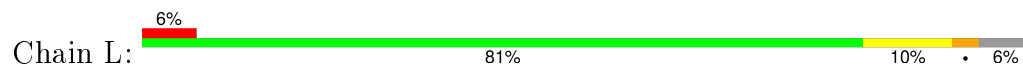
• Molecule 1: Beta-ketothiolase BktB



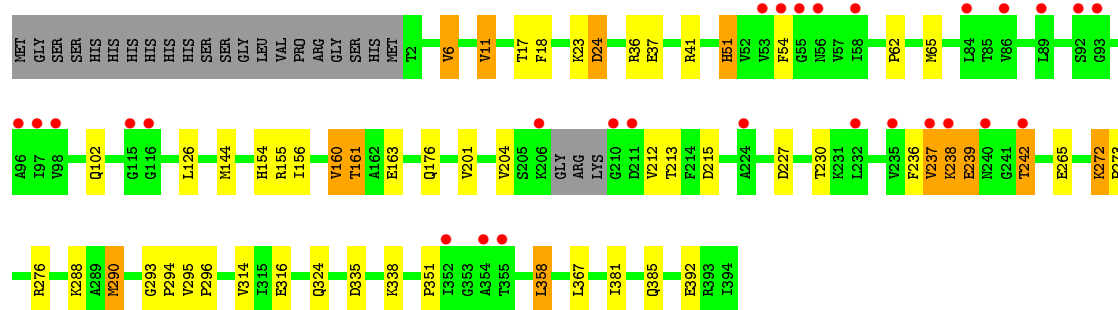
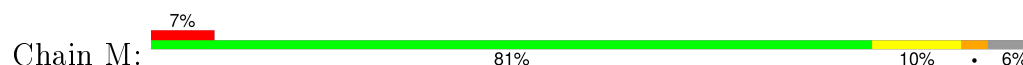




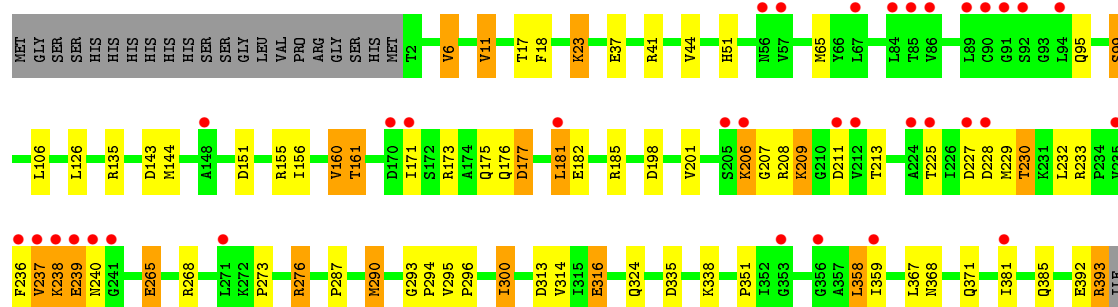
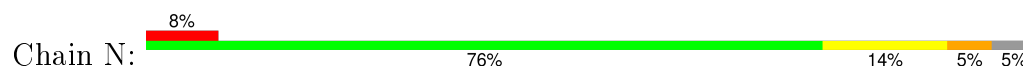
• Molecule 1: Beta-ketothiolase BktB




• Molecule 1: Beta-ketothiolase BktB

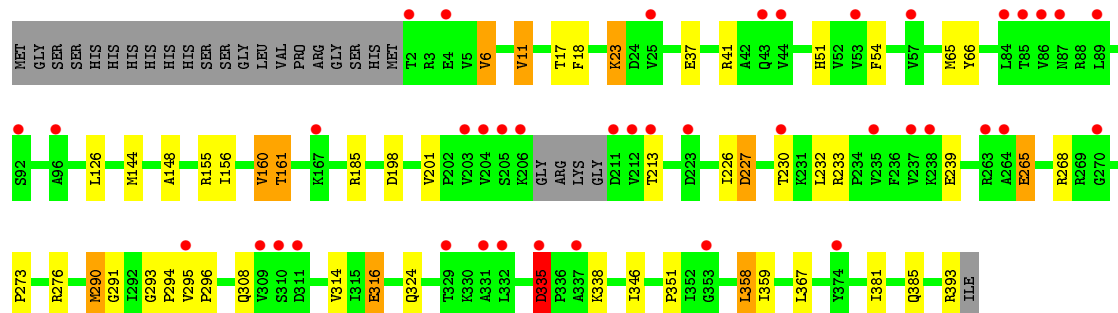


• Molecule 1: Beta-ketothiolase BktB




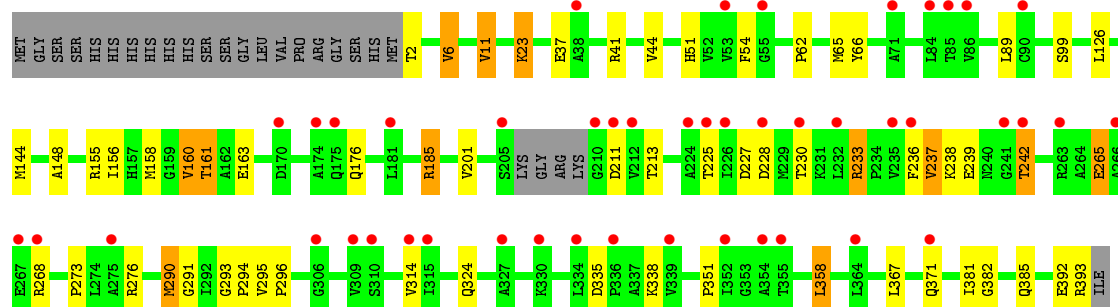
• Molecule 1: Beta-ketothiolase BktB

Chain O:  10% 81% 10% 6%



• Molecule 1: Beta-ketothiolase BktB

Chain P:  11% 79% 12% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.3 (41.79-2.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.176 , 0.208 0.185 , 0.213	Depositor DCC
$R_{free}$ test set	19985 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	EDS
Estimated twinning fraction	0.106 for h,-k,-l 0.125 for -h,k,-l 0.289 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 394878 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	46062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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 ⓘ

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:HD23	1:A:181:LEU:O	1.62	0.99
1:K:173:ARG:O	1:K:177:ASP:OD1	1.80	0.99
1:J:316:GLU:CG	1:J:359:ILE:HB	1.93	0.99
1:B:181:LEU:HD23	1:B:181:LEU:O	1.63	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:I:126:LEU:CD2	1:J:126:LEU:CD2	2.50	0.89
1:H:238:LYS:O	1:H:239:GLU:HB3	1.71	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:OD2	1:P:227:ASP:O	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:I:271:LEU:O	2:I:401:HOH:O	1.98	0.81
1:E:167:LYS:HG2	1:P:211:ASP:OD1	1.80	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:N:368:ASN:HA	1:N:393:ARG:NH2	1.95	0.81
1:L:225:THR:OG1	1:L:227:ASP:OD1	1.97	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:K:309:VAL:HG22	2:K:409:HOH:O	1.82	0.79
1:B:282:HIS:O	2:B:401:HOH:O	2.00	0.79
1:A:335:ASP:C	1:A:335:ASP:OD1	2.22	0.79
1:M:24:ASP:OD1	1:M:24:ASP:N	2.15	0.79
1:H:226:ILE:H	1:H:226:ILE:HD12	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:E:161:THR:CG2	2:E:422:HOH:O	2.27	0.78
1:A:66:TYR:CE2	1:B:89:LEU:CD1	2.67	0.78
1:P:276:ARG:NH1	1:P:392:GLU:OE1	2.16	0.78
1:L:161:THR:HG21	1:L:290:MET:HG3	1.66	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:M:276:ARG:NH1	1:M:392:GLU:OE1	2.19	0.76
1:J:236:PHE:O	1:J:237:VAL:HG12	1.86	0.76
1:B:181:LEU:C	1:B:181:LEU:HD23	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:CD2	1:B:181:LEU:C	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:N:238:LYS:O	1:N:239:GLU:HB2	1.90	0.71
1:E:329:THR:HG22	1:E:334:LEU:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:295:VAL:HG13	1:L:296:PRO:CD	2.20	0.71
1:K:65:MET:HE2	1:L:58:ILE:HA	1.71	0.71
1:I:161:THR:HG21	1:I:290:MET:HG3	1.73	0.71
1:F:316:GLU:OE1	1:F:316:GLU:HA	1.89	0.71
1:A:181:LEU:C	1:A:181:LEU:HD23	2.06	0.71
1:A:66:TYR:CE2	1:B:89:LEU:HD13	2.25	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:CD	1:L:233:ARG:H	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:G:126:LEU:CD2	1:H:126:LEU:HD23	2.22	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:C:58:ILE:HA	1:D:65:MET:HE2	1.73	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:E:126:LEU:HD23	1:F:126:LEU:CD2	2.23	0.67
1:A:126:LEU:HD23	1:B:126:LEU:CD2	2.25	0.67
1:F:161:THR:HG21	1:F:290:MET:HG3	1.76	0.67
1:P:371:GLN:HA	1:P:393:ARG:NH2	2.10	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: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:CD2	1:B:181:LEU:O	2.43	0.66
1:L:62:PRO:HA	1:L:65:MET:HE2	1.78	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:E:62:PRO:HA	1:E:65:MET:HE2	1.79	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:I:126:LEU:HD23	1:J:126:LEU:CD2	2.25	0.65
1:E:126:LEU:CD2	1:F:126:LEU:HD23	2.26	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:O:126:LEU:CD2	1:P:126:LEU:HD23	2.26	0.65
1:M:51:HIS:CE1	2:M:404:HOH:O	2.49	0.65
1:C:62:PRO:HA	1:C:65:MET:HE2	1.78	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:K:126:LEU:HD23	1:L:126:LEU:CD2	2.27	0.64
1:B:62:PRO:HA	1:B:65:MET:HE2	1.80	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:L:292:ILE:O	1:L:295:VAL:CG1	2.46	0.63
1:C:126:LEU:CD2	1:D:126:LEU:HD23	2.28	0.63
1:N:393:ARG:NE	2:N:402:HOH:O	2.31	0.63
1:N:44:VAL:HA	2:N:401:HOH:O	1.98	0.63
1:A:181:LEU:CD2	1:A:181:LEU:O	2.42	0.63
1:G:126:LEU:HD23	1:H:126:LEU:CD2	2.26	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:H:11:VAL:HG22	1:H: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:K:11:VAL:HG22	1:K:201:VAL:HG23	1.81	0.63
1:C:11:VAL:HG22	1:C: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:H:37:GLU:HG2	1:H:201:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:VAL:HG22	1:L:201:VAL:HG23	1.80	0.62
1:E:37:GLU:HG2	1:E:201:VAL:HG22	1.82	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:316:GLU:HA	1:N:316:GLU:OE2	1.99	0.62
1:N:208:ARG:CG	2:N:403:HOH:O	2.47	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:B:37:GLU:HG2	1:B:201:VAL:HG22	1.82	0.62
1:P:158:MET:CE	1:P:382:GLY:HA2	2.31	0.61
1:J:11:VAL:HG22	1:J:201:VAL:HG23	1.80	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:D:11:VAL:HG22	1:D:201:VAL:HG23	1.81	0.61
1:M:316:GLU:OE1	2:M:401:HOH:O	2.16	0.61
1:J:12:ARG:CZ	1:J:200:ILE:HD11	2.30	0.61
1:I:37:GLU:HG2	1:I:201:VAL:HG22	1.81	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:O:126:LEU:HD23	1:P:126:LEU:HD22	1.83	0.61
1:H:239:GLU:HG3	1:H:240:ASN:N	2.16	0.61
1:B:11:VAL:HG22	1:B:201:VAL:HG23	1.81	0.61
1:K:126:LEU:CD2	1:L:126:LEU:HD23	2.31	0.61
1:C:37:GLU:HG2	1:C:201:VAL:HG22	1.81	0.61
1:J:37:GLU:HG2	1:J:201:VAL:HG22	1.82	0.61
1:H:206:LYS:HB3	1:H:211:ASP:OD1	2.01	0.61
1:C:126:LEU:HD23	1:D:126:LEU:CD2	2.31	0.60
1:P:158:MET:CE	1:P:290:MET:SD	2.88	0.60
1:P:37:GLU:HG2	1:P:201:VAL:HG22	1.82	0.60
1:D:37:GLU:HG2	1:D: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:P:227:ASP:OD2	1:P:227:ASP:C	2.41	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:C:276:ARG:CZ	1:C:392:GLU:OE1	2.49	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:O:65:MET:CE	1:P:144:MET:CE	2.80	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
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:K:126:LEU:HD23	1:L:126:LEU:HD22	1.86	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:N:316:GLU:HG3	1:N:359:ILE:HB	1.86	0.57
1:C:167:LYS:HE3	2:C:456:HOH:O	2.04	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:I:126:LEU:HD22	1:J:126:LEU:HD23	1.86	0.57
1:G:126:LEU:HD23	1:H:126:LEU:HD22	1.87	0.57
1:O:335:ASP:O	1:O:335:ASP:OD1	2.22	0.56
1:D:265:GLU:OE1	1:D:268:ARG:NH1	2.38	0.56
1:K:177:ASP:N	1:K:177:ASP:OD1	2.32	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:D:372:GLY:O	1:D:393:ARG:CD	2.53	0.56
1:B:161:THR:HG21	1:B:290:MET:HG3	1.88	0.56
1:A:335:ASP:O	1:A:335:ASP:OD1	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: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:A:156:ILE:HD12	1:A:160:VAL:CG2	2.37	0.55
1:O:161:THR:HG21	1:O:290:MET:CG	2.34	0.55
1:D:206:LYS:NZ	1:G:264:ALA:C	2.61	0.55
1:C:156:ILE:HD12	1:C:160:VAL:CG2	2.36	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:M:156:ILE:HD12	1:M:160:VAL:CG2	2.37	0.54
1:G:156:ILE:HD12	1:G: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:A:207:GLY:C	1:A:209:LYS:H	2.10	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:O:65:MET:CE	1:P:144:MET:HE3	2.38	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:M:126:LEU:CD2	1:N:126:LEU:HD23	2.38	0.53
1:G:6:VAL:HG22	1:G:273:PRO:HB3	1.91	0.53
1:P:156:ILE:HD12	1:P:160:VAL:CG2	2.37	0.53
1:I:206:LYS:NZ	2:I:402:HOH:O	2.35	0.53
1:M:6:VAL:HG22	1:M:273:PRO:HB3	1.91	0.53
1:O:65:MET:HE3	1:P:144:MET:CE	2.39	0.53
1:K:126:LEU:HD22	1:L:126:LEU:HD23	1.89	0.53
1:C:265:GLU:HA	1:C:268:ARG:HH11	1.74	0.53
1:M:215:ASP:OD2	2:M:402:HOH:O	2.18	0.53
1:P:163:GLU:OE2	1:P:242:THR:CG2	2.57	0.53
1:K:6:VAL:HG22	1:K:273:PRO:HB3	1.91	0.53
1:J:158:MET:CA	1:J:158:MET:CE	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:N:6:VAL:HG22	1:N:273:PRO:HB3	1.92	0.52
1:H:381:ILE:HB	1:H:385:GLN:HB2	1.91	0.52
1:K:381:ILE:HB	1:K:385:GLN:HB2	1.92	0.52
1:H:6:VAL:HG22	1:H:273:PRO:HB3	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:279:SER:CA	2:A:404:HOH:O	2.57	0.52
1:N:208:ARG:HG3	2:N:403:HOH:O	2.07	0.52
1:L:381:ILE:HB	1:L:385:GLN:HB2	1.92	0.52
1:A:6:VAL:HG22	1:A:273:PRO:HB3	1.92	0.52
1:D:381:ILE:HB	1:D:385:GLN:HB2	1.92	0.52
1:M:381:ILE:HB	1:M:385:GLN:HB2	1.92	0.52
1:I:6:VAL:HG22	1:I:273:PRO:HB3	1.92	0.52
1:C:6:VAL:HG22	1:C:273:PRO:HB3	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:381:ILE:HB	1:B:385:GLN:HB2	1.92	0.51
1:B:6:VAL:HG22	1:B:273:PRO:HB3	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:381:ILE:HB	1:G:385:GLN:HB2	1.93	0.51
1:G:314:VAL:HG12	1:G:367:LEU:HD13	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:P:6:VAL:HG22	1:P:273:PRO:HB3	1.92	0.50
1:I:381:ILE:HB	1:I:385:GLN:HB2	1.93	0.50
1:E:239:GLU:N	2:E:405:HOH:O	2.43	0.50
1:C:100:ALA:HB3	1:C:260:MET:HE1	1.92	0.50
1:E:314:VAL:HG12	1:E:367:LEU:HD13	1.93	0.50
1:O:346:ILE:O	2:O:401:HOH:O	2.19	0.50
1:I:314:VAL:HG12	1:I:367:LEU:HD13	1.94	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:K:174:ALA:C	1:K:177:ASP:OD1	2.50	0.50
1:H:238:LYS:O	1:H:239:GLU:HB2	2.08	0.50
1:G:263:ARG:CD	2:G:404:HOH:O	2.59	0.50
1:E:195:TYR:OH	2:E:401:HOH:O	2.18	0.50
1:A:100:ALA:HB3	1:A:260:MET:HE1	1.93	0.50
1:F:381:ILE:HB	1:F:385:GLN:HB2	1.93	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:H:126:LEU:HG	1:H:144:MET:CG	2.43	0.49
1:E:371:GLN:HG3	1:E:393:ARG:NH1	2.27	0.49
1:C:293:GLY:N	1:C:294:PRO:CD	2.75	0.49
1:N:208:ARG:NE	2:N:403:HOH:O	2.45	0.49
1:J:172:SER:OG	1:J:175:GLN:HG3	2.12	0.49
1:L:233:ARG:N	1:L:233:ARG:HD2	2.10	0.49
1:K:126:LEU:HG	1:K:144:MET:CG	2.42	0.49
1:A:314:VAL:HG12	1:A:367:LEU:HD13	1.93	0.49
1:G:11:VAL:HG21	1:G:201:VAL:CG2	2.43	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:K:314:VAL:HG12	1:K:367:LEU:HD13	1.93	0.49
1:O:11:VAL:CG2	1:O:201:VAL:CG2	2.91	0.49
1:K:11:VAL:HG21	1:K:201:VAL:CG2	2.43	0.49
1:L:11:VAL:CG2	1:L:201:VAL:HG23	2.43	0.49
1:J:11:VAL:CG2	1:J:201:VAL:CG2	2.90	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:J:100:ALA:HB3	1:J:260:MET:HE1	1.95	0.49
1:P:314:VAL:HG12	1:P:367:LEU:HD13	1.94	0.49
1:N:314:VAL:HG12	1:N:367:LEU:HD13	1.94	0.49
1:L:126:LEU:HG	1:L:144:MET:CG	2.43	0.49
1:K:367:LEU:HG	1:K:393:ARG:HG2	1.94	0.49
1:P:11:VAL:CG2	1:P:201:VAL:CG2	2.91	0.49
1:O:314:VAL:HG12	1:O:367:LEU:HD13	1.94	0.49
1:B:100:ALA:HB3	1:B:260:MET:HE1	1.95	0.49
1:M:126:LEU:HG	1:M:144:MET:CG	2.43	0.49
1:J:37:GLU:HG2	1:J:201:VAL:CG2	2.43	0.49
1:D:37:GLU:HG2	1:D:201:VAL:CG2	2.43	0.49
1:K:100:ALA:HB3	1:K:260:MET:HE1	1.94	0.49
1:H:314:VAL:HG12	1:H:367:LEU:HD13	1.94	0.49
1:O:65:MET:HE2	1:P:144:MET:HE3	1.93	0.49
1:K:11:VAL:CG2	1:K:201:VAL:CG2	2.90	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: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:C:37:GLU:HG2	1:C:201:VAL:CG2	2.43	0.49
1:P:11:VAL:CG2	1:P:201:VAL:HG23	2.43	0.49
1:D:11:VAL:CG2	1:D:201:VAL:CG2	2.91	0.49
1:A:156:ILE:HB	1:A:160:VAL:HG21	1.95	0.49
1:C:314:VAL:HG12	1:C:367:LEU:HD13	1.95	0.49
1:G:11:VAL:CG2	1:G:201:VAL:HG23	2.42	0.49
1:B:126:LEU:HG	1:B:144:MET:CG	2.43	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:154:HIS:C	1:B:155:ARG:HG2	2.32	0.49
1:B:11:VAL:CG2	1:B:201:VAL:CG2	2.91	0.48
1:M:156:ILE:HB	1:M:160:VAL:HG21	1.95	0.48
1:F:373:ARG:NH1	1:F:374:TYR:OH	2.45	0.48
1:G:126:LEU:HG	1:G:144:MET:CG	2.44	0.48
1:A:126:LEU:HG	1:A:144:MET:CG	2.43	0.48
1:C:126:LEU:HG	1:C:144:MET:CG	2.43	0.48
1:L:11:VAL:HG21	1:L:201:VAL:CG2	2.43	0.48
1:B:11:VAL:CG2	1:B:201:VAL:HG23	2.43	0.48
1:K:156:ILE:HB	1:K:160:VAL:HG21	1.96	0.48
1:F:314:VAL:HG12	1:F:367:LEU:HD13	1.94	0.48
1:A:293:GLY:N	1:A:294:PRO:CD	2.75	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:P:126:LEU:HG	1:P:144:MET:CG	2.43	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: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:I:144:MET:CE	1:J:65:MET:HE2	2.44	0.48
1:M:11:VAL:HG21	1:M:201:VAL:CG2	2.44	0.48
1:H:11:VAL:CG2	1:H:201:VAL:CG2	2.90	0.48
1:K:37:GLU:HG2	1:K:201:VAL:CG2	2.43	0.48
1:I:11:VAL:CG2	1:I:201:VAL:HG23	2.43	0.48
1:H:156:ILE:HB	1:H:160:VAL:HG21	1.95	0.48
1:D:156:ILE:HB	1:D:160:VAL:HG21	1.95	0.48
1:L:156:ILE:HB	1:L:160:VAL:HG21	1.96	0.48
1:M:293:GLY:N	1:M:294:PRO:CD	2.77	0.48
1:F:335:ASP:C	1:F:335:ASP:OD1	2.52	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:K:11:VAL:CG2	1:K:201:VAL:HG23	2.43	0.48
1:C:11:VAL:CG2	1:C:201:VAL:HG23	2.43	0.48
1:P:37:GLU:HG2	1:P:201:VAL:CG2	2.43	0.48
1:D:11:VAL:HG21	1:D:201:VAL:CG2	2.44	0.48
1:G:11:VAL:CG2	1:G:201:VAL:CG2	2.90	0.48
1:N:135:ARG:CG	2:N:405:HOH:O	2.56	0.48
1:J:393:ARG:HG3	1:J:393:ARG:O	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:C:11:VAL:CG2	1:C:201:VAL:CG2	2.91	0.48
1:J:156:ILE:HB	1:J:160:VAL:HG21	1.95	0.48
1:G:293:GLY:N	1:G:294:PRO:CD	2.77	0.48
1:K:173:ARG:O	1:K:177:ASP:CG	2.48	0.48
1:G:37:GLU:HG2	1:G:201:VAL:HG22	1.96	0.48
1:J:126:LEU:HG	1:J:144:MET:CG	2.44	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:B:11:VAL:HG21	1:B:201:VAL:CG2	2.44	0.48
1:N:156:ILE:HB	1:N:160:VAL:HG21	1.96	0.48
1:G:156:ILE:HB	1:G:160:VAL:HG21	1.96	0.48
1:O:126:LEU:HG	1:O:144:MET:CG	2.44	0.48
1:A:280:TYR:N	2:A:404:HOH:O	2.28	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:B:156:ILE:HB	1:B:160:VAL:HG21	1.96	0.48
1:E:126:LEU:HG	1:E:144:MET:CG	2.44	0.48
1:M:37:GLU:HG2	1:M:201:VAL:CG2	2.44	0.48
1:L:37:GLU:HG2	1:L:201:VAL:CG2	2.43	0.48
1:I:148:ALA:O	1:J:66:TYR:OH	2.29	0.48
1:E:293:GLY:N	1:E:294:PRO:CD	2.77	0.47
1:N:37:GLU:HG2	1:N:201:VAL:CG2	2.44	0.47
1:E:37:GLU:HG2	1:E:201:VAL:CG2	2.43	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:O:156:ILE:HB	1:O:160:VAL:HG21	1.96	0.47
1:J:314:VAL:HG12	1:J:367:LEU:HD13	1.94	0.47
1:K:126:LEU:CD2	1:L:126:LEU:HD21	2.43	0.47
1:O:185:ARG:CZ	2:O:403:HOH:O	2.62	0.47
1:M:11:VAL:CG2	1:M:201:VAL:HG23	2.43	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:N:208:ARG:CD	2:N:403:HOH:O	2.62	0.47
1:C:156:ILE:HB	1:C:160:VAL:HG21	1.96	0.47
1:P:156:ILE:HB	1:P:160:VAL:HG21	1.95	0.47
1:O:148:ALA:O	1:P:66:TYR:OH	2.31	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:C	1:P:335:ASP:OD1	2.53	0.47
1:O:126:LEU:CD2	1:P:126:LEU:HD21	2.39	0.47
1:I:144:MET:HE3	1:J:65:MET:HE2	1.97	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:N:335:ASP:OD1	1:N:335:ASP:C	2.53	0.47
1:J:335:ASP:C	1:J:335:ASP:OD1	2.52	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:M:144:MET:CE	1:N:65:MET:HE2	2.44	0.47
1:I:37:GLU:HG2	1:I:201:VAL:CG2	2.43	0.47
1:F:293:GLY:N	1:F:294:PRO:CD	2.77	0.47
1:E:335:ASP:OD1	1:E:335:ASP:C	2.52	0.47
1:F:156:ILE:HB	1:F:160:VAL:HG21	1.96	0.46
1:H:209:LYS:HE2	1:H:209:LYS:HB2	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:65:MET:HE2	1:P:144:MET:CE	2.45	0.46
1:C:11:VAL:HG21	1:C:201:VAL:CG2	2.44	0.46
1:C:176:GLN:OE1	1:C:242:THR:OG1	2.27	0.46
1:C:89:LEU:HD11	1:D:66:TYR:CD1	2.50	0.46
1:N:198:ASP:HB2	2:N:411:HOH:O	2.15	0.46
1:K:19:GLY:O	1:K:23:LYS:CE	2.63	0.46
1:J:137:GLY:HA2	1:K:146:LEU:HD12	1.97	0.46
1:F:227:ASP:OD1	1:F:227:ASP:O	2.34	0.46
1:F:265:GLU:OE2	1:F:268:ARG:NH1	2.47	0.46
1:C:394:ILE:HD12	1:C:394:ILE:HA	1.71	0.46
1:E:23:LYS:HD2	2:E:410:HOH:O	2.15	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:I:286:ASP:OD2	1:I:288:LYS:CE	2.64	0.46
1:B:293:GLY:N	1:B:294:PRO:CD	2.77	0.46
1:L:335:ASP:C	1:L:335:ASP:OD1	2.52	0.46
1:G:358:LEU:C	1:G:358:LEU:HD12	2.36	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:O:226:ILE:HG23	1:O:227:ASP:OD1	2.16	0.46
1:L:368:ASN:HA	1:L:393:ARG:HD3	1.98	0.46
1:B:233:ARG:NH2	1:G:76:GLY:HA2	2.31	0.46
1:K:358:LEU:C	1:K:358:LEU:HD12	2.37	0.46
1:M:335:ASP:C	1:M:335:ASP:OD1	2.54	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:K:309:VAL:CG2	2:K:409:HOH:O	2.50	0.46
1:F:158:MET:CE	1:F:290:MET:SD	2.99	0.46
1:D:335:ASP:OD1	1:D:335:ASP:C	2.53	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:E:329:THR:HG23	1:E:339:VAL:HG21	1.97	0.45
1:B:265:GLU:CD	1:B:268[B]:ARG:HE	2.20	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:C:23:LYS:HE3	1:C:23:LYS:HB2	1.85	0.45
1:I:335:ASP:C	1:I:335:ASP:OD1	2.53	0.45
1:E:171:ILE:HA	1:E:175:GLN:OE1	2.17	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:C:176:GLN:CD	1:C:242:THR:HG1	2.18	0.45
1:B:358:LEU:HD12	1:B:358:LEU:C	2.36	0.45
1:P:293:GLY:N	1:P:294:PRO:CD	2.78	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:C:358:LEU:HD12	1:C:358:LEU:C	2.37	0.45
1:L:233:ARG:CD	1:L:233:ARG:N	2.73	0.45
1:G:263:ARG:HD3	2:G:404:HOH:O	2.17	0.45
1:E:126:LEU:HD21	1:F:126:LEU:HD21	1.98	0.45
1:I:238:LYS:HD2	1:I:238:LYS:HA	1.70	0.45
1:A:279:SER:HB2	2:A:404:HOH:O	2.16	0.45
1:F:100:ALA:HB3	1:F:260:MET:HE1	1.98	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: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:O:358:LEU:HD12	1:O:358:LEU:C	2.37	0.44
1:E:126:LEU:CD2	1:F:126:LEU:HD21	2.40	0.44
1:F:158:MET:CE	1:F:382:GLY:CA	2.95	0.44
1:J:238:LYS:HA	1:J:238:LYS:HD2	1.87	0.44
1:I:286:ASP:OD2	1:I:288:LYS:HE2	2.17	0.44
1:C:89:LEU:HD22	1:D:66:TYR:CE1	2.52	0.44
1:P:358:LEU:HD12	1:P:358:LEU:C	2.37	0.44
1:F:17:THR:HG22	1:F:18:PHE:N	2.32	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:O:66:TYR:CZ	1:P:89:LEU:HD22	2.52	0.44
1:N:182:GLU:OE1	1:N:185:ARG:NH2	2.49	0.44
1:O:126:LEU:HD21	1:P:126:LEU:HD21	1.98	0.44
1:H:126:LEU:HG	1:H:144:MET:HG2	1.99	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:M:358:LEU:C	1:M:358:LEU:HD12	2.37	0.44
1:J:171:ILE:HA	1:J:175:GLN:OE1	2.17	0.44
1:M:102:GLN:HG2	1:N:106:LEU:CD1	2.48	0.44
1:B:295:VAL:HB	1:B:296:PRO:CD	2.48	0.44
1:A:230:THR:CG2	1:A:230:THR:O	2.66	0.44
1:A:358:LEU:C	1:A:358:LEU:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:293:GLY:N	1:J:294:PRO:CD	2.80	0.44
1:N:161:THR:CG2	1:N:290:MET:HG3	2.44	0.44
1:O:23:LYS:HE3	1:O:23:LYS:HB2	1.84	0.44
1:F:158:MET:HE3	1:F:290:MET:CE	2.48	0.44
1:B:335:ASP:OD1	1:B:335:ASP:C	2.55	0.44
1:J:358:LEU:HD12	1:J:358:LEU:C	2.38	0.44
1:M:36:ARG:NE	2:M:403:HOH:O	2.25	0.44
1:G:204:VAL:HA	1:G:212:VAL:O	2.18	0.44
1:I:126:LEU:CD2	1:J:126:LEU:HD22	2.42	0.43
1:F:126:LEU:HG	1:F:144:MET:HG2	2.00	0.43
1:A:65:MET:CE	1:B:144:MET:CE	2.96	0.43
1:P:176:GLN:NE2	1:P:242:THR:OG1	2.51	0.43
1:K:89:LEU:HD22	1:L:66:TYR:CZ	2.53	0.43
1:D:233:ARG:CZ	2:D:428:HOH:O	2.66	0.43
1:G:319:GLU:CD	1:G:344:SER:HB3	2.39	0.43
1:B:272:LYS:H	1:B:272:LYS:HG3	1.63	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:D:293:GLY:N	1:D:294:PRO:CD	2.81	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:E:161:THR:CG2	1:E:290:MET:HG3	2.44	0.43
1:A:37:GLU:O	1:A:41:ARG:HG2	2.17	0.43
1:K:126:LEU:HG	1:K:144:MET:HG2	2.00	0.43
1:K:65:MET:CE	1:L:58:ILE:HA	2.46	0.43
1:K:17:THR:HG22	1:K:18:PHE:N	2.34	0.43
1:E:318:ASN:HB3	2:E:402:HOH:O	2.19	0.43
1:O:65:MET:HE3	1:P:144:MET:HE1	2.01	0.43
1:A:66:TYR:CD2	1:B:89:LEU:HD13	2.53	0.43
1:N:236:PHE:O	1:N:237:VAL:O	2.37	0.43
1:N:238:LYS:HA	1:N:238:LYS:HD2	1.85	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: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:L:11:VAL:HG21	1:L:201:VAL:HG22	2.01	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:H:290:MET:HE3	1:H:380:CYS:SG	2.59	0.43
1:P:126:LEU:HG	1:P:144:MET:HG2	2.00	0.43
1:M:126:LEU:HD23	1:N:126:LEU:HD22	2.01	0.43
1:L:276:ARG:NH2	1:L:392:GLU:OE1	2.49	0.43
1:N:151:ASP:OD2	1:N:287:PRO:HB3	2.19	0.43
1:K:19:GLY:C	1:K:23:LYS:HE2	2.40	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: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:P:265:GLU:OE2	1:P:268:ARG:NE	2.52	0.42
1:O:66:TYR:CE2	1:P:89:LEU:HD22	2.54	0.42
1:E:295:VAL:HB	1:E:296:PRO:CD	2.49	0.42
1:D:23:LYS:HB2	1:D:23:LYS:HE3	1.84	0.42
1:O:161:THR:CG2	1:O:290:MET:HG3	2.43	0.42
1:M:144:MET:HE3	1:N:65:MET:HE2	2.01	0.42
1:O:316:GLU:HG3	1:O:359:ILE:HB	1.99	0.42
1:D:358:LEU:HD12	1:D:358:LEU:C	2.39	0.42
1:N:358:LEU:C	1:N:358:LEU:HD12	2.39	0.42
1:K:174:ALA:HA	1:K:177:ASP:OD1	2.19	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:A:295:VAL:HB	1:A:296:PRO:CD	2.49	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:M:238:LYS:HD2	1:M:238:LYS:HA	1.61	0.42
1:K:89:LEU:HD11	1:L:66:TYR:CD2	2.54	0.42
1:E:66:TYR:CZ	1:F:89:LEU:HD22	2.53	0.42
1:I:17:THR:HG22	1:I:18:PHE:N	2.35	0.42
1:H:295:VAL:HB	1:H:296:PRO:CD	2.49	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:I:358:LEU:HD12	1:I:358:LEU:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:295:VAL:HB	1:N:296:PRO:CD	2.49	0.42
1:G:227:ASP:HA	1:G:230:THR:OG1	2.20	0.42
1:N:236:PHE:O	1:N:237:VAL:CG1	2.64	0.42
1:M:11:VAL:HG21	1:M:201:VAL:HG22	2.02	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
1:O:265:GLU:OE2	1:O:268:ARG:NH1	2.53	0.42
1:L:23:LYS:HB2	1:L:23:LYS:HE3	1.84	0.42
1:H:204:VAL:HA	1:H:212:VAL:O	2.19	0.42
1:E:126:LEU:HG	1:E:144:MET:HG2	2.01	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:J:295:VAL:HB	1:J:296:PRO:CD	2.50	0.42
1:J:161:THR:HG21	1:J:290:MET:CG	2.49	0.42
1:A:204:VAL:HA	1:A:212:VAL:O	2.20	0.42
1:N:23:LYS:HB2	1:N:23:LYS:HE3	1.84	0.42
1:N:181:LEU:O	1:N:181:LEU:HD13	2.20	0.42
1:O:126:LEU:HG	1:O:144:MET:HG2	2.01	0.41
1:N:368:ASN:HA	1:N:393:ARG:HH21	1.79	0.41
1:M:144:MET:CE	1:N:65:MET:HE3	2.49	0.41
1:M:126:LEU:HG	1:M:144:MET:HG2	2.01	0.41
1:D:265:GLU:OE2	1:D:268:ARG:NH1	2.53	0.41
1:K:168:GLU:OE1	2:K:401:HOH:O	2.22	0.41
1:I:204:VAL:HA	1:I:212:VAL:O	2.21	0.41
1:H:11:VAL:HG21	1:H:201:VAL:HG22	2.02	0.41
1:D:11:VAL:HG21	1:D:201:VAL:HG22	2.02	0.41
1:O:227:ASP:N	1:O:227:ASP:OD1	2.53	0.41
1:K:335:ASP:HA	1:K:336:PRO:HD3	1.90	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: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:N:227:ASP:HA	1:N:230:THR:OG1	2.21	0.41
1:J:158:MET:HA	1:J:158:MET:HE3	1.99	0.41
1:I:154:HIS:C	1:I:155:ARG:CG	2.87	0.41
1:O:17:THR:HG22	1:O:18:PHE:N	2.36	0.41
1:L:319:GLU:CD	1:L:344:SER:HB3	2.40	0.41
1:J:316:GLU:HG3	1:J:359:ILE:HD12	2.02	0.41
1:P:176:GLN:CD	1:P:242:THR:OG1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:THR:HG22	1:C:18:PHE:N	2.36	0.41
1:G:126:LEU:HG	1:G:144:MET:HG2	2.02	0.41
1:C:126:LEU:HD21	1:D:126:LEU:HD21	2.03	0.41
1:A:265:GLU:OE2	1:A:268:ARG:NH1	2.53	0.41
1:D:225:THR:O	1:D:228:ASP:HB2	2.21	0.41
1:N:171:ILE:HA	1:N:175:GLN:OE1	2.21	0.41
1:I:249:SER:HA	1:I:346:ILE:HA	2.03	0.41
1:K:11:VAL:HG21	1:K:201:VAL:HG22	2.01	0.41
1:C:89:LEU:HD22	1:D:66:TYR:CZ	2.55	0.41
1:K:204:VAL:HA	1:K:212:VAL:O	2.20	0.41
1:J:292:ILE:HG13	1:J:292:ILE:H	1.73	0.41
1:J:158:MET:CA	1:J:158:MET:HE3	2.50	0.41
1:G:204:VAL:HG12	1:G:213:THR:HB	2.02	0.41
1:B:172:SER:O	1:B:176:GLN:HG3	2.21	0.41
1:G:63:ARG:NH2	2:G:406:HOH:O	2.34	0.41
1:F:143:ASP:C	1:F:143:ASP:OD1	2.58	0.41
1:L:272:LYS:H	1:L:272:LYS:HG3	1.66	0.41
1:I:4:GLU:OE1	1:I:263:ARG:HD3	2.20	0.41
1:D:316:GLU:HG3	1:D:359:ILE:HB	2.02	0.41
1:K:106:LEU:CD1	1:L:102:GLN:HG2	2.51	0.41
1:F:225:THR:O	1:F:228:ASP:HB2	2.21	0.41
1:M:272:LYS:HG3	1:M:272:LYS:H	1.58	0.41
1:H:276:ARG:HH11	1:H:394:ILE:CD1	2.30	0.41
1:H:225:THR:O	1:H:228:ASP:HB2	2.21	0.41
1:B:227:ASP:HA	1:B:230:THR:OG1	2.21	0.41
1:N:11:VAL:HG21	1:N:201:VAL:HG22	2.02	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: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:K:225:THR:O	1:K:228:ASP:HB2	2.21	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:L:204:VAL:HA	1:L:212:VAL:O	2.21	0.40
1:N:143:ASP:C	1:N:143:ASP:OD1	2.60	0.40
1:F:249:SER:HA	1:F:346:ILE:HA	2.04	0.40
1:H:276:ARG:HD3	1:H:394:ILE:HD12	1.94	0.40
1:O:65:MET:CE	1:P:144:MET:HE1	2.49	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:F:204:VAL:HA	1:F:212:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:ILE:H	1:H:292:ILE:HG13	1.75	0.40
1:D:367:LEU:HG	1:D:393:ARG:HG2	2.02	0.40
1:A:143:ASP:C	1:A:143:ASP:OD1	2.59	0.40
1:E:225:THR:O	1:E:228:ASP:HB2	2.20	0.40
1:B:225:THR:O	1:B:228:ASP:HB2	2.21	0.40
1:I:161:THR:HG21	1:I:290:MET:CG	2.46	0.40
1:B:265:GLU:OE2	1:B:268[A]:ARG:NH1	2.53	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:A:225:THR:O	1:A:228:ASP:HB2	2.21	0.40
1:P:295:VAL:HB	1:P:296:PRO:CD	2.51	0.40
1:L:227:ASP:HA	1:L:230:THR:OG1	2.21	0.40
1:L:225:THR:O	1:L:228:ASP:HB2	2.21	0.40
1:P:158:MET:HE1	1:P:382:GLY:CA	2.42	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

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%)	46	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	388/414 (94%)	375 (97%)	11 (3%)	2 (0%)	34	26
1	I	387/414 (94%)	374 (97%)	13 (3%)	0	100	100
1	J	385/414 (93%)	372 (97%)	11 (3%)	2 (0%)	34	26
1	K	388/414 (94%)	377 (97%)	10 (3%)	1 (0%)	46	41
1	L	387/414 (94%)	377 (97%)	10 (3%)	0	100	100
1	M	386/414 (93%)	374 (97%)	10 (3%)	2 (0%)	34	26
1	N	390/414 (94%)	375 (96%)	13 (3%)	2 (0%)	34	26
1	O	384/414 (93%)	375 (98%)	9 (2%)	0	100	100
1	P	384/414 (93%)	371 (97%)	12 (3%)	1 (0%)	46	41
All	All	6179/6624 (93%)	6010 (97%)	158 (3%)	11 (0%)	52	48

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%)	262 (91%)	25 (9%)	13	7
1	B	287/305 (94%)	266 (93%)	21 (7%)	17	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	285/305 (93%)	260 (91%)	25 (9%)	12	7
1	D	285/305 (93%)	262 (92%)	23 (8%)	15	9
1	E	282/305 (92%)	262 (93%)	20 (7%)	18	12
1	F	284/305 (93%)	262 (92%)	22 (8%)	16	10
1	G	285/305 (93%)	265 (93%)	20 (7%)	19	12
1	H	286/305 (94%)	260 (91%)	26 (9%)	12	6
1	I	287/305 (94%)	264 (92%)	23 (8%)	15	9
1	J	284/305 (93%)	264 (93%)	20 (7%)	19	12
1	K	286/305 (94%)	264 (92%)	22 (8%)	16	10
1	L	285/305 (93%)	262 (92%)	23 (8%)	15	9
1	M	285/305 (93%)	264 (93%)	21 (7%)	17	11
1	N	286/305 (94%)	259 (91%)	27 (9%)	11	6
1	O	284/305 (93%)	258 (91%)	26 (9%)	11	6
1	P	283/305 (93%)	262 (93%)	21 (7%)	17	11
All	All	4561/4880 (94%)	4196 (92%)	365 (8%)	15	9

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	393/414 (94%)	0.22	21 (5%)	30 32	19, 35, 53, 75	0
1	B	391/414 (94%)	0.29	21 (5%)	29 31	17, 35, 57, 93	0
1	C	389/414 (93%)	0.22	9 (2%)	64 64	16, 32, 54, 87	0
1	D	390/414 (94%)	0.08	13 (3%)	50 51	15, 29, 53, 89	0
1	E	386/414 (93%)	0.55	39 (10%)	9 10	19, 39, 68, 104	0
1	F	388/414 (93%)	0.41	26 (6%)	21 22	19, 38, 61, 84	0
1	G	389/414 (93%)	0.19	12 (3%)	52 53	15, 31, 51, 75	0
1	H	392/414 (94%)	0.27	20 (5%)	32 33	17, 33, 59, 93	0
1	I	390/414 (94%)	0.16	15 (3%)	44 45	15, 28, 53, 81	0
1	J	389/414 (93%)	0.30	24 (6%)	24 25	18, 33, 57, 98	0
1	K	392/414 (94%)	0.39	23 (5%)	26 27	22, 39, 60, 81	0
1	L	390/414 (94%)	0.38	25 (6%)	23 24	20, 38, 60, 98	0
1	M	390/414 (94%)	0.38	28 (7%)	18 20	24, 38, 60, 95	0
1	N	392/414 (94%)	0.51	35 (8%)	12 13	22, 39, 64, 117	0
1	O	388/414 (93%)	0.59	41 (10%)	8 9	25, 44, 69, 99	0
1	P	388/414 (93%)	0.73	46 (11%)	6 6	23, 44, 73, 97	0
All	All	6237/6624 (94%)	0.35	398 (6%)	23 24	15, 36, 61, 117	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	THR	7.0
1	J	210	GLY	7.0
1	E	212	VAL	6.6
1	H	240	ASN	6.5
1	N	238	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	205	SER	5.5
1	O	212	VAL	5.3
1	P	235	VAL	5.1
1	F	84	LEU	4.9
1	P	225	THR	4.8
1	N	241	GLY	4.7
1	N	239	GLU	4.6
1	I	86	VAL	4.6
1	M	211	ASP	4.6
1	N	237	VAL	4.5
1	P	309	VAL	4.5
1	G	84	LEU	4.5
1	F	2	THR	4.4
1	L	84	LEU	4.3
1	L	224	ALA	4.2
1	M	84	LEU	4.2
1	J	237	VAL	4.2
1	N	271	LEU	4.1
1	O	223	ASP	4.1
1	J	57	VAL	4.0
1	O	206	LYS	4.0
1	A	86	VAL	4.0
1	N	240	ASN	4.0
1	O	203	VAL	4.0
1	H	241	GLY	4.0
1	O	2	THR	3.9
1	A	85	THR	3.9
1	L	205	SER	3.8
1	K	84	LEU	3.8
1	B	84	LEU	3.8
1	E	89	LEU	3.8
1	N	86	VAL	3.8
1	I	84	LEU	3.8
1	P	310	SER	3.8
1	F	53	VAL	3.8
1	O	167	LYS	3.8
1	P	226	ILE	3.7
1	A	84	LEU	3.7
1	O	309	VAL	3.7
1	G	86	VAL	3.7
1	J	89	LEU	3.7
1	E	239	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	226	ILE	3.7
1	K	89	LEU	3.7
1	G	53	VAL	3.6
1	H	85	THR	3.6
1	I	53	VAL	3.6
1	O	85	THR	3.5
1	P	205	SER	3.5
1	N	89	LEU	3.5
1	I	85	THR	3.5
1	M	240	ASN	3.5
1	O	235	VAL	3.5
1	N	225	THR	3.5
1	P	236	PHE	3.5
1	G	89	LEU	3.5
1	O	237	VAL	3.5
1	K	92	SER	3.4
1	L	53	VAL	3.4
1	N	227	ASP	3.4
1	C	86	VAL	3.4
1	O	53	VAL	3.4
1	O	57	VAL	3.4
1	E	57	VAL	3.4
1	H	57	VAL	3.4
1	L	86	VAL	3.4
1	J	211	ASP	3.4
1	P	241	GLY	3.4
1	N	236	PHE	3.4
1	G	67	LEU	3.4
1	O	332	LEU	3.4
1	K	225	THR	3.3
1	E	203	VAL	3.3
1	M	86	VAL	3.3
1	J	92	SER	3.3
1	A	225	THR	3.3
1	E	86	VAL	3.3
1	O	4	GLU	3.3
1	D	89	LEU	3.3
1	H	84	LEU	3.3
1	K	268	ARG	3.3
1	F	86	VAL	3.3
1	O	43	GLN	3.3
1	P	181	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	205	SER	3.2
1	D	84	LEU	3.2
1	B	57	VAL	3.2
1	L	55	GLY	3.2
1	P	224	ALA	3.2
1	M	235	VAL	3.2
1	P	53	VAL	3.2
1	A	92	SER	3.2
1	F	211	ASP	3.2
1	P	327	ALA	3.2
1	E	312	LEU	3.2
1	H	89	LEU	3.2
1	O	238	LYS	3.2
1	O	92	SER	3.1
1	K	210	GLY	3.1
1	P	211	ASP	3.1
1	L	42	ALA	3.1
1	C	85	THR	3.1
1	N	224	ALA	3.1
1	M	93	GLY	3.1
1	P	210	GLY	3.1
1	O	211	ASP	3.1
1	F	85	THR	3.1
1	B	86	VAL	3.1
1	D	212	VAL	3.1
1	H	237	VAL	3.1
1	J	86	VAL	3.1
1	L	237	VAL	3.1
1	P	84	LEU	3.1
1	K	91	GLY	3.0
1	O	264	ALA	3.0
1	O	270	GLY	3.0
1	J	85	THR	3.0
1	E	191	ILE	3.0
1	E	167	LYS	3.0
1	N	92	SER	3.0
1	L	85	THR	3.0
1	I	55	GLY	3.0
1	P	364	LEU	3.0
1	C	181	LEU	3.0
1	O	86	VAL	3.0
1	N	67	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	85	THR	3.0
1	N	90	CYS	3.0
1	H	86	VAL	2.9
1	K	86	VAL	2.9
1	P	268	ARG	2.9
1	E	84	LEU	2.9
1	D	210	GLY	2.9
1	J	309	VAL	2.9
1	H	239	GLU	2.9
1	E	233	ARG	2.9
1	K	57	VAL	2.9
1	O	204	VAL	2.9
1	L	242	THR	2.9
1	L	89	LEU	2.9
1	N	57	VAL	2.9
1	O	335	ASP	2.9
1	E	272	LYS	2.9
1	O	87	ASN	2.9
1	N	85	THR	2.9
1	M	238	LYS	2.9
1	B	89	LEU	2.8
1	C	84	LEU	2.8
1	L	98	VAL	2.8
1	P	330	LYS	2.8
1	D	86	VAL	2.8
1	N	181	LEU	2.8
1	M	224	ALA	2.8
1	O	89	LEU	2.8
1	L	227	ASP	2.7
1	P	242	THR	2.7
1	O	353	GLY	2.7
1	P	267	GLU	2.7
1	I	89	LEU	2.7
1	M	237	VAL	2.7
1	J	87	ASN	2.7
1	C	358	LEU	2.7
1	O	374	TYR	2.7
1	H	87	ASN	2.7
1	L	97	ILE	2.7
1	P	306	GLY	2.7
1	F	266	ALA	2.7
1	G	129	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	89	LEU	2.7
1	K	228	ASP	2.7
1	P	334	LEU	2.7
1	A	98	VAL	2.7
1	P	212	VAL	2.7
1	M	54	PHE	2.7
1	B	87	ASN	2.7
1	O	84	LEU	2.7
1	F	204	VAL	2.6
1	A	381	ILE	2.6
1	J	381	ILE	2.6
1	O	263	ARG	2.6
1	P	71	ALA	2.6
1	N	211	ASP	2.6
1	N	228	ASP	2.6
1	F	270	GLY	2.6
1	P	55	GLY	2.6
1	M	98	VAL	2.6
1	M	355	THR	2.6
1	J	212	VAL	2.6
1	B	381	ILE	2.6
1	H	92	SER	2.6
1	O	213	THR	2.6
1	K	90	CYS	2.6
1	P	336	PRO	2.6
1	B	53	VAL	2.6
1	A	94	LEU	2.6
1	E	223	ASP	2.5
1	A	57	VAL	2.5
1	K	237	VAL	2.5
1	K	240	ASN	2.5
1	I	96	ALA	2.5
1	P	266	ALA	2.5
1	L	240	ASN	2.5
1	E	338	LYS	2.5
1	H	238	LYS	2.5
1	N	94	LEU	2.5
1	N	235	VAL	2.5
1	L	67	LEU	2.5
1	E	42	ALA	2.5
1	P	354	ALA	2.5
1	E	330	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	92	SER	2.5
1	N	205	SER	2.5
1	P	263	ARG	2.5
1	E	353	GLY	2.5
1	I	54	PHE	2.5
1	M	89	LEU	2.5
1	J	2	THR	2.5
1	P	339	VAL	2.5
1	L	93	GLY	2.5
1	B	245	ALA	2.5
1	G	68	GLY	2.4
1	L	241	GLY	2.4
1	F	83	ALA	2.4
1	A	271	LEU	2.4
1	C	89	LEU	2.4
1	F	227	ASP	2.4
1	A	93	GLY	2.4
1	M	58	ILE	2.4
1	L	129	ALA	2.4
1	C	205	SER	2.4
1	L	57	VAL	2.4
1	D	211	ASP	2.4
1	A	359	ILE	2.4
1	I	354	ALA	2.4
1	F	115	GLY	2.4
1	F	353	GLY	2.4
1	M	53	VAL	2.4
1	J	223	ASP	2.4
1	P	275	ALA	2.4
1	B	85	THR	2.4
1	F	226	ILE	2.4
1	J	93	GLY	2.4
1	G	90	CYS	2.4
1	F	67	LEU	2.4
1	I	1	MET	2.4
1	M	55	GLY	2.4
1	O	329	THR	2.4
1	E	97	ILE	2.4
1	M	352	ILE	2.4
1	H	91	GLY	2.3
1	N	56	ASN	2.3
1	B	233	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	175	GLN	2.3
1	A	90	CYS	2.3
1	B	212	VAL	2.3
1	C	57	VAL	2.3
1	P	86	VAL	2.3
1	P	314	VAL	2.3
1	A	91	GLY	2.3
1	E	227	ASP	2.3
1	O	230	THR	2.3
1	P	85	THR	2.3
1	P	355	THR	2.3
1	B	67	LEU	2.3
1	K	181	LEU	2.3
1	P	170	ASP	2.3
1	D	85	THR	2.3
1	H	233	ARG	2.3
1	B	58	ILE	2.3
1	B	352	ILE	2.3
1	K	93	GLY	2.3
1	M	116	GLY	2.3
1	B	213	THR	2.3
1	E	85	THR	2.3
1	I	92	SER	2.3
1	B	174	ALA	2.3
1	G	117	ALA	2.3
1	H	224	ALA	2.3
1	E	53	VAL	2.3
1	J	53	VAL	2.3
1	N	206	LYS	2.3
1	J	90	CYS	2.3
1	L	58	ILE	2.3
1	N	359	ILE	2.3
1	F	331	ALA	2.2
1	J	96	ALA	2.2
1	P	232	LEU	2.2
1	E	309	VAL	2.2
1	F	306	GLY	2.2
1	H	94	LEU	2.2
1	M	96	ALA	2.2
1	H	242	THR	2.2
1	M	232	LEU	2.2
1	P	38	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	374	TYR	2.2
1	O	44	VAL	2.2
1	M	206	LYS	2.2
1	F	198	ASP	2.2
1	F	4	GLU	2.2
1	A	88	ARG	2.2
1	E	264	ALA	2.2
1	J	233	ARG	2.2
1	P	174	ALA	2.2
1	I	67	LEU	2.2
1	E	333	GLY	2.2
1	O	295	VAL	2.2
1	L	56	ASN	2.2
1	N	148	ALA	2.2
1	E	55	GLY	2.2
1	H	181	LEU	2.2
1	E	303	GLU	2.2
1	D	57	VAL	2.2
1	E	44	VAL	2.2
1	H	43	GLN	2.2
1	E	117	ALA	2.2
1	M	354	ALA	2.2
1	M	210	GLY	2.2
1	N	353	GLY	2.2
1	I	94	LEU	2.2
1	J	84	LEU	2.2
1	M	56	ASN	2.2
1	N	356	GLY	2.2
1	P	90	CYS	2.1
1	J	241	GLY	2.1
1	G	85	THR	2.1
1	J	56	ASN	2.1
1	N	84	LEU	2.1
1	A	167	LYS	2.1
1	A	212	VAL	2.1
1	B	211	ASP	2.1
1	O	311	ASP	2.1
1	K	356	GLY	2.1
1	N	91	GLY	2.1
1	B	224	ALA	2.1
1	M	92	SER	2.1
1	O	96	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	310	SER	2.1
1	C	352	ILE	2.1
1	D	97	ILE	2.1
1	D	381	ILE	2.1
1	F	268	ARG	2.1
1	J	55	GLY	2.1
1	M	115	GLY	2.1
1	P	230	THR	2.1
1	K	387	ILE	2.1
1	N	171	ILE	2.1
1	L	116	GLY	2.1
1	A	224	ALA	2.1
1	E	96	ALA	2.1
1	F	54	PHE	2.1
1	G	83	ALA	2.1
1	I	83	ALA	2.1
1	F	311	ASP	2.1
1	N	170	ASP	2.1
1	P	228	ASP	2.1
1	K	267	GLU	2.1
1	N	381	ILE	2.1
1	P	315	ILE	2.1
1	D	53	VAL	2.1
1	E	56	ASN	2.1
1	N	212	VAL	2.1
1	H	54	PHE	2.1
1	P	371	GLN	2.1
1	B	241	GLY	2.1
1	E	93	GLY	2.1
1	F	333	GLY	2.1
1	J	91	GLY	2.1
1	M	97	ILE	2.0
1	A	53	VAL	2.0
1	E	357	ALA	2.0
1	O	337	ALA	2.0
1	B	169	TYR	2.0
1	I	116	GLY	2.0
1	E	87	ASN	2.0
1	D	90	CYS	2.0
1	K	94	LEU	2.0
1	L	117	ALA	2.0
1	M	242	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	331	ALA	2.0
1	G	57	VAL	2.0
1	O	25	VAL	2.0
1	K	353	GLY	2.0
1	D	223	ASP	2.0
1	E	170	ASP	2.0
1	K	231	LYS	2.0
1	B	2	THR	2.0
1	P	352	ILE	2.0
1	E	160	VAL	2.0
1	E	221	ARG	2.0
1	A	353	GLY	2.0
1	F	170	ASP	2.0
1	F	228	ASP	2.0
1	L	353	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.