



# Full wwPDB X-ray Structure Validation Report

Oct 21, 2014 – 11:53 PM EDT

PDB ID : 4WL1  
Title : Structure of WzzE Polysaccharide Co-polymerase  
Authors : Kalynych, S.; Cherney, M.; Cygler, M.  
Deposited on : 2014-10-05  
Resolution : 5.99 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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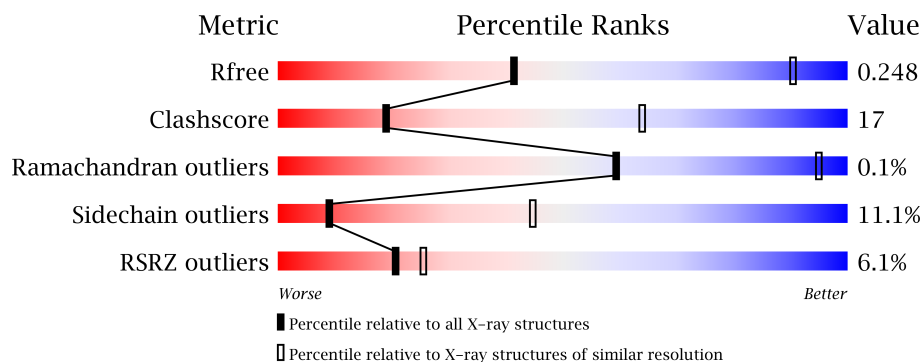
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 5.99 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.



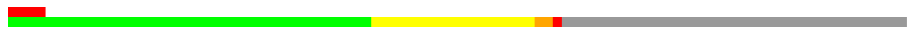


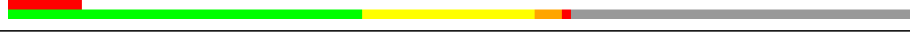
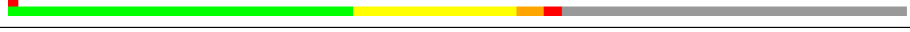
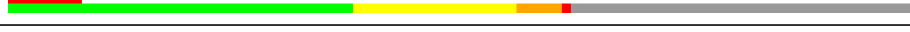
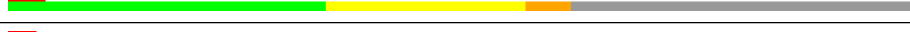

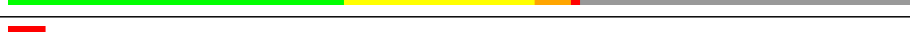

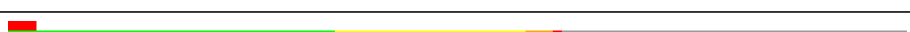
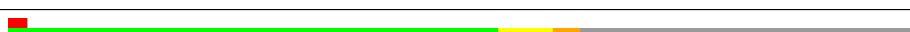


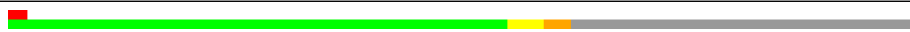



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1089 (8.20-3.50)
Clashscore	79885	1024 (8.20-3.52)
Ramachandran outliers	78287	1282 (8.20-3.50)
Sidechain outliers	78261	1258 (8.20-3.50)
RSRZ outliers	66119	1088 (8.20-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	356	
1	B	356	
1	C	356	
1	D	356	
1	E	356	
1	F	356	
1	G	356	
1	H	356	
1	I	356	
1	J	356	
1	K	356	
1	L	356	
1	M	356	
1	N	356	

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Mol	Chain	Length	Quality of chain
1	O	356	
1	P	356	
1	Q	356	
1	R	356	
1	S	356	
1	T	356	
1	U	356	
1	V	356	
1	W	356	
1	X	356	
1	Y	356	
1	Z	356	
1	a	356	
1	b	356	
1	c	356	
1	d	356	
1	e	356	
1	f	356	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 57504 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lipopolysaccharide biosynthesis protein WzzE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	B	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	C	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	D	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	E	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	F	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	G	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	H	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	I	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	J	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	K	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	L	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	M	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	N	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	O	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	P	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	R	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	S	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	T	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	U	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	V	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	W	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	X	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	Y	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	Z	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	a	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	b	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	c	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	d	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	e	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	f	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P0AG01
A	-5	GLY	-	expression tag	UNP P0AG01
A	-4	SER	-	expression tag	UNP P0AG01
A	-3	HIS	-	expression tag	UNP P0AG01
A	-2	HIS	-	expression tag	UNP P0AG01
A	-1	HIS	-	expression tag	UNP P0AG01
A	0	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P0AG01
A	2	HIS	-	expression tag	UNP P0AG01
B	-6	MET	-	initiating methionine	UNP P0AG01
B	-5	GLY	-	expression tag	UNP P0AG01
B	-4	SER	-	expression tag	UNP P0AG01
B	-3	HIS	-	expression tag	UNP P0AG01
B	-2	HIS	-	expression tag	UNP P0AG01
B	-1	HIS	-	expression tag	UNP P0AG01
B	0	HIS	-	expression tag	UNP P0AG01
B	1	HIS	-	expression tag	UNP P0AG01
B	2	HIS	-	expression tag	UNP P0AG01
C	-6	MET	-	initiating methionine	UNP P0AG01
C	-5	GLY	-	expression tag	UNP P0AG01
C	-4	SER	-	expression tag	UNP P0AG01
C	-3	HIS	-	expression tag	UNP P0AG01
C	-2	HIS	-	expression tag	UNP P0AG01
C	-1	HIS	-	expression tag	UNP P0AG01
C	0	HIS	-	expression tag	UNP P0AG01
C	1	HIS	-	expression tag	UNP P0AG01
C	2	HIS	-	expression tag	UNP P0AG01
D	-6	MET	-	initiating methionine	UNP P0AG01
D	-5	GLY	-	expression tag	UNP P0AG01
D	-4	SER	-	expression tag	UNP P0AG01
D	-3	HIS	-	expression tag	UNP P0AG01
D	-2	HIS	-	expression tag	UNP P0AG01
D	-1	HIS	-	expression tag	UNP P0AG01
D	0	HIS	-	expression tag	UNP P0AG01
D	1	HIS	-	expression tag	UNP P0AG01
D	2	HIS	-	expression tag	UNP P0AG01
E	-6	MET	-	initiating methionine	UNP P0AG01
E	-5	GLY	-	expression tag	UNP P0AG01
E	-4	SER	-	expression tag	UNP P0AG01
E	-3	HIS	-	expression tag	UNP P0AG01
E	-2	HIS	-	expression tag	UNP P0AG01
E	-1	HIS	-	expression tag	UNP P0AG01
E	0	HIS	-	expression tag	UNP P0AG01
E	1	HIS	-	expression tag	UNP P0AG01
E	2	HIS	-	expression tag	UNP P0AG01
F	-6	MET	-	initiating methionine	UNP P0AG01
F	-5	GLY	-	expression tag	UNP P0AG01
F	-4	SER	-	expression tag	UNP P0AG01
F	-3	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	HIS	-	expression tag	UNP P0AG01
F	-1	HIS	-	expression tag	UNP P0AG01
F	0	HIS	-	expression tag	UNP P0AG01
F	1	HIS	-	expression tag	UNP P0AG01
F	2	HIS	-	expression tag	UNP P0AG01
G	-6	MET	-	initiating methionine	UNP P0AG01
G	-5	GLY	-	expression tag	UNP P0AG01
G	-4	SER	-	expression tag	UNP P0AG01
G	-3	HIS	-	expression tag	UNP P0AG01
G	-2	HIS	-	expression tag	UNP P0AG01
G	-1	HIS	-	expression tag	UNP P0AG01
G	0	HIS	-	expression tag	UNP P0AG01
G	1	HIS	-	expression tag	UNP P0AG01
G	2	HIS	-	expression tag	UNP P0AG01
H	-6	MET	-	initiating methionine	UNP P0AG01
H	-5	GLY	-	expression tag	UNP P0AG01
H	-4	SER	-	expression tag	UNP P0AG01
H	-3	HIS	-	expression tag	UNP P0AG01
H	-2	HIS	-	expression tag	UNP P0AG01
H	-1	HIS	-	expression tag	UNP P0AG01
H	0	HIS	-	expression tag	UNP P0AG01
H	1	HIS	-	expression tag	UNP P0AG01
H	2	HIS	-	expression tag	UNP P0AG01
I	-6	MET	-	initiating methionine	UNP P0AG01
I	-5	GLY	-	expression tag	UNP P0AG01
I	-4	SER	-	expression tag	UNP P0AG01
I	-3	HIS	-	expression tag	UNP P0AG01
I	-2	HIS	-	expression tag	UNP P0AG01
I	-1	HIS	-	expression tag	UNP P0AG01
I	0	HIS	-	expression tag	UNP P0AG01
I	1	HIS	-	expression tag	UNP P0AG01
I	2	HIS	-	expression tag	UNP P0AG01
J	-6	MET	-	initiating methionine	UNP P0AG01
J	-5	GLY	-	expression tag	UNP P0AG01
J	-4	SER	-	expression tag	UNP P0AG01
J	-3	HIS	-	expression tag	UNP P0AG01
J	-2	HIS	-	expression tag	UNP P0AG01
J	-1	HIS	-	expression tag	UNP P0AG01
J	0	HIS	-	expression tag	UNP P0AG01
J	1	HIS	-	expression tag	UNP P0AG01
J	2	HIS	-	expression tag	UNP P0AG01
K	-6	MET	-	initiating methionine	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	GLY	-	expression tag	UNP P0AG01
K	-4	SER	-	expression tag	UNP P0AG01
K	-3	HIS	-	expression tag	UNP P0AG01
K	-2	HIS	-	expression tag	UNP P0AG01
K	-1	HIS	-	expression tag	UNP P0AG01
K	0	HIS	-	expression tag	UNP P0AG01
K	1	HIS	-	expression tag	UNP P0AG01
K	2	HIS	-	expression tag	UNP P0AG01
L	-6	MET	-	initiating methionine	UNP P0AG01
L	-5	GLY	-	expression tag	UNP P0AG01
L	-4	SER	-	expression tag	UNP P0AG01
L	-3	HIS	-	expression tag	UNP P0AG01
L	-2	HIS	-	expression tag	UNP P0AG01
L	-1	HIS	-	expression tag	UNP P0AG01
L	0	HIS	-	expression tag	UNP P0AG01
L	1	HIS	-	expression tag	UNP P0AG01
L	2	HIS	-	expression tag	UNP P0AG01
M	-6	MET	-	initiating methionine	UNP P0AG01
M	-5	GLY	-	expression tag	UNP P0AG01
M	-4	SER	-	expression tag	UNP P0AG01
M	-3	HIS	-	expression tag	UNP P0AG01
M	-2	HIS	-	expression tag	UNP P0AG01
M	-1	HIS	-	expression tag	UNP P0AG01
M	0	HIS	-	expression tag	UNP P0AG01
M	1	HIS	-	expression tag	UNP P0AG01
M	2	HIS	-	expression tag	UNP P0AG01
N	-6	MET	-	initiating methionine	UNP P0AG01
N	-5	GLY	-	expression tag	UNP P0AG01
N	-4	SER	-	expression tag	UNP P0AG01
N	-3	HIS	-	expression tag	UNP P0AG01
N	-2	HIS	-	expression tag	UNP P0AG01
N	-1	HIS	-	expression tag	UNP P0AG01
N	0	HIS	-	expression tag	UNP P0AG01
N	1	HIS	-	expression tag	UNP P0AG01
N	2	HIS	-	expression tag	UNP P0AG01
O	-6	MET	-	initiating methionine	UNP P0AG01
O	-5	GLY	-	expression tag	UNP P0AG01
O	-4	SER	-	expression tag	UNP P0AG01
O	-3	HIS	-	expression tag	UNP P0AG01
O	-2	HIS	-	expression tag	UNP P0AG01
O	-1	HIS	-	expression tag	UNP P0AG01
O	0	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
O	1	HIS	-	expression tag	UNP P0AG01
O	2	HIS	-	expression tag	UNP P0AG01
P	-6	MET	-	initiating methionine	UNP P0AG01
P	-5	GLY	-	expression tag	UNP P0AG01
P	-4	SER	-	expression tag	UNP P0AG01
P	-3	HIS	-	expression tag	UNP P0AG01
P	-2	HIS	-	expression tag	UNP P0AG01
P	-1	HIS	-	expression tag	UNP P0AG01
P	0	HIS	-	expression tag	UNP P0AG01
P	1	HIS	-	expression tag	UNP P0AG01
P	2	HIS	-	expression tag	UNP P0AG01
Q	-6	MET	-	initiating methionine	UNP P0AG01
Q	-5	GLY	-	expression tag	UNP P0AG01
Q	-4	SER	-	expression tag	UNP P0AG01
Q	-3	HIS	-	expression tag	UNP P0AG01
Q	-2	HIS	-	expression tag	UNP P0AG01
Q	-1	HIS	-	expression tag	UNP P0AG01
Q	0	HIS	-	expression tag	UNP P0AG01
Q	1	HIS	-	expression tag	UNP P0AG01
Q	2	HIS	-	expression tag	UNP P0AG01
R	-6	MET	-	initiating methionine	UNP P0AG01
R	-5	GLY	-	expression tag	UNP P0AG01
R	-4	SER	-	expression tag	UNP P0AG01
R	-3	HIS	-	expression tag	UNP P0AG01
R	-2	HIS	-	expression tag	UNP P0AG01
R	-1	HIS	-	expression tag	UNP P0AG01
R	0	HIS	-	expression tag	UNP P0AG01
R	1	HIS	-	expression tag	UNP P0AG01
R	2	HIS	-	expression tag	UNP P0AG01
S	-6	MET	-	initiating methionine	UNP P0AG01
S	-5	GLY	-	expression tag	UNP P0AG01
S	-4	SER	-	expression tag	UNP P0AG01
S	-3	HIS	-	expression tag	UNP P0AG01
S	-2	HIS	-	expression tag	UNP P0AG01
S	-1	HIS	-	expression tag	UNP P0AG01
S	0	HIS	-	expression tag	UNP P0AG01
S	1	HIS	-	expression tag	UNP P0AG01
S	2	HIS	-	expression tag	UNP P0AG01
T	-6	MET	-	initiating methionine	UNP P0AG01
T	-5	GLY	-	expression tag	UNP P0AG01
T	-4	SER	-	expression tag	UNP P0AG01
T	-3	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-2	HIS	-	expression tag	UNP P0AG01
T	-1	HIS	-	expression tag	UNP P0AG01
T	0	HIS	-	expression tag	UNP P0AG01
T	1	HIS	-	expression tag	UNP P0AG01
T	2	HIS	-	expression tag	UNP P0AG01
U	-6	MET	-	initiating methionine	UNP P0AG01
U	-5	GLY	-	expression tag	UNP P0AG01
U	-4	SER	-	expression tag	UNP P0AG01
U	-3	HIS	-	expression tag	UNP P0AG01
U	-2	HIS	-	expression tag	UNP P0AG01
U	-1	HIS	-	expression tag	UNP P0AG01
U	0	HIS	-	expression tag	UNP P0AG01
U	1	HIS	-	expression tag	UNP P0AG01
U	2	HIS	-	expression tag	UNP P0AG01
V	-6	MET	-	initiating methionine	UNP P0AG01
V	-5	GLY	-	expression tag	UNP P0AG01
V	-4	SER	-	expression tag	UNP P0AG01
V	-3	HIS	-	expression tag	UNP P0AG01
V	-2	HIS	-	expression tag	UNP P0AG01
V	-1	HIS	-	expression tag	UNP P0AG01
V	0	HIS	-	expression tag	UNP P0AG01
V	1	HIS	-	expression tag	UNP P0AG01
V	2	HIS	-	expression tag	UNP P0AG01
W	-6	MET	-	initiating methionine	UNP P0AG01
W	-5	GLY	-	expression tag	UNP P0AG01
W	-4	SER	-	expression tag	UNP P0AG01
W	-3	HIS	-	expression tag	UNP P0AG01
W	-2	HIS	-	expression tag	UNP P0AG01
W	-1	HIS	-	expression tag	UNP P0AG01
W	0	HIS	-	expression tag	UNP P0AG01
W	1	HIS	-	expression tag	UNP P0AG01
W	2	HIS	-	expression tag	UNP P0AG01
X	-6	MET	-	initiating methionine	UNP P0AG01
X	-5	GLY	-	expression tag	UNP P0AG01
X	-4	SER	-	expression tag	UNP P0AG01
X	-3	HIS	-	expression tag	UNP P0AG01
X	-2	HIS	-	expression tag	UNP P0AG01
X	-1	HIS	-	expression tag	UNP P0AG01
X	0	HIS	-	expression tag	UNP P0AG01
X	1	HIS	-	expression tag	UNP P0AG01
X	2	HIS	-	expression tag	UNP P0AG01
Y	-6	MET	-	initiating methionine	UNP P0AG01

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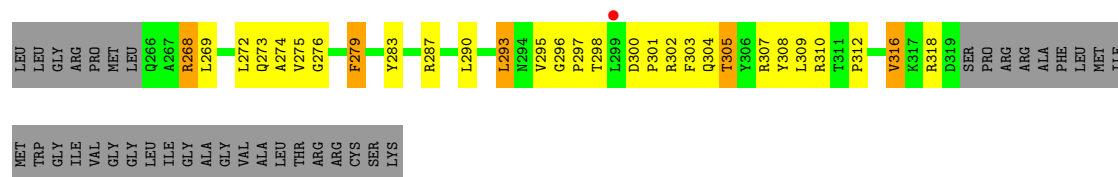
Chain	Residue	Modelled	Actual	Comment	Reference
Y	-5	GLY	-	expression tag	UNP P0AG01
Y	-4	SER	-	expression tag	UNP P0AG01
Y	-3	HIS	-	expression tag	UNP P0AG01
Y	-2	HIS	-	expression tag	UNP P0AG01
Y	-1	HIS	-	expression tag	UNP P0AG01
Y	0	HIS	-	expression tag	UNP P0AG01
Y	1	HIS	-	expression tag	UNP P0AG01
Y	2	HIS	-	expression tag	UNP P0AG01
Z	-6	MET	-	initiating methionine	UNP P0AG01
Z	-5	GLY	-	expression tag	UNP P0AG01
Z	-4	SER	-	expression tag	UNP P0AG01
Z	-3	HIS	-	expression tag	UNP P0AG01
Z	-2	HIS	-	expression tag	UNP P0AG01
Z	-1	HIS	-	expression tag	UNP P0AG01
Z	0	HIS	-	expression tag	UNP P0AG01
Z	1	HIS	-	expression tag	UNP P0AG01
Z	2	HIS	-	expression tag	UNP P0AG01
a	-6	MET	-	initiating methionine	UNP P0AG01
a	-5	GLY	-	expression tag	UNP P0AG01
a	-4	SER	-	expression tag	UNP P0AG01
a	-3	HIS	-	expression tag	UNP P0AG01
a	-2	HIS	-	expression tag	UNP P0AG01
a	-1	HIS	-	expression tag	UNP P0AG01
a	0	HIS	-	expression tag	UNP P0AG01
a	1	HIS	-	expression tag	UNP P0AG01
a	2	HIS	-	expression tag	UNP P0AG01
b	-6	MET	-	initiating methionine	UNP P0AG01
b	-5	GLY	-	expression tag	UNP P0AG01
b	-4	SER	-	expression tag	UNP P0AG01
b	-3	HIS	-	expression tag	UNP P0AG01
b	-2	HIS	-	expression tag	UNP P0AG01
b	-1	HIS	-	expression tag	UNP P0AG01
b	0	HIS	-	expression tag	UNP P0AG01
b	1	HIS	-	expression tag	UNP P0AG01
b	2	HIS	-	expression tag	UNP P0AG01
c	-6	MET	-	initiating methionine	UNP P0AG01
c	-5	GLY	-	expression tag	UNP P0AG01
c	-4	SER	-	expression tag	UNP P0AG01
c	-3	HIS	-	expression tag	UNP P0AG01
c	-2	HIS	-	expression tag	UNP P0AG01
c	-1	HIS	-	expression tag	UNP P0AG01
c	0	HIS	-	expression tag	UNP P0AG01

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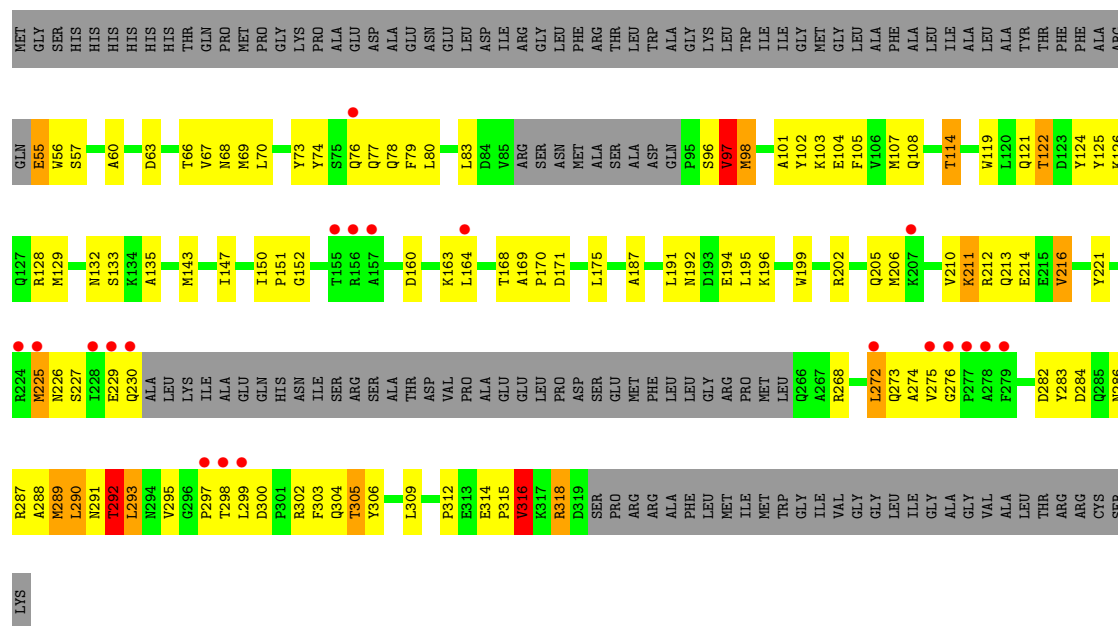
Chain	Residue	Modelled	Actual	Comment	Reference
c	1	HIS	-	expression tag	UNP P0AG01
c	2	HIS	-	expression tag	UNP P0AG01
d	-6	MET	-	initiating methionine	UNP P0AG01
d	-5	GLY	-	expression tag	UNP P0AG01
d	-4	SER	-	expression tag	UNP P0AG01
d	-3	HIS	-	expression tag	UNP P0AG01
d	-2	HIS	-	expression tag	UNP P0AG01
d	-1	HIS	-	expression tag	UNP P0AG01
d	0	HIS	-	expression tag	UNP P0AG01
d	1	HIS	-	expression tag	UNP P0AG01
d	2	HIS	-	expression tag	UNP P0AG01
e	-6	MET	-	initiating methionine	UNP P0AG01
e	-5	GLY	-	expression tag	UNP P0AG01
e	-4	SER	-	expression tag	UNP P0AG01
e	-3	HIS	-	expression tag	UNP P0AG01
e	-2	HIS	-	expression tag	UNP P0AG01
e	-1	HIS	-	expression tag	UNP P0AG01
e	0	HIS	-	expression tag	UNP P0AG01
e	1	HIS	-	expression tag	UNP P0AG01
e	2	HIS	-	expression tag	UNP P0AG01
f	-6	MET	-	initiating methionine	UNP P0AG01
f	-5	GLY	-	expression tag	UNP P0AG01
f	-4	SER	-	expression tag	UNP P0AG01
f	-3	HIS	-	expression tag	UNP P0AG01
f	-2	HIS	-	expression tag	UNP P0AG01
f	-1	HIS	-	expression tag	UNP P0AG01
f	0	HIS	-	expression tag	UNP P0AG01
f	1	HIS	-	expression tag	UNP P0AG01
f	2	HIS	-	expression tag	UNP P0AG01





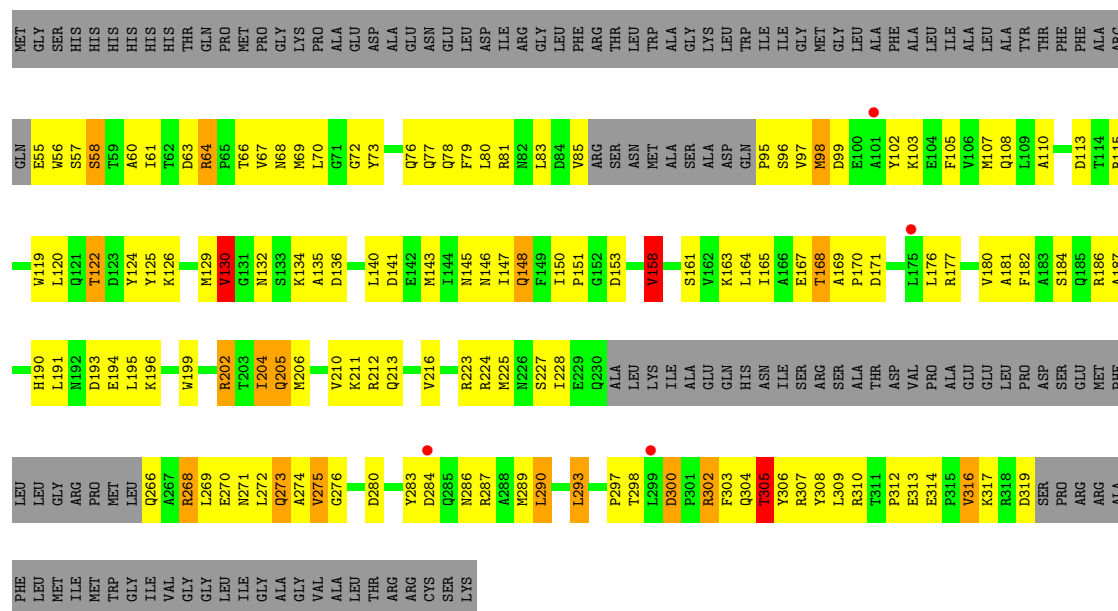
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain C:



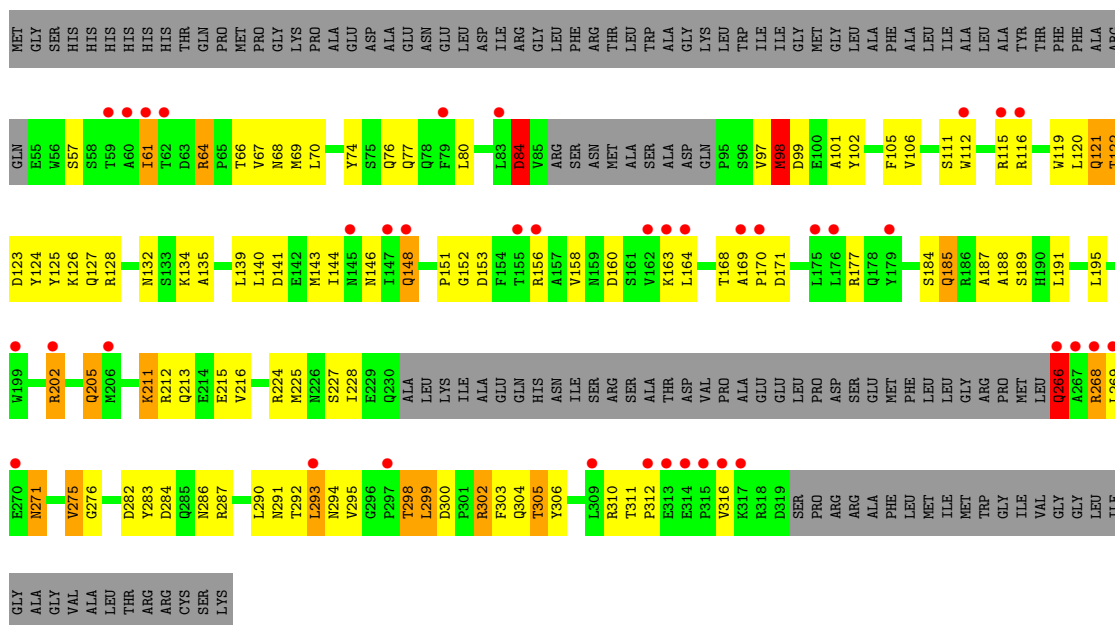
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain D:



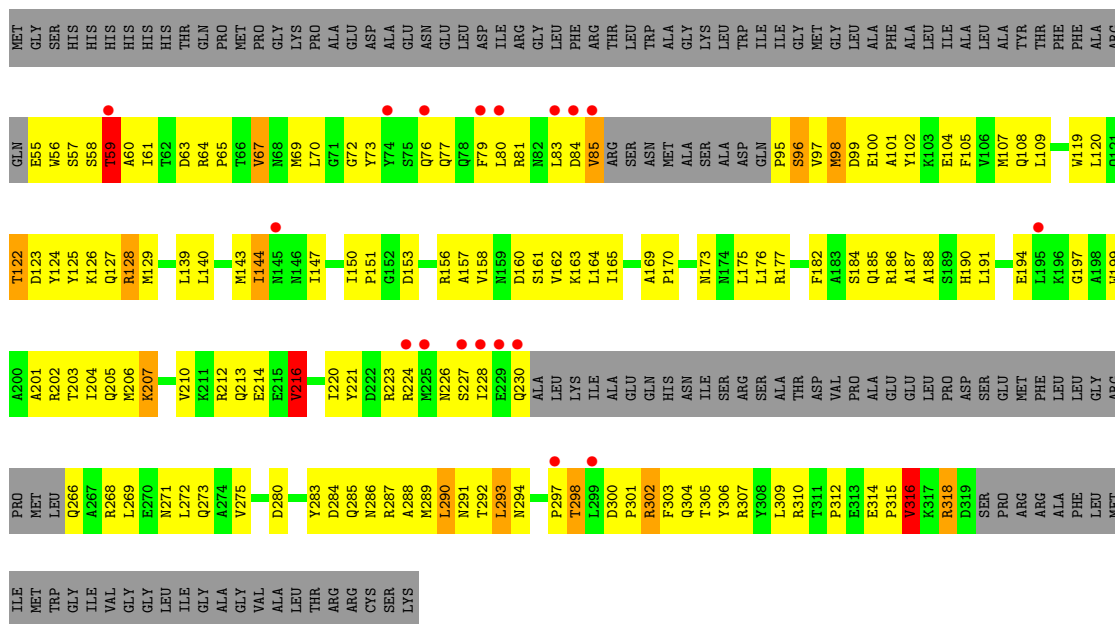
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain E:



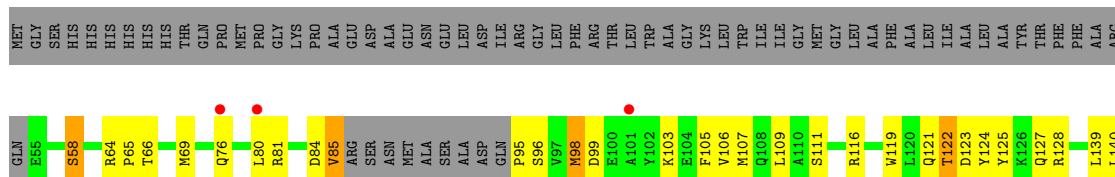
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

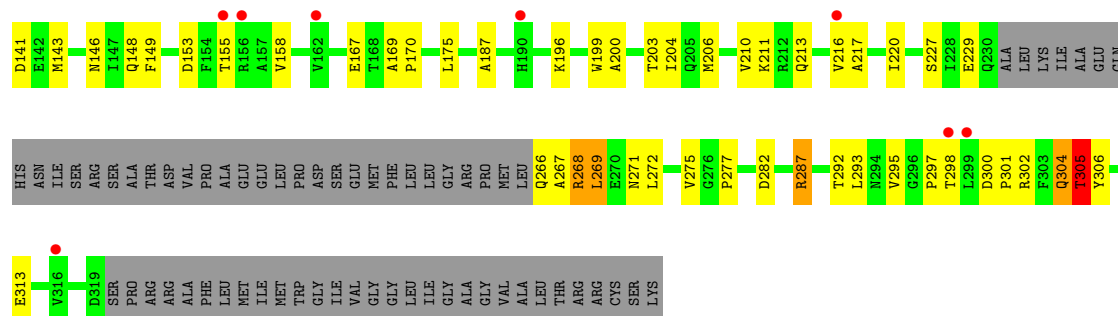
Chain F:



- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

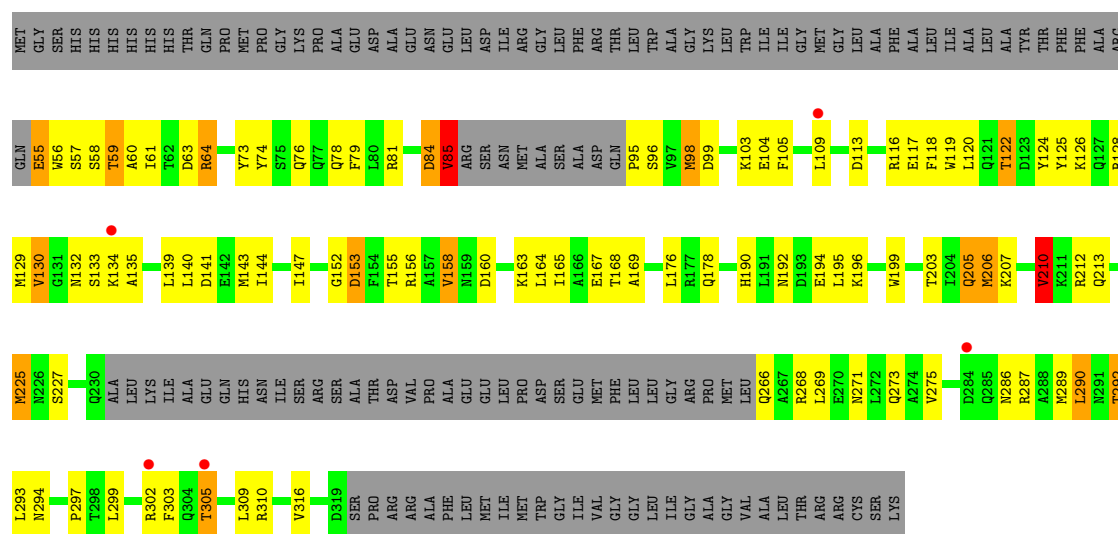
## Chain G:





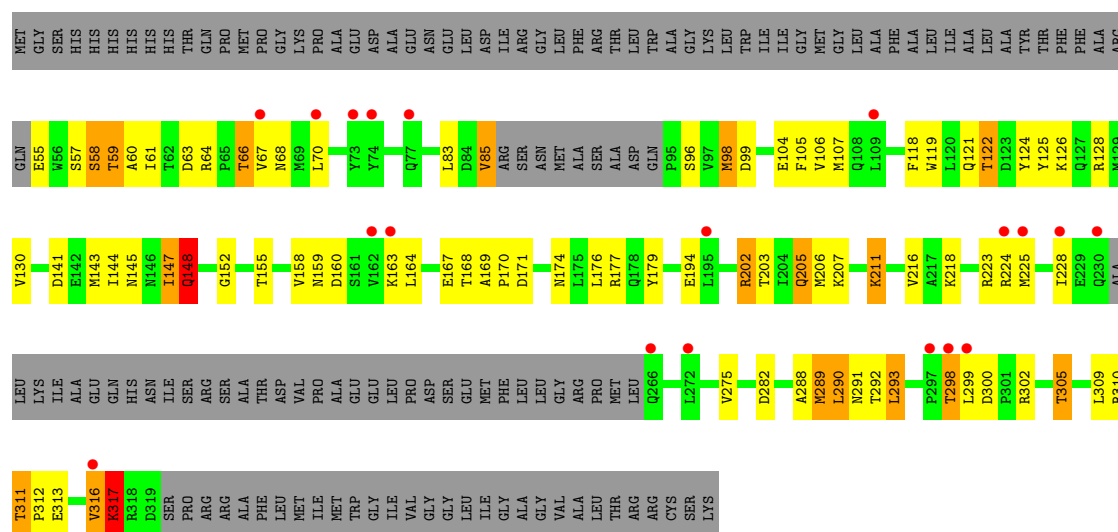
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain H:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

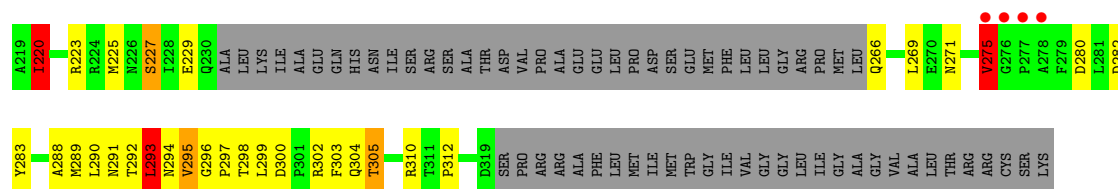
Chain I:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

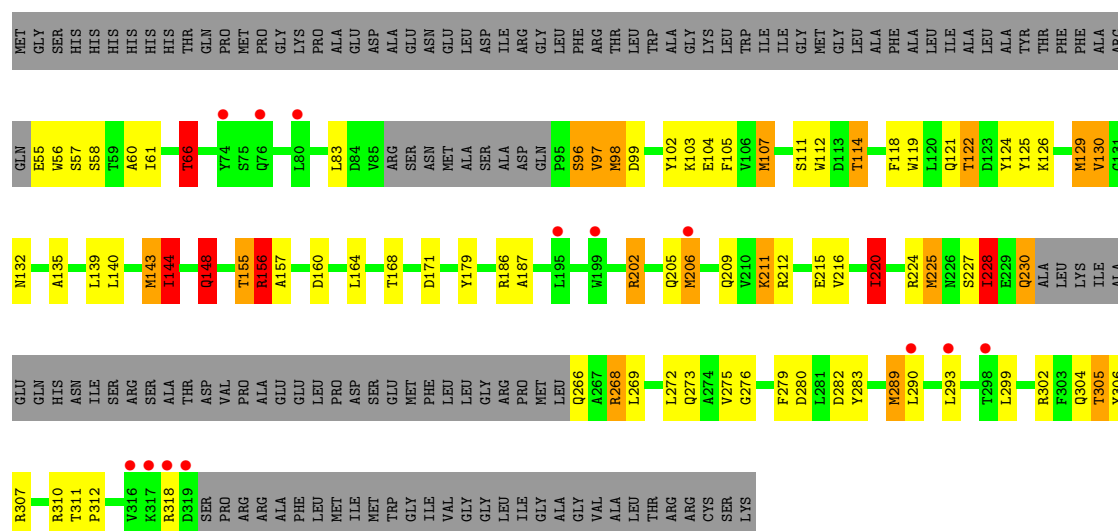






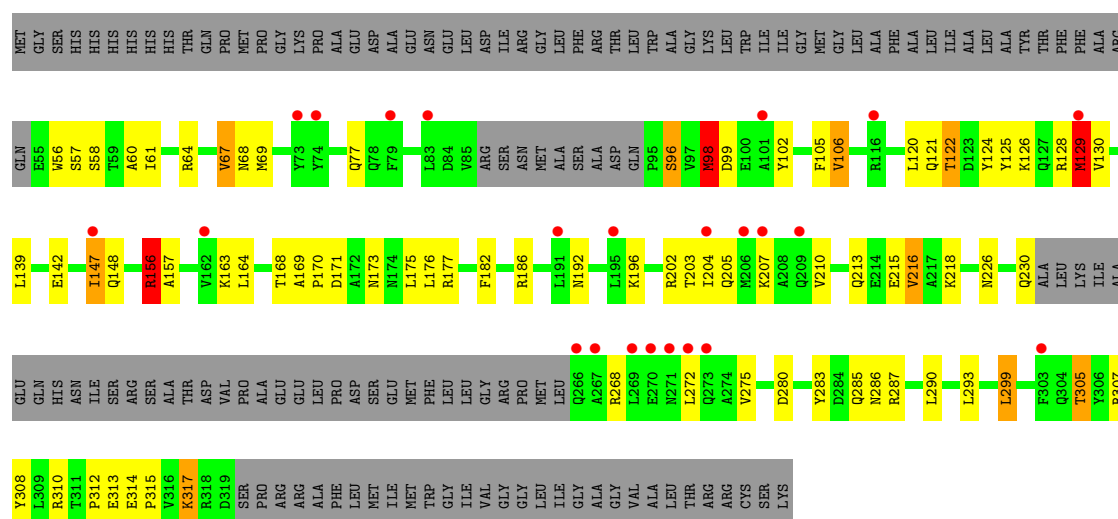
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain M:



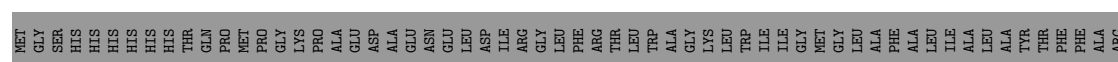
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

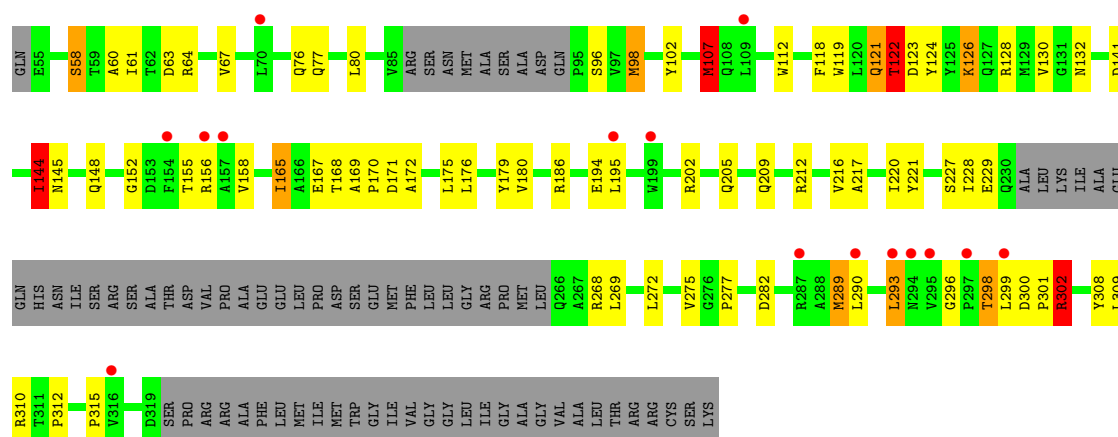
Chain N:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

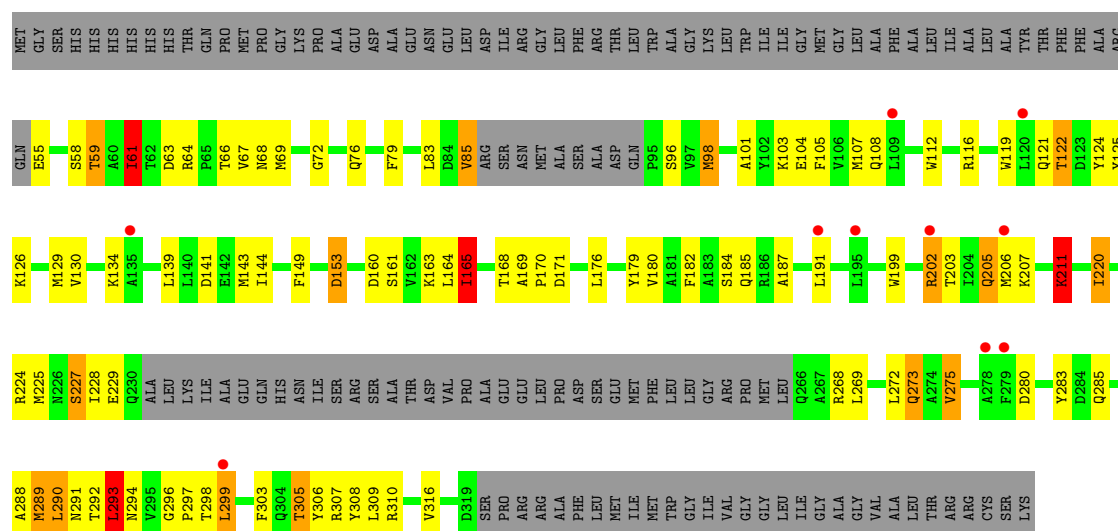
Chain O:





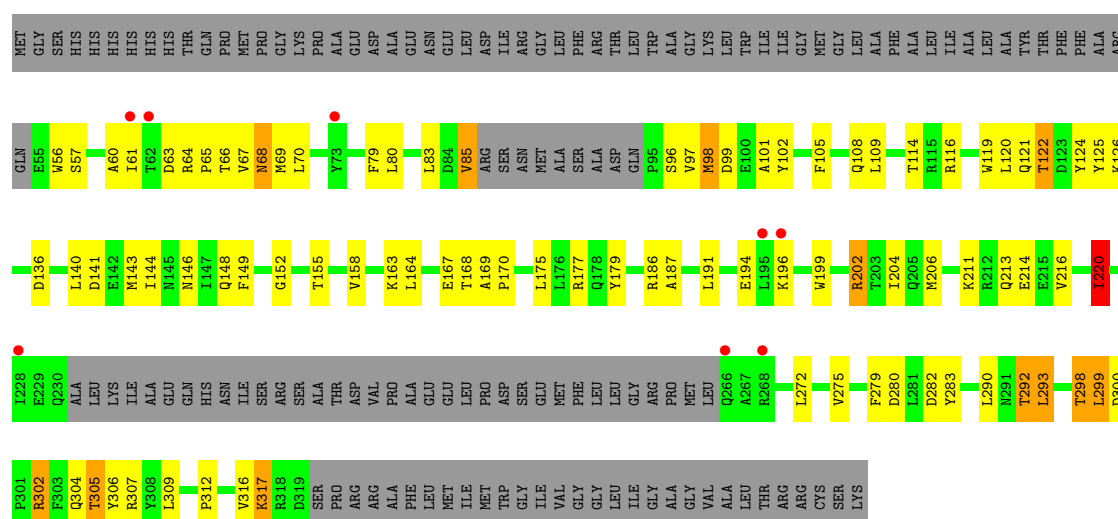
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain P:

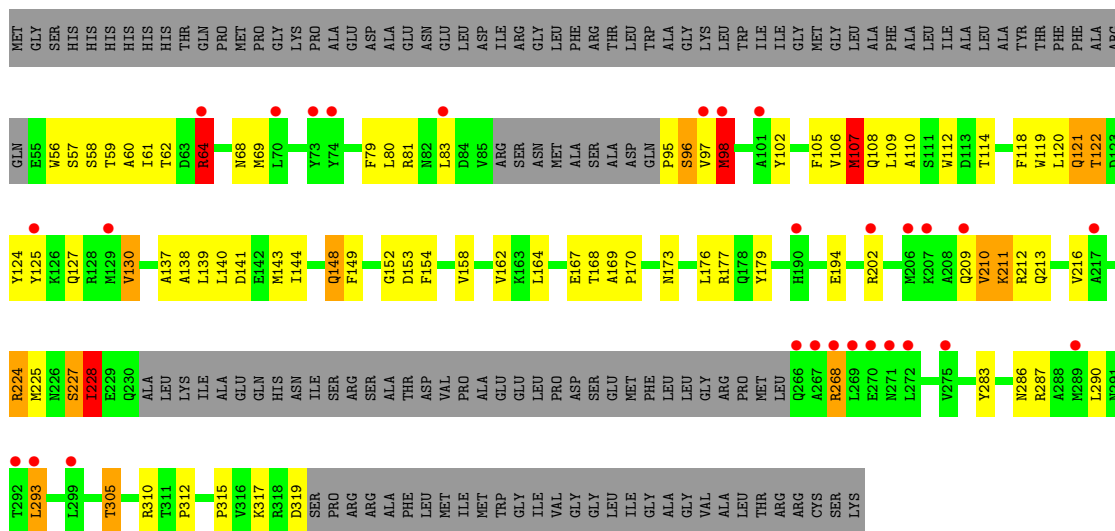


- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

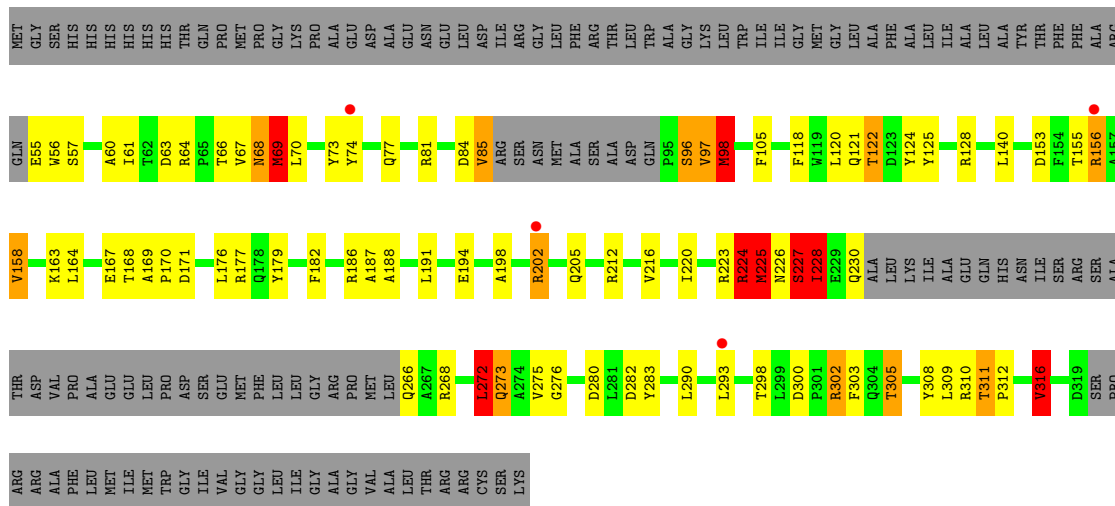
Chain Q:



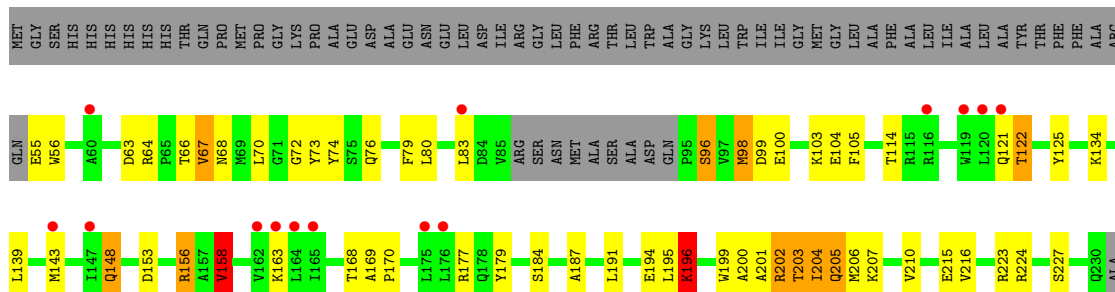
Chain R: 

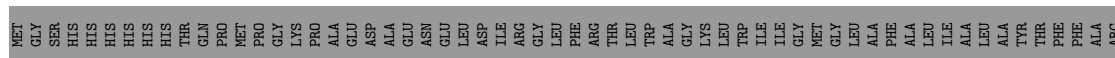


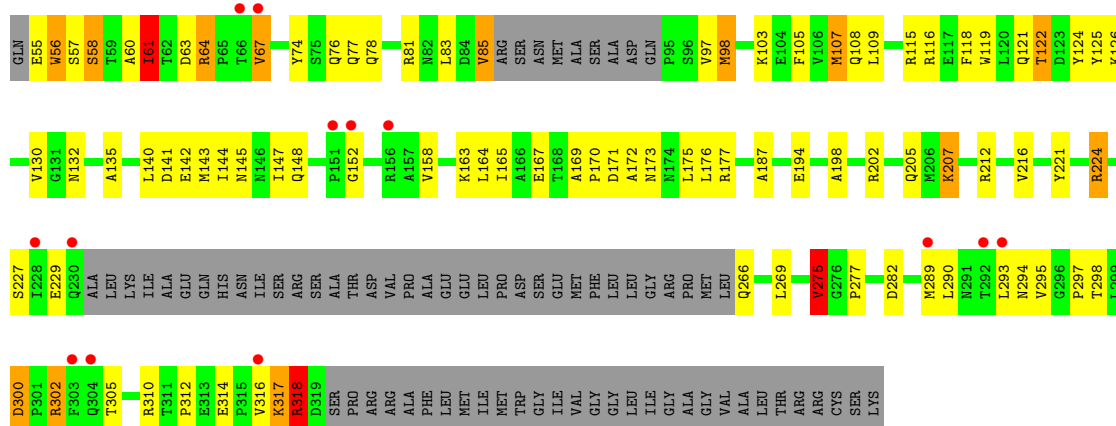
Chain S: 



Chain T: 

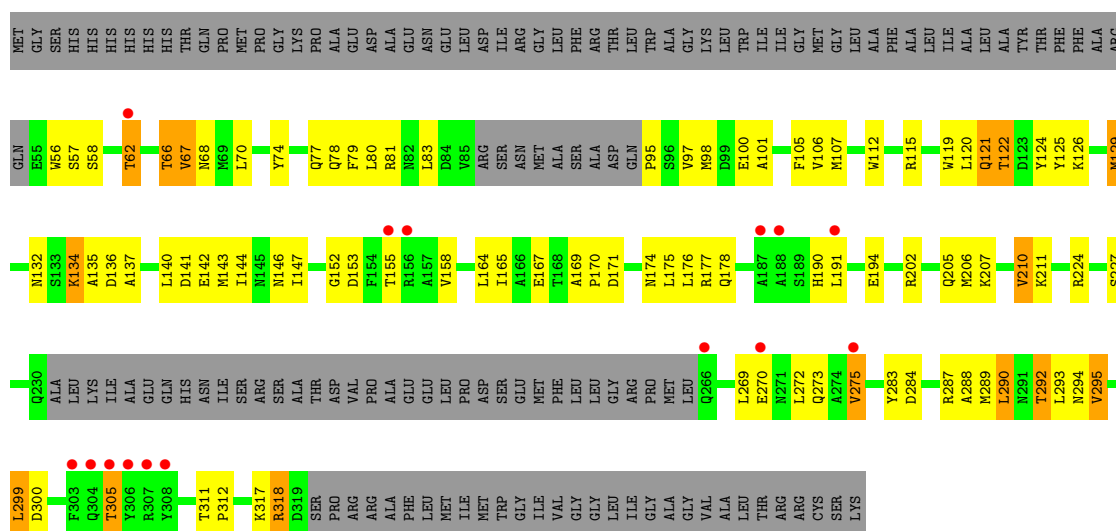






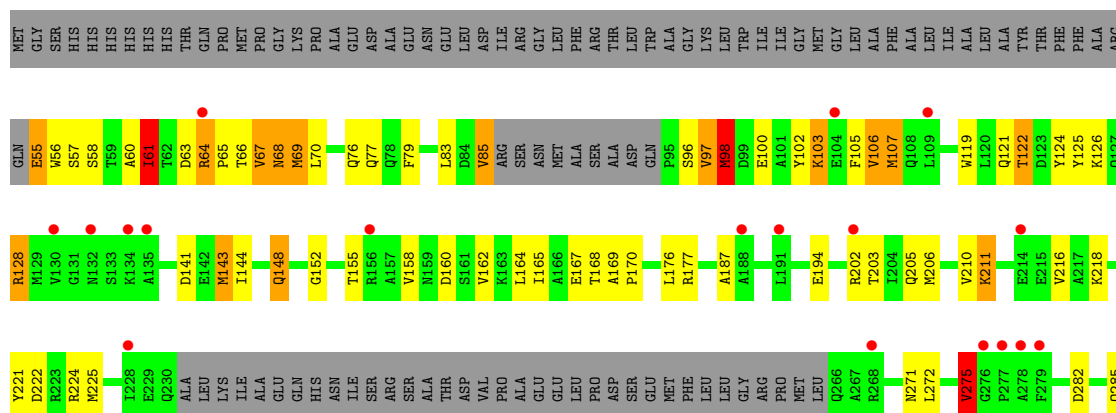
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain X:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

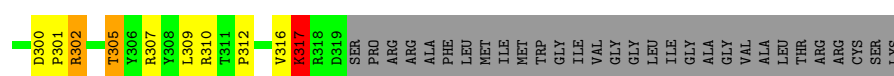
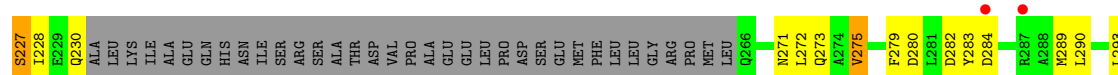
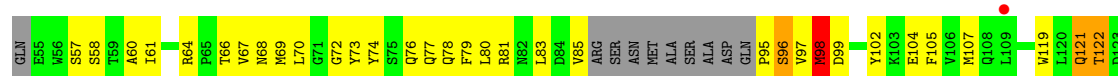
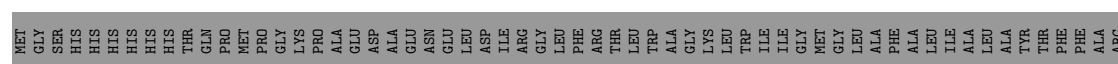
Chain Y:





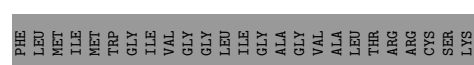
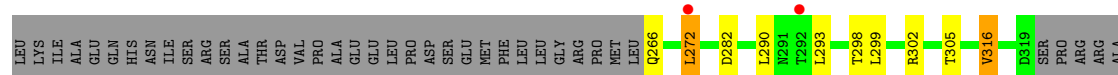
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain Z:



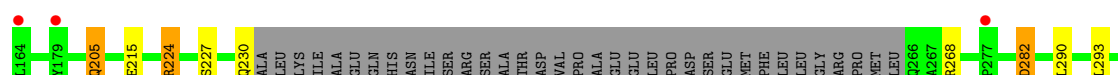
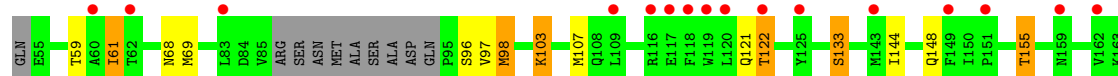
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

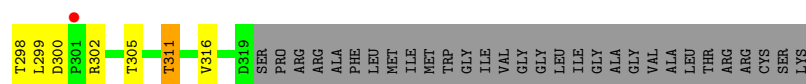
Chain a:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

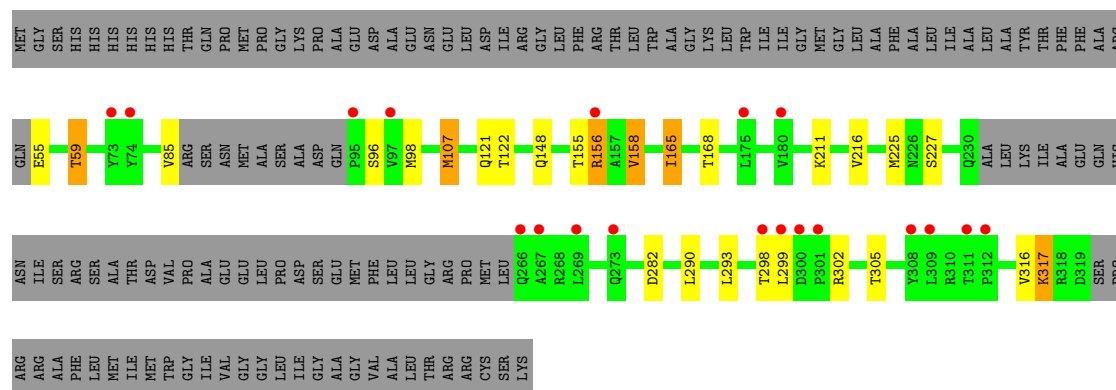
Chain b:





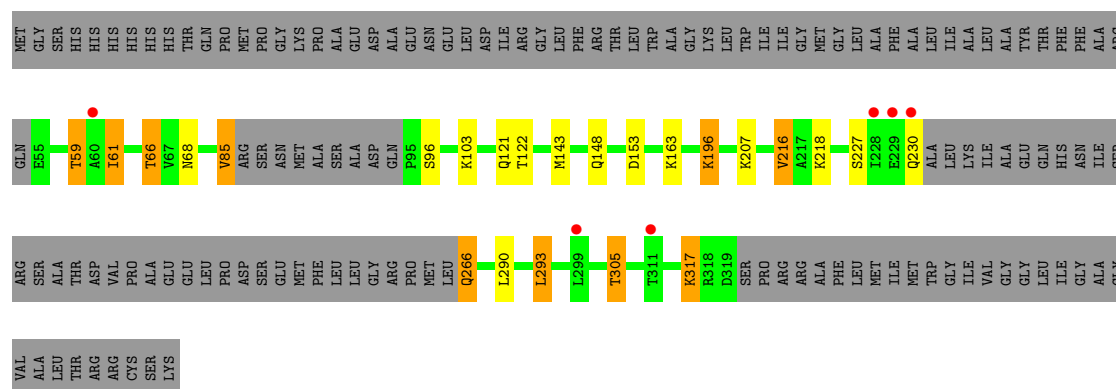
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain c:



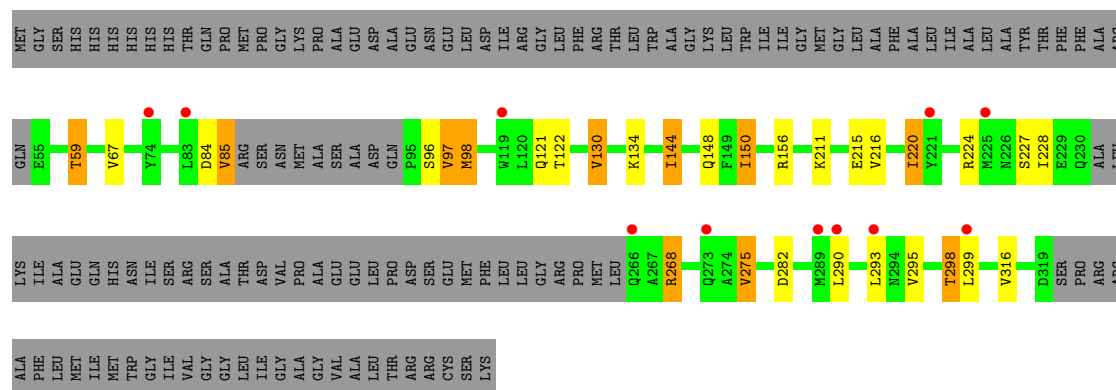
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain d:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

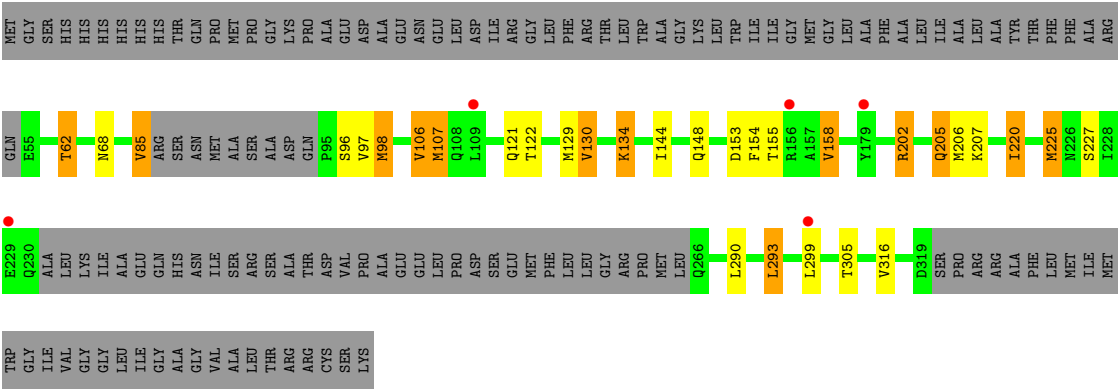
Chain e:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE



Chain f: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	276.85Å 246.31Å 133.20Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	47.81 – 5.99 47.81 – 5.99	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.81-5.99) 96.3 (47.81-5.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 6.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.234 , 0.245 0.236 , 0.248	Depositor DCC
$R_{free}$ test set	2169 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	234.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 134.2	EDS
Estimated twinning fraction	0.340 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 43381 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	57504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.52	1/1830 (0.1%)	1.17	9/2475 (0.4%)
1	B	0.56	0/1830	1.05	14/2475 (0.6%)
1	C	0.51	1/1830 (0.1%)	0.98	8/2475 (0.3%)
1	D	0.53	0/1830	1.01	10/2475 (0.4%)
1	E	0.57	0/1830	1.04	15/2475 (0.6%)
1	F	0.52	0/1830	1.01	11/2475 (0.4%)
1	G	0.46	0/1830	1.05	13/2475 (0.5%)
1	H	0.46	0/1830	0.93	8/2475 (0.3%)
1	I	0.48	0/1830	1.01	21/2475 (0.8%)
1	J	0.51	0/1830	1.10	16/2475 (0.6%)
1	K	0.51	1/1830 (0.1%)	1.02	13/2475 (0.5%)
1	L	0.53	0/1830	1.10	18/2475 (0.7%)
1	M	0.55	0/1830	1.14	20/2475 (0.8%)
1	N	0.57	0/1830	1.30	17/2475 (0.7%)
1	O	0.55	0/1830	1.02	12/2475 (0.5%)
1	P	0.59	1/1830 (0.1%)	1.21	20/2475 (0.8%)
1	Q	0.50	0/1830	1.02	13/2475 (0.5%)
1	R	0.60	1/1830 (0.1%)	1.22	23/2475 (0.9%)
1	S	0.54	1/1830 (0.1%)	1.12	21/2475 (0.8%)
1	T	0.61	2/1830 (0.1%)	1.21	19/2475 (0.8%)
1	U	0.57	1/1830 (0.1%)	1.16	12/2475 (0.5%)
1	V	0.52	0/1830	1.10	13/2475 (0.5%)
1	W	0.56	1/1830 (0.1%)	1.19	19/2475 (0.8%)
1	X	0.59	1/1830 (0.1%)	1.13	15/2475 (0.6%)
1	Y	0.61	1/1830 (0.1%)	1.33	22/2475 (0.9%)
1	Z	0.53	0/1830	1.10	21/2475 (0.8%)
1	a	0.59	1/1830 (0.1%)	1.18	19/2475 (0.8%)
1	b	0.61	1/1830 (0.1%)	1.19	22/2475 (0.9%)
1	c	0.51	0/1830	1.11	21/2475 (0.8%)
1	d	0.52	1/1830 (0.1%)	1.18	22/2475 (0.9%)
1	e	0.54	0/1830	1.19	26/2475 (1.1%)
1	f	0.57	0/1830	1.19	26/2475 (1.1%)
All	All	0.55	15/58560 (0.0%)	1.12	539/79200 (0.7%)

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	3	1
1	B	1	1
1	F	2	0
1	I	1	1
1	J	1	1
1	L	1	0
1	M	3	1
1	N	1	0
1	O	1	0
1	P	1	0
1	Q	3	0
1	R	2	0
1	S	0	1
1	T	0	1
1	U	1	0
1	V	0	1
1	W	1	1
1	X	1	1
1	Y	1	0
1	a	2	2
1	b	1	0
1	c	1	0
1	d	2	0
1	e	3	1
All	All	33	13

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	163	LYS	CD-CE	8.53	1.72	1.51
1	X	66	THR	CB-CG2	-7.76	1.26	1.52
1	b	59	THR	CB-CG2	-7.76	1.26	1.52
1	R	59	THR	CB-CG2	-6.83	1.29	1.52
1	d	305	THR	CB-CG2	-6.58	1.30	1.52
1	U	207	LYS	CD-CE	6.54	1.67	1.51
1	Y	128	ARG	CG-CD	6.19	1.67	1.51
1	A	59	THR	CB-CG2	-6.00	1.32	1.52
1	K	218	LYS	CG-CD	5.93	1.72	1.52
1	S	316	VAL	CB-CG1	-5.82	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	85	VAL	CB-CG1	5.76	1.65	1.52
1	T	163	LYS	CG-CD	5.76	1.72	1.52
1	a	218	LYS	CD-CE	5.76	1.65	1.51
1	C	103	LYS	CD-CE	5.63	1.65	1.51
1	W	56	TRP	CB-CG	-5.33	1.40	1.50

All (539) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	61	ILE	CG1-CB-CG2	-22.93	60.96	111.40
1	A	67	VAL	CG1-CB-CG2	-22.35	75.14	110.90
1	N	67	VAL	CG1-CB-CG2	-21.79	76.04	110.90
1	U	275	VAL	CG1-CB-CG2	-20.75	77.69	110.90
1	Y	128	ARG	NE-CZ-NH1	-20.73	109.94	120.30
1	T	275	VAL	CG1-CB-CG2	-20.46	78.17	110.90
1	N	216	VAL	CG1-CB-CG2	-20.27	78.47	110.90
1	Y	210	VAL	CG1-CB-CG2	-19.88	79.09	110.90
1	a	210	VAL	CG1-CB-CG2	-19.15	80.27	110.90
1	V	106	VAL	CG1-CB-CG2	-18.75	80.91	110.90
1	A	106	VAL	CG1-CB-CG2	-18.39	81.47	110.90
1	P	165	ILE	CG1-CB-CG2	-18.25	71.26	111.40
1	C	97	VAL	CG1-CB-CG2	-18.01	82.09	110.90
1	U	97	VAL	CG1-CB-CG2	-17.69	82.60	110.90
1	Y	295	VAL	CG1-CB-CG2	-17.43	83.01	110.90
1	R	97	VAL	CG1-CB-CG2	-17.13	83.49	110.90
1	Q	97	VAL	CG1-CB-CG2	-16.93	83.82	110.90
1	F	216	VAL	CG1-CB-CG2	-16.50	84.50	110.90
1	A	216	VAL	CG1-CB-CG2	-16.37	84.71	110.90
1	G	106	VAL	CG1-CB-CG2	-16.13	85.10	110.90
1	J	316	VAL	CG1-CB-CG2	-15.95	85.38	110.90
1	H	158	VAL	CG1-CB-CG2	-15.76	85.68	110.90
1	e	316	VAL	CG1-CB-CG2	-15.75	85.70	110.90
1	T	216	VAL	CG1-CB-CG2	-15.70	85.79	110.90
1	e	216	VAL	CG1-CB-CG2	-15.38	86.29	110.90
1	N	130	VAL	CG1-CB-CG2	-15.21	86.57	110.90
1	Y	275	VAL	CG1-CB-CG2	-15.19	86.60	110.90
1	b	97	VAL	CG1-CB-CG2	-14.98	86.92	110.90
1	A	150	ILE	CG1-CB-CG2	-14.94	78.53	111.40
1	W	61	ILE	CG1-CB-CG2	-14.94	78.53	111.40
1	Z	150	ILE	CG1-CB-CG2	-14.89	78.65	111.40
1	R	216	VAL	CG1-CB-CG2	-14.72	87.34	110.90
1	D	275	VAL	CG1-CB-CG2	-14.70	87.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	295	VAL	CG1-CB-CG2	-14.36	87.92	110.90
1	b	61	ILE	CG1-CB-CG2	-14.36	79.82	111.40
1	P	316	VAL	CG1-CB-CG2	-14.15	88.26	110.90
1	X	106	VAL	CG1-CB-CG2	-13.93	88.61	110.90
1	P	61	ILE	CG1-CB-CG2	-13.88	80.86	111.40
1	B	85	VAL	CG1-CB-CG2	-13.82	88.78	110.90
1	D	158	VAL	CG1-CB-CG2	-13.58	89.17	110.90
1	Y	67	VAL	CG1-CB-CG2	-13.57	89.18	110.90
1	G	220	ILE	CG1-CB-CG2	-13.30	82.14	111.40
1	T	210	VAL	CG1-CB-CG2	-13.22	89.75	110.90
1	M	156	ARG	CA-CB-CG	13.11	142.25	113.40
1	X	210	VAL	CG1-CB-CG2	-12.92	90.23	110.90
1	W	224	ARG	NE-CZ-NH2	-12.85	113.87	120.30
1	a	272	LEU	CA-CB-CG	12.82	144.78	115.30
1	f	158	VAL	CG1-CB-CG2	-12.61	90.72	110.90
1	E	61	ILE	CG1-CB-CG2	-12.49	83.92	111.40
1	G	305	THR	OG1-CB-CG2	-12.44	81.39	110.00
1	c	158	VAL	CG1-CB-CG2	-12.37	91.11	110.90
1	F	144	ILE	CG1-CB-CG2	-12.33	84.28	111.40
1	V	220	ILE	CG1-CB-CG2	-12.31	84.32	111.40
1	H	130	VAL	CG1-CB-CG2	-12.12	91.50	110.90
1	I	317	LYS	CB-CA-C	-11.99	86.41	110.40
1	S	228	ILE	CG1-CB-CG2	-11.95	85.12	111.40
1	f	97	VAL	CG1-CB-CG2	-11.89	91.88	110.90
1	I	311	THR	OG1-CB-CG2	-11.84	82.77	110.00
1	W	224	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	K	85	VAL	CG1-CB-CG2	-11.66	92.25	110.90
1	N	129	MET	CA-CB-CG	11.66	133.12	113.30
1	S	224	ARG	NE-CZ-NH1	11.63	126.12	120.30
1	B	67	VAL	CG1-CB-CG2	-11.55	92.41	110.90
1	R	130	VAL	CG1-CB-CG2	-11.44	92.60	110.90
1	B	61	ILE	CG1-CB-CG2	-11.41	86.29	111.40
1	B	122	THR	OG1-CB-CG2	-11.30	84.01	110.00
1	C	316	VAL	CG1-CB-CG2	-11.26	92.88	110.90
1	E	298	THR	OG1-CB-CG2	-11.26	84.10	110.00
1	b	316	VAL	CG1-CB-CG2	-11.23	92.93	110.90
1	C	114	THR	OG1-CB-CG2	-11.16	84.34	110.00
1	c	216	VAL	CG1-CB-CG2	-11.15	93.06	110.90
1	A	147	ILE	CG1-CB-CG2	-11.05	87.08	111.40
1	J	205	GLN	CA-CB-CG	11.01	137.61	113.40
1	e	228	ILE	CG1-CB-CG2	-10.89	87.45	111.40
1	c	225	MET	CG-SD-CE	-10.79	82.94	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	122	THR	OG1-CB-CG2	-10.76	85.26	110.00
1	Y	128	ARG	NE-CZ-NH2	10.75	125.68	120.30
1	f	316	VAL	CG1-CB-CG2	-10.63	93.88	110.90
1	c	316	VAL	CG1-CB-CG2	-10.55	94.03	110.90
1	D	204	ILE	CG1-CB-CG2	-10.51	88.28	111.40
1	J	216	VAL	CG1-CB-CG2	-10.41	94.24	110.90
1	Y	97	VAL	CG1-CB-CG2	-10.39	94.28	110.90
1	A	98	MET	CA-CB-CG	10.34	130.88	113.30
1	c	156	ARG	CA-CB-CG	10.30	136.06	113.40
1	I	66	THR	OG1-CB-CG2	-10.13	86.71	110.00
1	Y	107	MET	CA-CB-CG	10.12	130.50	113.30
1	U	107	MET	CB-CG-SD	-10.10	82.11	112.40
1	O	298	THR	OG1-CB-CG2	-9.81	87.44	110.00
1	d	122	THR	OG1-CB-CG2	-9.77	87.53	110.00
1	K	225	MET	CA-CB-CG	9.75	129.87	113.30
1	Y	103	LYS	CB-CA-C	-9.74	90.92	110.40
1	N	106	VAL	CG1-CB-CG2	-9.74	95.32	110.90
1	W	67	VAL	CG1-CB-CG2	-9.72	95.35	110.90
1	N	156	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	F	316	VAL	CG1-CB-CG2	-9.64	95.47	110.90
1	E	299	LEU	CB-CG-CD2	9.63	127.36	111.00
1	W	298	THR	OG1-CB-CG2	-9.62	87.88	110.00
1	G	85	VAL	CG1-CB-CG2	-9.59	95.56	110.90
1	f	207	LYS	CA-CB-CG	9.56	134.44	113.40
1	f	130	VAL	CG1-CB-CG2	-9.50	95.70	110.90
1	V	127	GLN	CA-CB-CG	9.47	134.23	113.40
1	Z	143	MET	CA-CB-CG	9.45	129.37	113.30
1	K	155	THR	OG1-CB-CG2	-9.34	88.53	110.00
1	G	216	VAL	CG1-CB-CG2	-9.32	95.99	110.90
1	R	98	MET	CB-CG-SD	9.26	140.19	112.40
1	D	216	VAL	CG1-CB-CG2	-9.24	96.12	110.90
1	P	275	VAL	CG1-CB-CG2	-9.23	96.14	110.90
1	W	207	LYS	CA-CB-CG	9.00	133.21	113.40
1	R	268	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	N	156	ARG	CA-CB-CG	8.96	133.12	113.40
1	W	275	VAL	CG1-CB-CG2	-8.91	96.64	110.90
1	Z	216	VAL	CG1-CB-CG2	8.89	125.13	110.90
1	S	227	SER	CB-CA-C	-8.88	93.23	110.10
1	a	103	LYS	CB-CA-C	-8.88	92.65	110.40
1	T	122	THR	OG1-CB-CG2	-8.86	89.63	110.00
1	H	292	THR	OG1-CB-CG2	-8.85	89.64	110.00
1	M	156	ARG	CB-CG-CD	8.85	134.60	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	VAL	CG1-CB-CG2	-8.78	96.85	110.90
1	a	272	LEU	CB-CA-C	-8.77	93.55	110.20
1	X	66	THR	OG1-CB-CG2	-8.76	89.84	110.00
1	e	67	VAL	CG1-CB-CG2	8.75	124.90	110.90
1	P	98	MET	CA-CB-CG	8.73	128.15	113.30
1	D	202	ARG	CB-CG-CD	8.73	134.29	111.60
1	V	156	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	E	98	MET	CA-CB-CG	8.60	127.92	113.30
1	O	293	LEU	CB-CG-CD2	-8.59	96.39	111.00
1	f	205	GLN	CA-CB-CG	8.58	132.28	113.40
1	O	67	VAL	CG1-CB-CG2	8.56	124.61	110.90
1	P	225	MET	CA-CB-CG	-8.53	98.79	113.30
1	b	230	GLN	CA-CB-CG	8.53	132.17	113.40
1	Q	317	LYS	CA-CB-CG	8.51	132.13	113.40
1	a	298	THR	OG1-CB-CG2	-8.50	90.44	110.00
1	U	165	ILE	CG1-CB-CG2	8.48	130.06	111.40
1	D	168	THR	OG1-CB-CG2	-8.43	90.60	110.00
1	M	289	MET	CB-CG-SD	-8.42	87.13	112.40
1	e	134	LYS	CD-CE-NZ	8.40	131.02	111.70
1	d	85	VAL	CG1-CB-CG2	8.40	124.33	110.90
1	X	62	THR	OG1-CB-CG2	-8.39	90.70	110.00
1	M	130	VAL	CG1-CB-CG2	8.36	124.27	110.90
1	I	106	VAL	CG1-CB-CG2	8.33	124.23	110.90
1	b	282	ASP	CB-CA-C	-8.32	93.76	110.40
1	T	163	LYS	CA-CB-CG	8.30	131.66	113.40
1	T	67	VAL	CG1-CB-CG2	8.29	124.17	110.90
1	C	67	VAL	CG1-CB-CG2	8.29	124.16	110.90
1	N	147	ILE	CG1-CB-CG2	8.28	129.61	111.40
1	e	268	ARG	CA-CB-CG	-8.26	95.22	113.40
1	M	97	VAL	CG1-CB-CG2	8.26	124.12	110.90
1	e	275	VAL	CG1-CB-CG2	8.26	124.12	110.90
1	K	211	LYS	CB-CA-C	-8.26	93.88	110.40
1	c	156	ARG	N-CA-CB	-8.24	95.76	110.60
1	R	224	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	I	317	LYS	CA-CB-CG	8.23	131.51	113.40
1	Y	106	VAL	CG1-CB-CG2	8.22	124.05	110.90
1	e	150	ILE	CG1-CB-CG2	8.22	129.47	111.40
1	U	317	LYS	CA-CB-CG	8.20	131.45	113.40
1	U	62	THR	OG1-CB-CG2	-8.19	91.15	110.00
1	M	225	MET	CA-CB-CG	8.19	127.22	113.30
1	U	107	MET	CA-CB-CG	8.18	127.21	113.30
1	P	211	LYS	CD-CE-NZ	-8.16	92.93	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	289	MET	CB-CA-C	-8.16	94.09	110.40
1	J	210	VAL	CG1-CB-CG2	8.14	123.92	110.90
1	E	266	GLN	N-CA-C	-8.12	89.07	111.00
1	C	216	VAL	CG1-CB-CG2	-8.05	98.02	110.90
1	H	210	VAL	CG1-CB-CG2	8.05	123.79	110.90
1	V	156	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	E	189	SER	CB-CA-C	8.02	125.34	110.10
1	E	67	VAL	CG1-CB-CG2	8.02	123.73	110.90
1	d	216	VAL	CG1-CB-CG2	8.01	123.72	110.90
1	Z	317	LYS	CB-CA-C	8.01	126.42	110.40
1	a	163	LYS	CB-CG-CD	-8.00	90.80	111.60
1	E	295	VAL	CG1-CB-CG2	7.94	123.60	110.90
1	Q	204	ILE	CG1-CB-CG2	7.93	128.85	111.40
1	a	163	LYS	CA-CB-CG	7.90	130.78	113.40
1	b	144	ILE	CG1-CB-CG2	7.88	128.74	111.40
1	f	220	ILE	CG1-CB-CG2	7.88	128.74	111.40
1	D	211	LYS	CB-CG-CD	-7.87	91.13	111.60
1	K	225	MET	CB-CG-SD	7.87	136.02	112.40
1	L	130	VAL	CG1-CB-CG2	7.86	123.47	110.90
1	T	205	GLN	CA-CB-CG	7.84	130.65	113.40
1	O	122	THR	OG1-CB-CG2	-7.79	92.08	110.00
1	G	287	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	f	85	VAL	CG1-CB-CG2	7.79	123.36	110.90
1	e	215	GLU	CA-CB-CG	-7.79	96.27	113.40
1	R	228	ILE	CG1-CB-CG2	7.78	128.52	111.40
1	S	298	THR	OG1-CB-CG2	-7.78	92.11	110.00
1	S	97	VAL	CG1-CB-CG2	7.77	123.33	110.90
1	J	275	VAL	CG1-CB-CG2	-7.76	98.48	110.90
1	S	85	VAL	CG1-CB-CG2	7.75	123.30	110.90
1	L	67	VAL	CG1-CB-CG2	7.68	123.19	110.90
1	d	293	LEU	CB-CG-CD2	-7.67	97.95	111.00
1	A	98	MET	CB-CG-SD	7.64	135.32	112.40
1	e	85	VAL	CG1-CB-CG2	7.64	123.12	110.90
1	e	97	VAL	CG1-CB-CG2	-7.62	98.70	110.90
1	f	106	VAL	CG1-CB-CG2	7.61	123.08	110.90
1	L	211	LYS	CD-CE-NZ	-7.60	94.22	111.70
1	L	66	THR	OG1-CB-CG2	-7.60	92.52	110.00
1	a	61	ILE	CG1-CB-CG2	7.59	128.11	111.40
1	e	144	ILE	CG1-CB-CG2	7.59	128.10	111.40
1	b	298	THR	CA-CB-CG2	-7.58	101.78	112.40
1	M	220	ILE	CG1-CB-CG2	7.58	128.07	111.40
1	D	130	VAL	CG1-CB-CG2	7.58	123.02	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	228	ILE	CG1-CB-CG2	7.57	128.05	111.40
1	c	156	ARG	CB-CA-C	7.54	125.48	110.40
1	K	97	VAL	CG1-CB-CG2	7.54	122.97	110.90
1	X	107	MET	CB-CG-SD	-7.54	89.78	112.40
1	O	165	ILE	CG1-CB-CG2	7.50	127.91	111.40
1	a	316	VAL	CG1-CB-CG2	7.50	122.89	110.90
1	a	163	LYS	N-CA-CB	7.49	124.08	110.60
1	L	220	ILE	CG1-CB-CG2	7.49	127.87	111.40
1	J	218	LYS	CD-CE-NZ	7.48	128.90	111.70
1	e	130	VAL	CG1-CB-CG2	7.47	122.86	110.90
1	J	147	ILE	CG1-CB-CG2	7.47	127.83	111.40
1	O	156	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	a	163	LYS	CB-CA-C	-7.46	95.49	110.40
1	P	85	VAL	CB-CA-C	-7.45	97.25	111.40
1	c	85	VAL	CG1-CB-CG2	7.43	122.79	110.90
1	R	210	VAL	CG1-CB-CG2	7.42	122.78	110.90
1	V	163	LYS	N-CA-CB	7.42	123.96	110.60
1	c	165	ILE	CG1-CB-CG2	7.40	127.69	111.40
1	e	295	VAL	CG1-CB-CG2	7.38	122.70	110.90
1	S	69	MET	CB-CA-C	-7.37	95.65	110.40
1	R	224	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	b	268	ARG	CB-CG-CD	7.37	130.76	111.60
1	I	130	VAL	CG1-CB-CG2	7.36	122.68	110.90
1	f	206	MET	CA-CB-CG	7.34	125.78	113.30
1	b	298	THR	OG1-CB-CG2	-7.34	93.13	110.00
1	X	202	ARG	CB-CG-CD	7.32	130.64	111.60
1	Y	61	ILE	CG1-CB-CG2	7.31	127.49	111.40
1	A	61	ILE	CG1-CB-CG2	7.28	127.42	111.40
1	L	153	ASP	N-CA-C	-7.27	91.38	111.00
1	K	211	LYS	CB-CG-CD	7.25	130.45	111.60
1	c	168	THR	OG1-CB-CG2	-7.25	93.33	110.00
1	I	85	VAL	CG1-CB-CG2	7.24	122.48	110.90
1	S	224	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	f	134	LYS	CD-CE-NZ	7.22	128.31	111.70
1	Q	67	VAL	CG1-CB-CG2	7.21	122.43	110.90
1	N	69	MET	CB-CG-SD	7.18	133.93	112.40
1	L	85	VAL	CG1-CB-CG2	7.17	122.38	110.90
1	d	66	THR	OG1-CB-CG2	-7.17	93.50	110.00
1	T	204	ILE	CG1-CB-CG2	7.17	127.17	111.40
1	V	302	ARG	CA-CB-CG	7.16	129.15	113.40
1	F	293	LEU	CB-CG-CD2	-7.15	98.85	111.00
1	M	144	ILE	CG1-CB-CG2	7.13	127.09	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	211	LYS	CD-CE-NZ	-7.11	95.35	111.70
1	Y	206	MET	CB-CG-SD	7.11	133.72	112.40
1	Q	85	VAL	CG1-CB-CG2	7.09	122.25	110.90
1	U	143	MET	CG-SD-CE	-7.08	88.88	100.20
1	R	69	MET	CB-CG-SD	-7.07	91.18	112.40
1	Y	85	VAL	CG1-CB-CG2	7.05	122.19	110.90
1	T	163	LYS	CD-CE-NZ	-7.04	95.51	111.70
1	T	163	LYS	CB-CG-CD	-7.03	93.34	111.60
1	Z	85	VAL	CG1-CB-CG2	7.02	122.13	110.90
1	G	148	GLN	N-CA-CB	-7.01	97.98	110.60
1	S	158	VAL	CG1-CB-CG2	7.01	122.11	110.90
1	c	317	LYS	CB-CG-CD	7.00	129.81	111.60
1	U	107	MET	CB-CA-C	7.00	124.40	110.40
1	S	224	ARG	CD-NE-CZ	6.99	133.39	123.60
1	B	153	ASP	CB-CG-OD2	6.97	124.57	118.30
1	Q	220	ILE	CG1-CB-CG2	6.96	126.71	111.40
1	c	298	THR	OG1-CB-CG2	-6.95	94.01	110.00
1	Y	98	MET	CA-CB-CG	6.94	125.10	113.30
1	R	211	LYS	CB-CA-C	6.94	124.28	110.40
1	B	153	ASP	CB-CG-OD1	-6.94	112.06	118.30
1	b	103	LYS	CB-CG-CD	6.93	129.63	111.60
1	L	293	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	H	85	VAL	CG1-CB-CG2	6.87	121.89	110.90
1	f	305	THR	OG1-CB-CG2	-6.85	94.25	110.00
1	G	98	MET	CA-CB-CG	-6.85	101.66	113.30
1	f	225	MET	CB-CG-SD	6.84	132.93	112.40
1	W	317	LYS	N-CA-CB	6.83	122.90	110.60
1	U	180	VAL	CG1-CB-CG2	6.83	121.82	110.90
1	U	207	LYS	CD-CE-NZ	-6.79	96.08	111.70
1	f	62	THR	OG1-CB-CG2	-6.75	94.46	110.00
1	O	98	MET	CA-CB-CG	6.75	124.77	113.30
1	f	153	ASP	N-CA-C	-6.75	92.78	111.00
1	Q	155	THR	OG1-CB-CG2	-6.74	94.50	110.00
1	b	205	GLN	CA-CB-CG	6.74	128.23	113.40
1	V	163	LYS	CA-CB-CG	6.72	128.18	113.40
1	O	107	MET	CB-CG-SD	-6.71	92.26	112.40
1	M	268	ARG	CB-CG-CD	-6.69	94.20	111.60
1	L	143	MET	CA-CB-CG	6.69	124.67	113.30
1	Z	130	VAL	CG1-CB-CG2	6.69	121.60	110.90
1	T	156	ARG	CB-CG-CD	-6.68	94.23	111.60
1	I	205	GLN	CB-CA-C	-6.66	97.09	110.40
1	P	103	LYS	CA-CB-CG	6.62	127.96	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	300	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	d	317	LYS	CB-CA-C	6.60	123.61	110.40
1	I	147	ILE	CG1-CB-CG2	6.60	125.91	111.40
1	I	107	MET	CB-CA-C	6.54	123.47	110.40
1	X	295	VAL	CG1-CB-CG2	6.53	121.34	110.90
1	N	317	LYS	CB-CG-CD	6.52	128.56	111.60
1	b	103	LYS	CD-CE-NZ	6.51	126.67	111.70
1	f	129	MET	CB-CG-SD	-6.50	92.89	112.40
1	S	225	MET	CG-SD-CE	-6.50	89.80	100.20
1	Z	205	GLN	CB-CA-C	6.50	123.40	110.40
1	Z	275	VAL	CG1-CB-CG2	-6.50	100.50	110.90
1	W	224	ARG	CD-NE-CZ	6.50	132.70	123.60
1	Z	98	MET	CA-CB-CG	6.48	124.31	113.30
1	R	69	MET	CB-CA-C	6.47	123.34	110.40
1	X	142	GLU	CB-CA-C	-6.46	97.48	110.40
1	E	299	LEU	CB-CG-CD1	-6.46	100.02	111.00
1	L	295	VAL	CG1-CB-CG2	6.46	121.23	110.90
1	f	154	PHE	N-CA-CB	-6.44	99.01	110.60
1	R	107	MET	CB-CG-SD	-6.43	93.10	112.40
1	E	84	ASP	CB-CG-OD1	6.42	124.08	118.30
1	E	225	MET	CG-SD-CE	-6.41	89.95	100.20
1	G	287	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	J	218	LYS	CB-CG-CD	6.39	128.21	111.60
1	J	153	ASP	N-CA-C	-6.38	93.79	111.00
1	N	129	MET	CG-SD-CE	6.37	110.39	100.20
1	Y	143	MET	CB-CG-SD	6.35	131.46	112.40
1	C	196	LYS	CB-CG-CD	-6.34	95.10	111.60
1	e	134	LYS	CB-CG-CD	6.33	128.05	111.60
1	b	59	THR	OG1-CB-CG2	-6.31	95.49	110.00
1	X	275	VAL	CG1-CB-CG2	6.30	120.98	110.90
1	R	224	ARG	CD-NE-CZ	6.30	132.42	123.60
1	I	218	LYS	CB-CA-C	-6.29	97.83	110.40
1	a	155	THR	OG1-CB-CG2	-6.29	95.54	110.00
1	H	225	MET	CA-CB-CG	-6.28	102.62	113.30
1	K	207	LYS	CA-CB-CG	6.27	127.20	113.40
1	X	311	THR	OG1-CB-CG2	-6.26	95.59	110.00
1	K	211	LYS	CG-CD-CE	6.26	130.69	111.90
1	e	98	MET	CB-CG-SD	6.25	131.14	112.40
1	c	156	ARG	CD-NE-CZ	6.22	132.31	123.60
1	I	289	MET	CB-CG-SD	-6.21	93.75	112.40
1	J	300	ASP	CB-CA-C	-6.20	98.01	110.40
1	b	300	ASP	C-N-CD	6.18	141.38	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	156	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	L	59	THR	CA-CB-CG2	6.16	121.03	112.40
1	G	287	ARG	CA-CB-CG	-6.16	99.85	113.40
1	W	318	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	d	266	GLN	N-CA-C	-6.15	94.39	111.00
1	b	98	MET	CA-CB-CG	-6.15	102.84	113.30
1	c	156	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	R	211	LYS	CD-CE-NZ	6.12	125.77	111.70
1	L	275	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	Z	143	MET	N-CA-CB	6.10	121.58	110.60
1	Q	122	THR	CA-CB-CG2	6.09	120.92	112.40
1	F	128	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	R	121	GLN	CA-CB-CG	6.08	126.78	113.40
1	K	295	VAL	CG1-CB-CG2	6.08	120.62	110.90
1	P	293	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	W	207	LYS	CB-CA-C	-6.05	98.30	110.40
1	W	58	SER	N-CA-C	-6.05	94.67	111.00
1	T	153	ASP	N-CA-C	-6.04	94.68	111.00
1	M	143	MET	N-CA-CB	-6.04	99.72	110.60
1	R	153	ASP	N-CA-C	-6.02	94.74	111.00
1	M	155	THR	OG1-CB-CG2	-6.02	96.16	110.00
1	a	85	VAL	CG1-CB-CG2	6.01	120.51	110.90
1	B	196	LYS	CD-CE-NZ	-6.00	97.89	111.70
1	H	155	THR	OG1-CB-CG2	-5.99	96.21	110.00
1	W	316	VAL	CG1-CB-CG2	-5.99	101.32	110.90
1	L	211	LYS	CG-CD-CE	5.95	129.76	111.90
1	S	156	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	d	153	ASP	N-CA-C	-5.94	94.97	111.00
1	P	273	GLN	CA-CB-CG	5.92	126.44	113.40
1	X	318	ARG	CB-CG-CD	5.90	126.95	111.60
1	f	144	ILE	CG1-CB-CG2	-5.90	98.42	111.40
1	d	59	THR	CA-CB-CG2	5.88	120.64	112.40
1	W	122	THR	CA-CB-CG2	5.88	120.64	112.40
1	b	133	SER	CB-CA-C	5.88	121.27	110.10
1	Z	317	LYS	N-CA-CB	-5.88	100.02	110.60
1	d	103	LYS	CB-CA-C	-5.87	98.65	110.40
1	T	202	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	a	202	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	P	153	ASP	N-CA-C	-5.84	95.23	111.00
1	Z	98	MET	CB-CA-C	5.83	122.06	110.40
1	P	220	ILE	CG1-CB-CG2	5.82	124.21	111.40
1	W	64	ARG	NE-CZ-NH2	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	106	VAL	N-CA-CB	5.82	124.30	111.50
1	b	155	THR	OG1-CB-CG2	-5.81	96.63	110.00
1	R	64	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	O	302	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	T	316	VAL	CG1-CB-CG2	5.80	120.19	110.90
1	b	268	ARG	CG-CD-NE	-5.80	99.62	111.80
1	Y	143	MET	CG-SD-CE	-5.79	90.93	100.20
1	Y	206	MET	CA-CB-CG	5.79	123.14	113.30
1	B	207	LYS	N-CA-CB	5.77	120.99	110.60
1	W	300	ASP	CB-CG-OD1	5.77	123.49	118.30
1	d	317	LYS	CG-CD-CE	-5.77	94.59	111.90
1	U	289	MET	CG-SD-CE	5.77	109.43	100.20
1	T	280	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	a	66	THR	OG1-CB-CG2	5.76	123.24	110.00
1	e	268	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	S	272	LEU	CA-CB-CG	5.75	128.54	115.30
1	Z	289	MET	CB-CG-SD	5.75	129.64	112.40
1	N	142	GLU	CB-CA-C	-5.73	98.94	110.40
1	M	66	THR	OG1-CB-CG2	-5.73	96.83	110.00
1	F	67	VAL	CG1-CB-CG2	5.72	120.06	110.90
1	Z	98	MET	CB-CG-SD	5.72	129.57	112.40
1	J	203	THR	OG1-CB-CG2	5.72	123.16	110.00
1	f	206	MET	CB-CG-SD	-5.72	95.23	112.40
1	I	59	THR	CA-CB-CG2	5.70	120.38	112.40
1	F	59	THR	OG1-CB-CG2	5.69	123.08	110.00
1	d	317	LYS	CD-CE-NZ	5.69	124.79	111.70
1	d	153	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	O	156	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	316	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	P	55	GLU	N-CA-C	-5.66	95.72	111.00
1	S	266	GLN	N-CA-C	-5.65	95.74	111.00
1	R	98	MET	N-CA-CB	-5.64	100.45	110.60
1	b	224	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	N	196	LYS	CG-CD-CE	-5.61	95.07	111.90
1	J	218	LYS	CG-CD-CE	-5.61	95.08	111.90
1	Q	292	THR	CA-CB-CG2	5.61	120.25	112.40
1	L	218	LYS	CD-CE-NZ	-5.61	98.81	111.70
1	Z	153	ASP	CB-CA-C	5.59	121.59	110.40
1	c	107	MET	CG-SD-CE	5.59	109.14	100.20
1	e	59	THR	CA-CB-CG2	5.58	120.22	112.40
1	Q	206	MET	CB-CG-SD	-5.58	95.67	112.40
1	a	107	MET	CB-CG-SD	-5.57	95.71	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	298	THR	OG1-CB-CG2	5.56	122.79	110.00
1	e	268	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	K	207	LYS	CB-CG-CD	-5.55	97.17	111.60
1	d	317	LYS	CB-CG-CD	5.55	126.03	111.60
1	Z	203	THR	CA-CB-CG2	5.55	120.17	112.40
1	N	317	LYS	CA-CB-CG	5.54	125.59	113.40
1	c	156	ARG	CG-CD-NE	-5.52	100.20	111.80
1	N	129	MET	N-CA-CB	-5.52	100.67	110.60
1	L	98	MET	CB-CG-SD	5.52	128.95	112.40
1	Y	69	MET	N-CA-CB	-5.51	100.68	110.60
1	d	103	LYS	N-CA-CB	5.51	120.51	110.60
1	S	220	ILE	CB-CA-C	-5.50	100.59	111.60
1	f	107	MET	N-CA-CB	5.50	120.51	110.60
1	P	59	THR	OG1-CB-CG2	5.50	122.65	110.00
1	d	143	MET	CB-CG-SD	5.50	128.90	112.40
1	C	289	MET	CG-SD-CE	-5.49	91.41	100.20
1	R	59	THR	OG1-CB-CG2	-5.49	97.38	110.00
1	b	122	THR	OG1-CB-CG2	-5.49	97.38	110.00
1	Z	153	ASP	N-CA-C	-5.48	96.20	111.00
1	b	282	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	f	293	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	N	98	MET	CA-CB-CG	-5.47	104.00	113.30
1	M	206	MET	CB-CG-SD	-5.47	96.00	112.40
1	d	196	LYS	CA-CB-CG	5.47	125.43	113.40
1	F	298	THR	CA-CB-CG2	5.46	120.04	112.40
1	F	298	THR	OG1-CB-CG2	5.46	122.55	110.00
1	e	59	THR	OG1-CB-CG2	5.45	122.55	110.00
1	I	59	THR	OG1-CB-CG2	5.45	122.52	110.00
1	X	299	LEU	CB-CG-CD2	5.43	120.24	111.00
1	B	62	THR	OG1-CB-CG2	5.43	122.48	110.00
1	I	316	VAL	CG1-CB-CG2	-5.43	102.22	110.90
1	K	225	MET	CB-CA-C	5.43	121.25	110.40
1	S	156	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	W	300	ASP	CB-CA-C	5.42	121.23	110.40
1	R	154	PHE	N-CA-CB	-5.41	100.85	110.60
1	S	224	ARG	N-CA-CB	5.39	120.30	110.60
1	B	196	LYS	CB-CA-C	5.39	121.17	110.40
1	B	279	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	Q	317	LYS	CB-CG-CD	5.39	125.61	111.60
1	Z	317	LYS	CD-CE-NZ	5.39	124.09	111.70
1	c	225	MET	CB-CG-SD	5.38	128.55	112.40
1	e	220	ILE	CG1-CB-CG2	5.38	123.24	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	98	MET	CA-CB-CG	5.37	122.44	113.30
1	Y	203	THR	OG1-CB-CG2	-5.37	97.65	110.00
1	E	106	VAL	CA-CB-CG2	5.36	118.95	110.90
1	d	59	THR	OG1-CB-CG2	5.36	122.33	110.00
1	A	158	VAL	CG1-CB-CG2	5.36	119.47	110.90
1	T	158	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	c	156	ARG	CB-CG-CD	5.33	125.47	111.60
1	Q	292	THR	OG1-CB-CG2	5.33	122.26	110.00
1	Y	292	THR	CA-CB-CG2	5.33	119.86	112.40
1	T	317	LYS	CB-CG-CD	5.33	125.45	111.60
1	Z	218	LYS	CB-CG-CD	-5.32	97.76	111.60
1	I	218	LYS	CG-CD-CE	-5.32	95.94	111.90
1	f	148	GLN	N-CA-CB	-5.31	101.04	110.60
1	c	298	THR	CA-CB-CG2	-5.30	104.98	112.40
1	R	107	MET	CG-SD-CE	5.29	108.66	100.20
1	Y	97	VAL	CB-CA-C	-5.28	101.37	111.40
1	M	143	MET	CA-CB-CG	5.28	122.27	113.30
1	I	206	MET	CB-CA-C	5.27	120.95	110.40
1	B	55	GLU	CB-CA-C	5.27	120.94	110.40
1	P	103	LYS	CG-CD-CE	-5.27	96.09	111.90
1	S	98	MET	CB-CG-SD	5.26	128.19	112.40
1	D	305	THR	OG1-CB-CG2	5.26	122.10	110.00
1	P	130	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	a	272	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	O	144	ILE	CB-CA-C	5.25	122.09	111.60
1	C	292	THR	OG1-CB-CG2	-5.25	97.94	110.00
1	G	206	MET	CB-CA-C	5.25	120.89	110.40
1	T	196	LYS	CA-CB-CG	5.25	124.94	113.40
1	f	202	ARG	CB-CG-CD	-5.24	97.99	111.60
1	M	225	MET	CG-SD-CE	5.22	108.55	100.20
1	e	134	LYS	CB-CA-C	-5.21	99.97	110.40
1	e	156	ARG	CG-CD-NE	-5.21	100.85	111.80
1	c	59	THR	OG1-CB-CG2	5.21	121.98	110.00
1	I	107	MET	CG-SD-CE	5.20	108.52	100.20
1	E	98	MET	CB-CG-SD	5.20	127.99	112.40
1	X	129	MET	CA-CB-CG	5.19	122.12	113.30
1	a	142	GLU	CB-CA-C	-5.19	100.03	110.40
1	H	59	THR	OG1-CB-CG2	5.17	121.90	110.00
1	I	225	MET	CB-CG-SD	5.17	127.91	112.40
1	d	143	MET	CG-SD-CE	-5.17	91.93	100.20
1	F	59	THR	CA-CB-CG2	5.16	119.63	112.40
1	N	156	ARG	CB-CA-C	5.16	120.73	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	302	ARG	CB-CA-C	-5.16	100.07	110.40
1	V	163	LYS	CB-CG-CD	-5.16	98.18	111.60
1	I	206	MET	CG-SD-CE	-5.16	91.95	100.20
1	M	225	MET	CB-CG-SD	-5.16	96.92	112.40
1	J	225	MET	CB-CG-SD	-5.16	96.93	112.40
1	M	156	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	J	66	THR	OG1-CB-CG2	-5.15	98.15	110.00
1	f	107	MET	CA-CB-CG	5.15	122.06	113.30
1	I	298	THR	OG1-CB-CG2	5.14	121.83	110.00
1	G	287	ARG	CD-NE-CZ	5.13	130.79	123.60
1	G	98	MET	N-CA-CB	-5.13	101.36	110.60
1	M	129	MET	CB-CG-SD	-5.13	97.00	112.40
1	S	156	ARG	CG-CD-NE	-5.13	101.03	111.80
1	E	106	VAL	CB-CA-C	-5.13	101.66	111.40
1	T	156	ARG	CG-CD-NE	5.13	122.57	111.80
1	X	153	ASP	N-CA-C	-5.13	97.16	111.00
1	f	98	MET	CA-CB-CG	5.12	122.00	113.30
1	Y	103	LYS	N-CA-CB	5.11	119.81	110.60
1	Z	203	THR	OG1-CB-CG2	5.11	121.74	110.00
1	f	85	VAL	CA-CB-CG1	5.10	118.55	110.90
1	B	62	THR	CA-CB-CG2	5.09	119.53	112.40
1	J	64	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	L	59	THR	OG1-CB-CG2	5.09	121.71	110.00
1	R	69	MET	CG-SD-CE	5.08	108.33	100.20
1	b	311	THR	OG1-CB-CG2	5.08	121.69	110.00
1	Z	150	ILE	C-N-CD	5.08	139.06	128.40
1	P	299	LEU	CB-CG-CD2	5.08	119.63	111.00
1	e	85	VAL	CA-CB-CG2	5.07	118.51	110.90
1	d	305	THR	OG1-CB-CG2	-5.06	98.35	110.00
1	e	298	THR	OG1-CB-CG2	5.06	121.64	110.00
1	S	97	VAL	CA-CB-CG1	5.06	118.49	110.90
1	S	69	MET	N-CA-CB	5.05	119.70	110.60
1	O	289	MET	CB-CG-SD	-5.05	97.25	112.40
1	F	85	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	a	129	MET	N-CA-CB	-5.03	101.54	110.60
1	V	218	LYS	CD-CE-NZ	5.03	123.27	111.70
1	d	163	LYS	CB-CG-CD	-5.03	98.53	111.60
1	L	130	VAL	CA-CB-CG1	5.02	118.43	110.90
1	X	67	VAL	CG1-CB-CG2	5.01	118.92	110.90
1	V	302	ARG	CD-NE-CZ	5.01	130.62	123.60
1	P	107	MET	CB-CG-SD	-5.01	97.37	112.40
1	P	85	VAL	N-CA-C	-5.01	97.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	107	MET	CB-CG-SD	-5.01	97.38	112.40
1	e	134	LYS	CG-CD-CE	-5.00	96.89	111.90

All (33) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	59	THR	CB
1	A	168	THR	CB
1	A	305	THR	CB
1	B	62	THR	CB
1	F	59	THR	CB
1	F	298	THR	CB
1	I	59	THR	CB
1	J	203	THR	CB
1	L	59	THR	CB
1	M	144	ILE	CB
1	M	220	ILE	CB
1	M	228	ILE	CB
1	N	147	ILE	CB
1	O	144	ILE	CB
1	P	220	ILE	CB
1	Q	122	THR	CB
1	Q	292	THR	CB
1	Q	298	THR	CB
1	R	59	THR	CB
1	R	298	THR	CB
1	U	155	THR	CB
1	W	122	THR	CB
1	X	66	THR	CB
1	Y	292	THR	CB
1	a	59	THR	CB
1	a	66	THR	CB
1	b	59	THR	CB
1	c	165	ILE	CB
1	d	59	THR	CB
1	d	305	THR	CB
1	e	59	THR	CB
1	e	144	ILE	CB
1	e	220	ILE	CB

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	GLU	Sidechain
1	B	279	PHE	Sidechain
1	I	148	GLN	Sidechain
1	J	300	ASP	Sidechain
1	M	148	GLN	Sidechain
1	S	273	GLN	Sidechain
1	T	280	ASP	Sidechain
1	V	148	GLN	Sidechain
1	W	142	GLU	Sidechain
1	X	300	ASP	Sidechain
1	a	148	GLN	Sidechain
1	a	266	GLN	Sidechain
1	e	84	ASP	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1797	0	1748	121	0
1	B	1797	0	1748	140	0
1	C	1797	0	1748	95	0
1	D	1797	0	1748	125	1
1	E	1797	0	1748	103	0
1	F	1797	0	1748	154	0
1	G	1797	0	1748	68	0
1	H	1797	0	1748	77	0
1	I	1797	0	1748	50	0
1	J	1797	0	1748	61	0
1	K	1797	0	1748	55	0
1	L	1797	0	1748	66	1
1	M	1797	0	1748	65	0
1	N	1797	0	1748	51	0
1	O	1797	0	1748	60	0
1	P	1797	0	1748	78	0
1	Q	1797	0	1748	63	0
1	R	1797	0	1748	60	0
1	S	1797	0	1748	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1797	0	1747	78	0
1	U	1797	0	1748	80	0
1	V	1797	0	1748	57	0
1	W	1797	0	1748	74	0
1	X	1797	0	1748	63	0
1	Y	1797	0	1748	57	0
1	Z	1797	0	1748	64	0
1	a	1797	0	1748	0	0
1	b	1797	0	1748	0	0
1	c	1797	0	1748	0	0
1	d	1797	0	1748	0	0
1	e	1797	0	1748	0	0
1	f	1797	0	1748	0	0
All	All	57504	0	55935	1873	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (1873) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:96:SER:OG	1:T:98:MET:SD	1.93	1.26
1:T:196:LYS:HG3	1:T:299:LEU:HD21	1.38	1.04
1:Q:105:PHE:HB2	1:Q:305:THR:HG23	1.35	1.03
1:X:126:LYS:HA	1:X:129:MET:HG3	1.40	1.01
1:B:225:MET:HE1	1:B:273:GLN:HG2	1.38	1.01
1:S:96:SER:OG	1:S:98:MET:SD	2.20	0.99
1:M:105:PHE:HB2	1:M:305:THR:HG23	1.45	0.98
1:W:194:GLU:OE2	1:X:66:THR:OG1	1.84	0.96
1:U:126:LYS:HA	1:U:129:MET:HG3	1.46	0.95
1:E:211:LYS:HA	1:E:211:LYS:HE3	1.44	0.95
1:W:61:ILE:HB	1:W:310:ARG:HB3	1.46	0.95
1:P:187:ALA:HB3	1:P:305:THR:HG21	1.48	0.95
1:B:61:ILE:HB	1:B:310:ARG:HB3	1.85	0.95
1:A:61:ILE:HG13	1:A:310:ARG:HB3	1.50	0.93
1:J:211:LYS:HE3	1:J:211:LYS:HA	1.50	0.93
1:P:105:PHE:HB2	1:P:305:THR:HG23	1.48	0.93
1:B:105:PHE:HB2	1:B:305:THR:HG23	1.49	0.93
1:E:268:ARG:HH11	1:E:268:ARG:HG2	3.23	0.92
1:Z:72:GLY:O	1:Z:76:GLN:NE2	2.01	0.92
1:P:83:LEU:HB3	1:P:202:ARG:HH11	1.33	0.91
1:E:61:ILE:HB	1:E:310:ARG:HB3	1.52	0.91
1:J:64:ARG:HD3	1:J:99:ASP:HA	1.51	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:61:ILE:HB	1:D:310:ARG:HB3	2.08	0.90
1:U:230:GLN:OE1	1:U:230:GLN:N	2.04	0.89
1:T:98:MET:N	1:T:98:MET:SD	2.45	0.89
1:A:126:LYS:HA	1:A:129:MET:HG3	1.55	0.89
1:M:230:GLN:OE1	1:M:230:GLN:N	2.06	0.88
1:F:98:MET:SD	1:F:98:MET:N	2.47	0.88
1:F:105:PHE:HB2	1:F:305:THR:HG23	1.72	0.88
1:F:290:LEU:O	1:F:294:ASN:ND2	2.05	0.88
1:A:207:LYS:HE3	1:A:294:ASN:HD21	2.98	0.87
1:G:200:ALA:O	1:O:302:ARG:NH2	2.07	0.87
1:K:225:MET:HA	1:K:272:LEU:HD21	1.55	0.87
1:D:187:ALA:HB3	1:D:305:THR:HG21	1.54	0.87
1:K:105:PHE:HB2	1:K:305:THR:HG23	1.57	0.87
1:S:105:PHE:HB2	1:S:305:THR:HG23	1.55	0.87
1:H:207:LYS:HG3	1:H:290:LEU:HD21	1.55	0.86
1:P:203:THR:O	1:P:207:LYS:HG3	1.74	0.86
1:F:187:ALA:HB3	1:F:305:THR:HG21	1.57	0.86
1:B:225:MET:CE	1:B:273:GLN:HG2	2.05	0.86
1:D:105:PHE:HB2	1:D:305:THR:HG23	1.56	0.85
1:E:300:ASP:OD1	1:E:302:ARG:NH1	2.10	0.85
1:J:202:ARG:HH21	1:J:205:GLN:HG2	1.41	0.85
1:J:271:ASN:O	1:J:275:VAL:HG23	1.75	0.85
1:E:275:VAL:HG13	1:E:276:GLY:H	1.42	0.84
1:C:168:THR:OG1	1:C:171:ASP:OD2	2.26	0.84
1:L:72:GLY:O	1:L:76:GLN:HG3	1.78	0.83
1:G:122:THR:HG22	1:G:125:TYR:H	1.44	0.82
1:S:68:ASN:H	1:S:68:ASN:HD22	1.25	0.82
1:D:180:VAL:HG21	1:D:308:TYR:OH	1.80	0.82
1:B:229:GLU:HG3	1:B:269:LEU:HD11	2.55	0.81
1:A:275:VAL:HG23	1:Z:227:SER:HB2	148.58	0.81
1:F:202:ARG:HH21	1:F:205:GLN:NE2	3.77	0.81
1:C:105:PHE:HB2	1:C:305:THR:HG23	1.62	0.81
1:U:134:LYS:NZ	1:V:316:VAL:O	2.13	0.80
1:K:70:LEU:HD11	1:K:98:MET:HB3	1.63	0.80
1:V:177:ARG:NH2	1:V:312:PRO:O	2.15	0.80
1:T:199:TRP:NE1	1:T:293:LEU:O	2.10	0.80
1:R:224:ARG:O	1:R:228:ILE:HG13	1.81	0.80
1:A:105:PHE:HB2	1:A:305:THR:HG23	1.62	0.80
1:Q:316:VAL:O	1:X:134:LYS:NZ	2.14	0.80
1:I:105:PHE:HB2	1:I:305:THR:HG23	1.62	0.80
1:L:105:PHE:HB2	1:L:305:THR:HG23	1.64	0.80
1:P:83:LEU:HB3	1:P:202:ARG:NH1	1.96	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:185:GLN:O	1:L:189:SER:OG	2.00	0.79
1:Z:105:PHE:HB2	1:Z:305:THR:HG23	1.62	0.79
1:T:187:ALA:HB3	1:T:305:THR:HG21	1.64	0.79
1:F:61:ILE:HG12	1:F:161:SER:HB3	1.64	0.79
1:X:81:ARG:NH1	1:X:95:PRO:O	2.15	0.79
1:Z:271:ASN:O	1:Z:275:VAL:HG23	1.83	0.79
1:G:125:TYR:HD1	1:G:143:MET:CE	1.95	0.79
1:P:72:GLY:O	1:P:76:GLN:HG3	1.83	0.79
1:E:105:PHE:HB2	1:E:305:THR:HG23	1.65	0.78
1:J:202:ARG:NH2	1:J:205:GLN:HG2	1.99	0.78
1:T:202:ARG:HE	1:T:205:GLN:HG3	1.50	0.77
1:B:163:LYS:HG2	1:B:164:LEU:N	2.66	0.77
1:K:225:MET:HB2	1:K:272:LEU:HD11	1.66	0.77
1:F:202:ARG:HH21	1:F:205:GLN:HE21	4.34	0.77
1:U:96:SER:OG	1:U:98:MET:HG2	1.85	0.77
1:B:117:GLU:OE1	1:B:186:ARG:NH1	2.17	0.76
1:W:173:ASN:OD1	1:W:177:ARG:NE	2.17	0.76
1:C:187:ALA:HB3	1:C:305:THR:HG21	1.72	0.76
1:C:132:ASN:HD22	1:C:135:ALA:H	1.32	0.76
1:Z:228:ILE:HD12	1:Z:272:LEU:HD22	1.68	0.76
1:V:300:ASP:OD1	1:V:302:ARG:HD3	1.85	0.75
1:W:105:PHE:HB2	1:W:305:THR:HG22	1.68	0.75
1:W:207:LYS:NZ	1:W:294:ASN:HD21	1.83	0.75
1:G:204:ILE:HD12	1:O:302:ARG:CZ	2.16	0.75
1:U:132:ASN:HD22	1:U:135:ALA:H	1.32	0.75
1:S:68:ASN:ND2	1:S:68:ASN:H	1.81	0.75
1:Y:61:ILE:HG13	1:Y:310:ARG:HB3	1.69	0.75
1:A:292:THR:HG21	1:H:212:ARG:HD3	1.70	0.74
1:L:119:TRP:CE2	1:L:143:MET:HB3	2.22	0.74
1:T:105:PHE:HB2	1:T:305:THR:HG23	1.70	0.74
1:P:228:ILE:HD12	1:P:272:LEU:HD22	1.67	0.74
1:I:98:MET:N	1:I:98:MET:SD	2.61	0.74
1:J:203:THR:HG23	1:J:293:LEU:HB3	1.70	0.74
1:V:227:SER:HB2	1:W:275:VAL:HG23	1.70	0.74
1:D:70:LEU:HD11	1:D:98:MET:HG2	5.65	0.73
1:E:140:LEU:O	1:E:144:ILE:HG13	2.51	0.73
1:H:213:GLN:HE22	1:H:286:ASN:HD22	1.36	0.73
1:S:68:ASN:N	1:S:68:ASN:HD22	1.83	0.73
1:T:196:LYS:CG	1:T:299:LEU:HD21	2.17	0.73
1:B:80:LEU:HD12	1:B:195:LEU:HD12	2.50	0.73
1:A:202:ARG:NH2	1:A:205:GLN:OE1	2.47	0.73
1:A:316:VAL:HG23	1:A:317:LYS:HD3	1.70	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:105:PHE:HB2	1:H:305:THR:HG23	1.71	0.73
1:A:70:LEU:HD11	1:A:98:MET:HB3	1.69	0.73
1:G:125:TYR:HD1	1:G:143:MET:HE3	1.53	0.73
1:A:60:ALA:HB2	1:A:312:PRO:HG3	1.71	0.72
1:E:64:ARG:NE	1:E:99:ASP:OD1	2.20	0.72
1:Q:187:ALA:HB3	1:Q:305:THR:HG21	1.70	0.72
1:F:122:THR:HG22	1:F:125:TYR:H	1.54	0.72
1:A:132:ASN:HD22	1:A:135:ALA:H	4.83	0.72
1:B:64:ARG:NE	1:B:99:ASP:OD1	2.34	0.72
1:O:228:ILE:HD13	1:O:268:ARG:HB3	1.70	0.72
1:H:199:TRP:CD1	1:H:297:PRO:HD3	2.25	0.72
1:U:63:ASP:OD1	1:U:64:ARG:HG2	1.90	0.71
1:J:115:ARG:HG2	1:J:147:ILE:HD12	1.73	0.71
1:I:207:LYS:HG3	1:I:290:LEU:HD11	1.73	0.71
1:F:107:MET:SD	1:Y:307:ARG:NH2	178.49	0.71
1:C:318:ARG:H	1:C:318:ARG:HD2	1.56	0.71
1:I:152:GLY:N	1:I:160:ASP:OD2	2.20	0.71
1:Z:81:ARG:NH1	1:Z:95:PRO:O	2.22	0.71
1:B:187:ALA:HB3	1:B:305:THR:HG21	1.70	0.71
1:N:60:ALA:HB2	1:N:312:PRO:HG3	1.71	0.71
1:K:132:ASN:HD22	1:K:135:ALA:H	1.38	0.71
1:M:103:LYS:O	1:M:107:MET:HG2	1.90	0.71
1:E:77:GLN:HG2	1:E:97:VAL:HG11	3.34	0.71
1:S:212:ARG:HG2	1:T:288:ALA:HB1	1.73	0.71
1:H:210:VAL:HG22	1:H:286:ASN:HB3	1.73	0.70
1:P:203:THR:HG22	1:P:207:LYS:HE3	1.72	0.70
1:X:119:TRP:CE2	1:X:143:MET:HB3	2.26	0.70
1:U:132:ASN:ND2	1:U:135:ALA:H	1.89	0.70
1:L:57:SER:HB2	1:L:163:LYS:HE3	1.73	0.70
1:S:225:MET:HA	1:S:272:LEU:HD21	1.73	0.70
1:W:124:TYR:CG	1:W:175:LEU:HD11	2.26	0.70
1:W:164:LEU:HB2	1:W:176:LEU:HD13	1.72	0.70
1:W:202:ARG:NH2	1:W:205:GLN:OE1	2.24	0.70
1:J:105:PHE:HB2	1:J:305:THR:HG23	1.74	0.70
1:O:212:ARG:HH11	1:P:292:THR:HG21	1.57	0.70
1:Z:211:LYS:HE3	1:Z:211:LYS:HA	1.73	0.70
1:X:80:LEU:HD23	1:X:83:LEU:HD12	1.73	0.70
1:D:98:MET:N	1:D:98:MET:SD	2.59	0.70
1:B:295:VAL:O	1:T:287:ARG:NH2	177.77	0.70
1:A:224:ARG:HA	1:A:227:SER:OG	1.92	0.69
1:F:210:VAL:HA	1:F:213:GLN:HE21	1.55	0.69
1:G:210:VAL:HA	1:G:213:GLN:HE21	1.55	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Z:70:LEU:HD11	1:Z:98:MET:HB3	1.73	0.69
1:P:61:ILE:HB	1:P:310:ARG:HB3	1.74	0.69
1:B:141:ASP:HA	1:B:144:ILE:HD12	1.73	0.69
1:F:80:LEU:HD23	1:F:83:LEU:HD12	3.33	0.69
1:P:119:TRP:NE1	1:P:143:MET:O	2.25	0.69
1:T:83:LEU:HB3	1:T:202:ARG:HH11	1.57	0.69
1:J:122:THR:HG23	1:J:125:TYR:H	1.57	0.69
1:J:194:GLU:OE2	1:K:68:ASN:ND2	2.25	0.69
1:Q:304:GLN:NE2	1:Q:306:TYR:O	2.24	0.69
1:U:80:LEU:HD23	1:U:83:LEU:HD12	1.73	0.69
1:R:194:GLU:OE2	1:S:68:ASN:ND2	2.26	0.69
1:B:300:ASP:HB2	1:T:295:VAL:HG21	174.85	0.69
1:V:316:VAL:HG23	1:V:317:LYS:HD3	1.74	0.69
1:H:147:ILE:HG12	1:H:164:LEU:HD12	1.75	0.68
1:G:200:ALA:C	1:O:302:ARG:HH22	1.96	0.68
1:U:83:LEU:HB3	1:U:202:ARG:HH11	1.58	0.68
1:J:64:ARG:CD	1:J:99:ASP:HA	2.24	0.68
1:R:106:VAL:HG13	1:R:149:PHE:CZ	2.29	0.68
1:E:132:ASN:HD22	1:E:135:ALA:H	1.40	0.68
1:B:76:GLN:OE1	1:B:298:THR:N	2.92	0.68
1:D:64:ARG:HE	1:D:99:ASP:HA	2.43	0.68
1:G:300:ASP:OD1	1:G:302:ARG:NH1	2.27	0.68
1:Y:60:ALA:HB2	1:Y:312:PRO:HG3	1.76	0.68
1:R:80:LEU:HD23	1:R:83:LEU:HD12	1.73	0.68
1:B:134:LYS:NZ	1:C:316:VAL:O	3.98	0.68
1:C:213:GLN:HE22	1:C:286:ASN:HD22	1.40	0.67
1:K:210:VAL:HG13	1:K:283:TYR:HE1	1.57	0.67
1:M:132:ASN:HD22	1:M:135:ALA:H	1.42	0.67
1:B:298:THR:HG21	1:T:294:ASN:CB	172.05	0.67
1:D:228:ILE:HD12	1:D:272:LEU:HD22	1.75	0.67
1:K:60:ALA:HB2	1:K:312:PRO:HG3	1.76	0.67
1:D:70:LEU:CD1	1:D:98:MET:HG2	6.32	0.67
1:J:211:LYS:HE3	1:J:211:LYS:CA	2.21	0.67
1:L:96:SER:OG	1:L:98:MET:HG2	1.95	0.67
1:T:207:LYS:HE3	1:T:294:ASN:HD21	1.58	0.67
1:B:60:ALA:HB2	1:B:312:PRO:HG3	1.77	0.67
1:E:185:GLN:HA	1:E:185:GLN:HE21	1.59	0.67
1:T:156:ARG:HB3	1:T:158:VAL:HG23	1.76	0.67
1:B:224:ARG:HB3	1:B:272:LEU:HD21	3.40	0.67
1:B:300:ASP:HB2	1:T:295:VAL:CG2	173.97	0.67
1:V:173:ASN:OD1	1:V:177:ARG:NE	2.26	0.67
1:F:128:ARG:HB3	1:F:139:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:173:ASN:OD1	1:N:177:ARG:NE	2.26	0.67
1:P:207:LYS:HE2	1:P:294:ASN:HD21	1.60	0.67
1:M:96:SER:OG	1:M:98:MET:HG2	1.95	0.67
1:B:302:ARG:HH12	1:T:292:THR:HG22	178.40	0.67
1:F:224:ARG:O	1:F:228:ILE:HG13	2.55	0.67
1:I:177:ARG:NH2	1:I:312:PRO:O	2.28	0.67
1:R:112:TRP:HB3	1:S:310:ARG:HB2	1.77	0.67
1:X:207:LYS:HE3	1:X:294:ASN:HD21	1.59	0.67
1:F:216:VAL:O	1:F:220:ILE:HG13	2.59	0.67
1:T:63:ASP:OD1	1:T:64:ARG:HG2	1.95	0.67
1:S:187:ALA:HB3	1:S:305:THR:HG21	1.77	0.66
1:H:207:LYS:HE3	1:H:294:ASN:HD21	1.61	0.66
1:R:164:LEU:HB2	1:R:176:LEU:HD13	1.76	0.66
1:R:177:ARG:NH2	1:R:312:PRO:O	2.27	0.66
1:D:168:THR:OG1	1:D:171:ASP:OD2	2.11	0.66
1:D:72:GLY:O	1:D:76:GLN:HG3	2.31	0.66
1:E:69:MET:HB3	1:E:304:GLN:HB3	1.77	0.66
1:F:83:LEU:HB3	1:F:202:ARG:HH11	3.26	0.66
1:S:224:ARG:HA	1:S:227:SER:OG	1.96	0.66
1:G:200:ALA:HB1	1:O:302:ARG:HH12	1.60	0.66
1:N:202:ARG:NH2	1:N:205:GLN:OE1	2.28	0.66
1:Q:216:VAL:O	1:Q:220:ILE:HG13	1.95	0.66
1:L:83:LEU:HB3	1:L:202:ARG:HH11	1.61	0.66
1:C:288:ALA:O	1:C:291:ASN:HB2	1.96	0.66
1:F:283:TYR:CZ	1:F:287:ARG:HD3	2.30	0.66
1:T:177:ARG:NH2	1:T:312:PRO:O	2.29	0.66
1:L:187:ALA:HB3	1:L:305:THR:HG21	1.78	0.66
1:M:216:VAL:O	1:M:220:ILE:HG13	1.95	0.65
1:S:225:MET:HB2	1:S:272:LEU:HD11	1.78	0.65
1:Y:141:ASP:HA	1:Y:144:ILE:HD12	1.78	0.65
1:D:126:LYS:O	1:D:129:MET:HG2	1.95	0.65
1:N:126:LYS:O	1:N:129:MET:HG3	1.96	0.65
1:J:202:ARG:HH21	1:J:205:GLN:CG	2.09	0.65
1:D:76:GLN:NE2	1:D:298:THR:O	2.21	0.65
1:F:64:ARG:HE	1:F:99:ASP:HA	1.59	0.65
1:E:70:LEU:HB2	1:E:74:TYR:HB2	1.78	0.65
1:N:64:ARG:HE	1:N:99:ASP:HA	1.61	0.65
1:O:202:ARG:NH2	1:O:205:GLN:OE1	2.30	0.65
1:B:225:MET:HE1	1:B:273:GLN:CG	2.22	0.65
1:D:113:ASP:OD2	1:E:311:THR:OG1	3.34	0.65
1:F:164:LEU:HB2	1:F:176:LEU:HD13	2.11	0.65
1:M:114:THR:HG23	1:M:186:ARG:HD3	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:64:ARG:HB3	1:R:102:TYR:HB2	1.79	0.65
1:A:66:THR:HG21	1:H:190:HIS:HE1	1.62	0.65
1:R:122:THR:HG22	1:R:125:TYR:H	1.61	0.65
1:U:211:LYS:HA	1:U:211:LYS:HE3	1.78	0.65
1:G:125:TYR:CD1	1:G:143:MET:HE3	2.31	0.65
1:R:105:PHE:HB2	1:R:305:THR:HG23	1.79	0.65
1:N:61:ILE:HB	1:N:310:ARG:HB3	1.79	0.64
1:S:226:ASN:OD1	1:S:230:GLN:NE2	2.30	0.64
1:W:132:ASN:HB3	1:W:135:ALA:HB3	1.78	0.64
1:C:56:TRP:HB3	1:C:315:PRO:HG2	2.99	0.64
1:M:112:TRP:HB3	1:N:310:ARG:HB2	1.78	0.64
1:M:122:THR:HG22	1:M:125:TYR:H	1.62	0.64
1:F:177:ARG:NH2	1:F:312:PRO:O	2.31	0.64
1:H:210:VAL:CG2	1:H:286:ASN:HB3	2.27	0.64
1:A:66:THR:HG21	1:Z:190:HIS:CE1	147.53	0.64
1:B:61:ILE:HG22	1:B:309:LEU:HB2	1.80	0.64
1:F:210:VAL:HG11	1:F:290:LEU:HD12	1.80	0.64
1:K:202:ARG:NH2	1:K:205:GLN:OE1	2.28	0.64
1:L:60:ALA:HB2	1:L:312:PRO:HG3	1.80	0.64
1:R:173:ASN:OD1	1:R:177:ARG:NE	2.27	0.64
1:Z:64:ARG:HG2	1:Z:102:TYR:CG	2.32	0.64
1:I:124:TYR:OH	1:I:167:GLU:N	2.31	0.64
1:W:58:SER:HB2	1:W:176:LEU:HD23	1.79	0.64
1:A:66:THR:HG21	1:H:190:HIS:CE1	2.32	0.64
1:C:226:ASN:OD1	1:C:230:GLN:NE2	3.12	0.64
1:D:66:THR:H	1:D:69:MET:HB2	2.92	0.64
1:F:206:MET:HE1	1:F:289:MET:HG2	3.47	0.64
1:H:141:ASP:HA	1:H:144:ILE:HD12	1.79	0.64
1:H:302:ARG:HH22	1:O:186:ARG:HG2	1.61	0.64
1:C:132:ASN:ND2	1:C:135:ALA:H	1.95	0.64
1:N:177:ARG:NH2	1:N:312:PRO:O	2.31	0.63
1:W:124:TYR:CD2	1:W:175:LEU:HD11	2.33	0.63
1:D:61:ILE:HG22	1:D:309:LEU:HB2	1.97	0.63
1:F:56:TRP:O	1:F:165:ILE:HA	2.58	0.63
1:B:69:MET:CG	1:B:304:GLN:HB3	3.33	0.63
1:O:112:TRP:CZ2	1:O:144:ILE:HD12	2.33	0.63
1:O:122:THR:O	1:O:126:LYS:HG2	1.97	0.63
1:V:64:ARG:HE	1:V:99:ASP:HA	1.63	0.63
1:A:307:ARG:HH22	1:H:104:GLU:CD	2.01	0.63
1:H:210:VAL:HA	1:H:213:GLN:HE21	1.63	0.63
1:V:230:GLN:OE1	1:V:230:GLN:N	2.30	0.63
1:B:69:MET:HG2	1:B:304:GLN:HB3	3.10	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:266:GLN:O	1:E:266:GLN:HG2	1.99	0.63
1:I:58:SER:OG	1:I:313:GLU:O	2.16	0.63
1:T:223:ARG:NH1	1:U:284:ASP:OD2	2.29	0.63
1:B:96:SER:OG	1:B:98:MET:HG2	2.86	0.63
1:G:196:LYS:HE2	1:O:298:THR:HG22	1.79	0.63
1:F:182:PHE:CE2	1:F:186:ARG:HD2	2.34	0.62
1:F:290:LEU:HD22	1:F:294:ASN:HD21	1.64	0.62
1:K:61:ILE:HB	1:K:310:ARG:HB3	1.80	0.62
1:M:111:SER:HB3	1:M:114:THR:OG1	1.99	0.62
1:Q:66:THR:HG21	1:X:190:HIS:CE1	2.34	0.62
1:G:196:LYS:NZ	1:O:296:GLY:O	2.32	0.62
1:P:205:GLN:HG3	1:P:206:MET:N	2.14	0.62
1:Q:119:TRP:NE1	1:Q:143:MET:O	2.32	0.62
1:A:66:THR:HG21	1:Z:190:HIS:NE2	147.62	0.62
1:W:207:LYS:HZ1	1:W:294:ASN:HD21	1.47	0.62
1:A:284:ASP:OD1	1:Z:223:ARG:NH2	147.84	0.62
1:A:101:ALA:HA	1:A:191:LEU:HD11	2.48	0.62
1:M:122:THR:CG2	1:M:125:TYR:H	2.12	0.62
1:X:206:MET:O	1:X:210:VAL:HG22	1.99	0.62
1:D:119:TRP:CD2	1:D:143:MET:HG3	2.35	0.62
1:H:116:ARG:HG3	1:H:144:ILE:HD11	1.81	0.62
1:J:74:TYR:OH	1:J:78:GLN:NE2	2.33	0.62
1:Q:63:ASP:OD2	1:Q:64:ARG:N	2.29	0.62
1:Z:226:ASN:O	1:Z:230:GLN:HG3	1.99	0.62
1:Y:119:TRP:CE2	1:Y:143:MET:HB3	2.35	0.62
1:H:126:LYS:HA	1:H:129:MET:SD	2.40	0.62
1:Q:98:MET:N	1:Q:98:MET:SD	2.72	0.62
1:U:83:LEU:O	1:U:202:ARG:NH1	2.33	0.62
1:E:119:TRP:NE1	1:E:143:MET:O	2.60	0.62
1:F:204:ILE:O	1:F:207:LYS:HB2	2.98	0.61
1:Q:83:LEU:HB3	1:Q:202:ARG:HH11	1.65	0.61
1:Z:96:SER:OG	1:Z:98:MET:SD	2.58	0.61
1:I:119:TRP:NE1	1:I:143:MET:O	2.33	0.61
1:F:187:ALA:CB	1:F:305:THR:HG21	2.30	0.61
1:H:113:ASP:O	1:H:117:GLU:HG3	2.00	0.61
1:I:141:ASP:HA	1:I:144:ILE:HD12	1.82	0.61
1:K:228:ILE:HD12	1:K:272:LEU:HD22	1.82	0.61
1:T:72:GLY:O	1:T:76:GLN:HG3	2.00	0.61
1:A:177:ARG:NH2	1:A:312:PRO:O	2.32	0.61
1:B:168:THR:OG1	1:B:171:ASP:OD2	2.50	0.61
1:J:63:ASP:HB2	1:J:309:LEU:HD11	1.83	0.61
1:O:229:GLU:HG3	1:O:269:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:GLY:HA2	1:A:158:VAL:HG12	1.81	0.61
1:I:141:ASP:O	1:I:145:ASN:ND2	2.33	0.61
1:K:227:SER:HB2	1:L:275:VAL:HG23	1.82	0.61
1:E:152:GLY:HA2	1:E:158:VAL:HG12	2.60	0.61
1:G:128:ARG:HE	1:G:167:GLU:CD	2.04	0.61
1:C:83:LEU:HD21	1:C:289:MET:SD	2.41	0.61
1:E:177:ARG:NH2	1:E:312:PRO:O	2.25	0.61
1:H:164:LEU:HB2	1:H:176:LEU:HD13	1.82	0.61
1:T:80:LEU:HD12	1:T:195:LEU:HD12	1.81	0.61
1:Y:124:TYR:OH	1:Y:167:GLU:N	2.28	0.61
1:E:98:MET:CE	1:E:98:MET:H	2.14	0.61
1:F:59:THR:HB	1:F:310:ARG:CZ	3.12	0.61
1:J:70:LEU:HD11	1:J:98:MET:HB3	1.81	0.61
1:S:177:ARG:NH2	1:S:312:PRO:O	2.34	0.61
1:Y:105:PHE:HB2	1:Y:305:THR:HG23	1.83	0.61
1:F:101:ALA:HA	1:F:191:LEU:HD11	2.16	0.60
1:B:177:ARG:NH2	1:B:312:PRO:O	2.34	0.60
1:C:79:PHE:HE2	1:C:293:LEU:HD13	2.34	0.60
1:G:76:GLN:NE2	1:G:298:THR:H	1.99	0.60
1:P:139:LEU:O	1:P:143:MET:HG2	2.01	0.60
1:V:202:ARG:NH2	1:V:205:GLN:OE1	2.34	0.60
1:X:105:PHE:HB2	1:X:305:THR:HG23	1.83	0.60
1:Y:122:THR:HG22	1:Y:125:TYR:H	1.67	0.60
1:A:132:ASN:ND2	1:A:135:ALA:H	4.16	0.60
1:D:108:GLN:HG3	1:D:187:ALA:HB2	1.82	0.60
1:E:119:TRP:CD2	1:E:143:MET:HB3	2.83	0.60
1:F:202:ARG:NH2	1:F:205:GLN:HE21	4.07	0.60
1:I:60:ALA:HB2	1:I:312:PRO:HG3	1.84	0.60
1:D:190:HIS:NE2	1:E:66:THR:HG21	2.17	0.60
1:D:228:ILE:HG21	1:D:269:LEU:HA	1.82	0.60
1:F:184:SER:HB2	1:F:306:TYR:CE1	2.36	0.60
1:J:124:TYR:O	1:J:128:ARG:NH1	2.28	0.60
1:L:112:TRP:HB3	1:M:310:ARG:HB2	1.84	0.60
1:E:132:ASN:ND2	1:E:135:ALA:H	1.99	0.60
1:E:168:THR:OG1	1:E:171:ASP:OD2	2.19	0.60
1:R:227:SER:HB2	1:S:275:VAL:HG23	1.84	0.60
1:A:210:VAL:HG21	1:A:290:LEU:HD12	3.21	0.60
1:L:73:TYR:CZ	1:L:191:LEU:HB3	2.37	0.60
1:P:187:ALA:CB	1:P:305:THR:HG21	2.29	0.60
1:Y:152:GLY:HA2	1:Y:158:VAL:HG12	1.83	0.60
1:B:77:GLN:HG2	1:B:97:VAL:HG13	1.84	0.59
1:E:268:ARG:HA	1:E:271:ASN:HB2	1.82	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:316:VAL:HG23	1:I:317:LYS:HD2	1.84	0.59
1:J:223:ARG:HH12	1:K:284:ASP:CG	2.06	0.59
1:B:302:ARG:NH1	1:T:292:THR:HG22	177.74	0.59
1:U:139:LEU:HG	1:U:143:MET:HE3	1.84	0.59
1:F:268:ARG:HA	1:F:271:ASN:HB2	1.83	0.59
1:F:290:LEU:HD22	1:F:294:ASN:ND2	2.17	0.59
1:M:132:ASN:ND2	1:M:135:ALA:H	2.00	0.59
1:A:227:SER:HB3	1:B:275:VAL:HG22	1.85	0.59
1:J:210:VAL:HA	1:J:213:GLN:HE21	1.67	0.59
1:T:223:ARG:HH12	1:U:284:ASP:CG	2.04	0.59
1:Z:173:ASN:OD1	1:Z:177:ARG:NE	2.35	0.59
1:A:228:ILE:HD12	1:A:272:LEU:HD22	1.85	0.59
1:S:73:TYR:CE1	1:S:191:LEU:HB3	2.37	0.59
1:Y:122:THR:CG2	1:Y:125:TYR:H	2.14	0.59
1:E:123:ASP:HB3	1:E:127:GLN:HE21	1.68	0.59
1:K:69:MET:SD	1:K:307:ARG:HB3	2.43	0.59
1:F:122:THR:O	1:F:126:LYS:HG3	2.75	0.59
1:M:224:ARG:O	1:M:228:ILE:HG13	2.02	0.59
1:Z:126:LYS:HG2	1:Z:129:MET:HE2	1.84	0.59
1:Z:126:LYS:O	1:Z:129:MET:HG3	2.03	0.59
1:A:207:LYS:HE3	1:A:294:ASN:ND2	3.76	0.59
1:E:125:TYR:HD1	1:E:143:MET:HE3	3.41	0.59
1:E:120:LEU:HD21	1:E:140:LEU:HD22	2.18	0.59
1:M:275:VAL:HG13	1:M:276:GLY:H	1.67	0.59
1:N:122:THR:HG22	1:N:125:TYR:H	1.68	0.59
1:O:119:TRP:CE3	1:O:122:THR:HG21	2.37	0.59
1:U:122:THR:HG22	1:U:125:TYR:H	1.67	0.59
1:A:169:ALA:HB3	1:A:170:PRO:HD3	1.85	0.59
1:B:119:TRP:NE1	1:B:143:MET:O	2.35	0.59
1:E:268:ARG:NH1	1:E:268:ARG:HG2	3.55	0.59
1:L:103:LYS:O	1:L:107:MET:HG3	2.03	0.59
1:L:223:ARG:O	1:L:227:SER:OG	2.20	0.59
1:F:61:ILE:HG22	1:F:309:LEU:HB2	1.85	0.59
1:G:227:SER:HB2	1:H:275:VAL:HG23	1.85	0.59
1:R:56:TRP:HB3	1:R:315:PRO:HG2	1.85	0.59
1:P:207:LYS:HG2	1:P:290:LEU:HD21	1.85	0.59
1:C:225:MET:HG3	1:C:272:LEU:HD21	1.84	0.58
1:L:80:LEU:HD21	1:L:199:TRP:HA	1.85	0.58
1:I:164:LEU:HB2	1:I:176:LEU:HD13	1.84	0.58
1:O:217:ALA:HA	1:O:220:ILE:HD12	1.84	0.58
1:D:227:SER:HB2	1:E:275:VAL:HG23	4.22	0.58
1:D:223:ARG:HH12	1:E:284:ASP:CG	2.06	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:214:GLU:HG3	1:F:283:TYR:CE1	2.59	0.58
1:H:203:THR:HA	1:H:293:LEU:HD23	1.83	0.58
1:B:140:LEU:O	1:B:144:ILE:HG13	2.44	0.58
1:D:202:ARG:NH2	1:D:205:GLN:OE1	3.74	0.58
1:W:56:TRP:O	1:W:165:ILE:HA	2.04	0.58
1:C:202:ARG:NH2	1:C:205:GLN:OE1	2.67	0.58
1:G:125:TYR:CD1	1:G:143:MET:CE	2.83	0.58
1:K:212:ARG:HH11	1:L:292:THR:HG21	1.69	0.58
1:P:76:GLN:NE2	1:P:298:THR:O	2.36	0.58
1:S:212:ARG:O	1:S:216:VAL:HG23	2.04	0.58
1:I:223:ARG:NH2	1:J:284:ASP:OD1	2.26	0.58
1:W:58:SER:HB2	1:W:176:LEU:CD2	2.33	0.58
1:Z:316:VAL:HG23	1:Z:317:LYS:HG2	1.85	0.58
1:D:58:SER:OG	1:D:313:GLU:O	2.22	0.58
1:E:122:THR:HG22	1:E:125:TYR:H	2.30	0.58
1:F:73:TYR:CZ	1:F:191:LEU:HB3	2.38	0.58
1:J:64:ARG:HG2	1:J:102:TYR:CB	2.33	0.58
1:J:66:THR:H	1:J:69:MET:HB2	1.68	0.58
1:M:212:ARG:O	1:M:216:VAL:HG23	2.04	0.58
1:Q:177:ARG:NH2	1:Q:312:PRO:O	2.36	0.58
1:V:164:LEU:HB2	1:V:176:LEU:HD13	1.85	0.58
1:Y:79:PHE:O	1:Y:83:LEU:HG	2.03	0.58
1:Z:122:THR:HG22	1:Z:125:TYR:H	1.68	0.58
1:A:74:TYR:CE1	1:A:98:MET:HE1	2.50	0.57
1:W:57:SER:HA	1:W:164:LEU:O	2.04	0.57
1:X:136:ASP:O	1:X:140:LEU:HB2	2.03	0.57
1:B:130:VAL:HG23	1:B:132:ASN:H	2.29	0.57
1:B:298:THR:HG21	1:T:294:ASN:HB2	172.71	0.57
1:D:205:GLN:HG3	1:D:206:MET:N	2.19	0.57
1:I:122:THR:HG22	1:I:125:TYR:H	1.70	0.57
1:Q:122:THR:CG2	1:Q:124:TYR:HB3	2.34	0.57
1:R:162:VAL:HG13	1:R:176:LEU:HD11	1.86	0.57
1:E:268:ARG:HH11	1:E:268:ARG:CG	2.61	0.57
1:N:283:TYR:CZ	1:N:287:ARG:HD3	2.38	0.57
1:U:169:ALA:HB1	1:U:314:GLU:HG2	1.85	0.57
1:W:58:SER:HG	1:W:172:ALA:C	2.06	0.57
1:Y:187:ALA:HB3	1:Y:305:THR:HG21	1.86	0.57
1:D:124:TYR:OH	1:D:167:GLU:HG3	2.48	0.57
1:M:187:ALA:HB3	1:M:305:THR:HG21	1.86	0.57
1:U:55:GLU:O	1:U:318:ARG:HG2	2.05	0.57
1:H:124:TYR:OH	1:H:167:GLU:HG3	2.05	0.57
1:Y:56:TRP:CE3	1:Y:169:ALA:HB2	2.40	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:MET:CE	1:A:98:MET:H	2.17	0.57
1:E:187:ALA:HB3	1:E:305:THR:HG21	1.85	0.57
1:G:302:ARG:HH21	1:N:215:GLU:CD	2.06	0.57
1:Q:122:THR:HG23	1:Q:124:TYR:HB3	1.86	0.57
1:V:168:THR:OG1	1:V:170:PRO:HD2	2.04	0.57
1:X:56:TRP:CZ2	1:X:318:ARG:HD2	2.40	0.57
1:F:216:VAL:HG12	1:F:220:ILE:HD11	3.21	0.57
1:M:168:THR:OG1	1:M:171:ASP:OD2	2.19	0.57
1:O:124:TYR:CG	1:O:175:LEU:HD11	2.39	0.57
1:U:122:THR:CG2	1:U:125:TYR:H	2.17	0.57
1:F:119:TRP:NE1	1:F:143:MET:O	2.50	0.57
1:K:56:TRP:CE3	1:K:169:ALA:HB2	2.39	0.57
1:P:202:ARG:HE	1:P:205:GLN:HG2	1.70	0.57
1:A:226:ASN:O	1:A:230:GLN:HG3	2.05	0.57
1:I:148:GLN:N	1:I:148:GLN:HE21	2.03	0.57
1:W:115:ARG:HD3	1:W:147:ILE:HB	1.87	0.57
1:L:76:GLN:NE2	1:L:298:THR:OG1	2.37	0.56
1:M:119:TRP:NE1	1:M:143:MET:O	2.38	0.56
1:P:199:TRP:NE1	1:P:293:LEU:O	2.29	0.56
1:P:63:ASP:O	1:P:307:ARG:N	2.28	0.56
1:Q:105:PHE:HB2	1:Q:305:THR:CG2	2.23	0.56
1:R:56:TRP:CE3	1:R:169:ALA:HB2	2.40	0.56
1:R:61:ILE:HB	1:R:310:ARG:HB3	1.87	0.56
1:B:199:TRP:NE1	1:B:296:GLY:HA2	2.41	0.56
1:D:199:TRP:CD2	1:D:297:PRO:HD3	2.40	0.56
1:D:190:HIS:CE1	1:E:66:THR:HG21	2.71	0.56
1:L:196:LYS:HG3	1:L:299:LEU:HD21	1.87	0.56
1:S:164:LEU:HB2	1:S:176:LEU:HD13	1.86	0.56
1:W:97:VAL:HB	1:W:98:MET:HE2	1.87	0.56
1:X:164:LEU:HB2	1:X:176:LEU:HD13	1.87	0.56
1:Y:152:GLY:N	1:Y:160:ASP:OD2	2.28	0.56
1:F:188:ALA:HA	1:F:303:PHE:CZ	2.40	0.56
1:G:125:TYR:HD1	1:G:143:MET:HE2	1.67	0.56
1:K:132:ASN:ND2	1:K:135:ALA:H	2.01	0.56
1:E:271:ASN:O	1:E:275:VAL:HG12	2.21	0.56
1:F:120:LEU:O	1:F:126:LYS:HE2	2.05	0.56
1:L:113:ASP:OD2	1:M:311:THR:OG1	2.23	0.56
1:P:69:MET:O	1:P:303:PHE:HB2	2.06	0.56
1:C:122:THR:O	1:C:126:LYS:HG3	2.05	0.56
1:F:190:HIS:NE2	1:Y:66:THR:HG21	176.01	0.56
1:X:132:ASN:HB3	1:X:135:ALA:HB3	1.88	0.56
1:C:152:GLY:N	1:C:160:ASP:OD2	2.20	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:56:TRP:CE3	1:D:169:ALA:HB2	2.40	0.56
1:F:64:ARG:O	1:F:307:ARG:HG2	2.05	0.56
1:X:283:TYR:CZ	1:X:287:ARG:HD3	2.41	0.56
1:G:105:PHE:HB2	1:G:305:THR:HG22	1.87	0.56
1:M:269:LEU:O	1:M:273:GLN:HB2	2.05	0.56
1:Q:124:TYR:OH	1:Q:167:GLU:N	2.37	0.56
1:U:115:ARG:HD3	1:U:147:ILE:HB	1.87	0.56
1:Y:177:ARG:NH2	1:Y:312:PRO:O	2.38	0.56
1:A:194:GLU:OE2	1:B:67:VAL:HG23	3.45	0.56
1:C:96:SER:OG	1:C:98:MET:SD	3.11	0.56
1:M:139:LEU:O	1:M:143:MET:HG3	2.06	0.56
1:B:190:HIS:NE2	1:C:66:THR:HG21	2.58	0.56
1:B:55:GLU:N	1:B:166:ALA:O	3.53	0.56
1:O:118:PHE:O	1:O:122:THR:HB	2.06	0.56
1:O:123:ASP:HA	1:O:126:LYS:HG3	1.87	0.56
1:S:77:GLN:HB3	1:S:97:VAL:HG11	1.88	0.56
1:A:307:ARG:NH2	1:Z:104:GLU:OE1	146.47	0.56
1:A:119:TRP:CZ2	1:A:143:MET:HG2	2.41	0.56
1:A:141:ASP:HA	1:A:144:ILE:HD12	1.88	0.56
1:C:122:THR:HG22	1:C:125:TYR:H	1.71	0.56
1:J:223:ARG:NH2	1:K:284:ASP:OD1	2.33	0.56
1:M:124:TYR:CD1	1:M:143:MET:HE1	2.41	0.56
1:M:225:MET:HE1	1:M:273:GLN:HG3	1.88	0.56
1:Q:65:PRO:HD2	1:Q:102:TYR:HB2	1.88	0.56
1:X:122:THR:HG22	1:X:125:TYR:H	1.71	0.56
1:Z:64:ARG:HG2	1:Z:102:TYR:CD2	2.40	0.56
1:Z:79:PHE:O	1:Z:83:LEU:HG	2.06	0.56
1:A:211:LYS:HA	1:A:211:LYS:HE3	1.88	0.56
1:A:76:GLN:NE2	1:A:298:THR:H	2.22	0.56
1:B:58:SER:OG	1:B:172:ALA:C	3.40	0.56
1:C:192:ASN:HB3	1:C:299:LEU:HD22	1.88	0.56
1:D:57:SER:HB3	1:D:165:ILE:HG12	2.17	0.55
1:E:122:THR:CG2	1:E:124:TYR:HB3	2.72	0.55
1:H:124:TYR:OH	1:H:167:GLU:N	2.37	0.55
1:U:173:ASN:OD1	1:U:177:ARG:NE	2.38	0.55
1:L:190:HIS:NE2	1:M:66:THR:HG21	2.21	0.55
1:B:182:PHE:CE2	1:B:186:ARG:HD2	2.41	0.55
1:C:101:ALA:HA	1:C:191:LEU:HD11	2.13	0.55
1:D:76:GLN:OE1	1:D:298:THR:N	2.38	0.55
1:L:152:GLY:HA2	1:L:158:VAL:HG12	1.87	0.55
1:U:120:LEU:HD23	1:U:125:TYR:HE2	1.69	0.55
1:V:56:TRP:HE3	1:V:315:PRO:HG2	1.71	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:96:SER:HB3	1:V:99:ASP:OD2	2.06	0.55
1:L:76:GLN:HB3	1:L:195:LEU:HD11	1.88	0.55
1:O:194:GLU:OE2	1:P:67:VAL:HG23	2.07	0.55
1:B:269:LEU:O	1:B:273:GLN:HG3	2.05	0.55
1:B:69:MET:O	1:B:303:PHE:HB2	2.07	0.55
1:D:300:ASP:O	1:D:303:PHE:HD2	1.89	0.55
1:D:79:PHE:CE2	1:D:83:LEU:HD11	2.42	0.55
1:E:202:ARG:NH2	1:E:205:GLN:OE1	2.95	0.55
1:J:223:ARG:NH1	1:K:284:ASP:OD2	2.29	0.55
1:R:96:SER:OG	1:R:98:MET:HG3	2.05	0.55
1:U:132:ASN:HD22	1:U:135:ALA:N	2.01	0.55
1:V:206:MET:HE2	1:V:289:MET:HG2	1.88	0.55
1:W:229:GLU:HG3	1:W:269:LEU:HD11	1.89	0.55
1:B:210:VAL:HA	1:B:213:GLN:HE21	1.71	0.55
1:B:72:GLY:HA3	1:T:295:VAL:HA	170.85	0.55
1:B:302:ARG:HH22	1:T:292:THR:CG2	176.54	0.55
1:F:221:TYR:OH	1:F:273:GLN:HA	2.79	0.55
1:K:63:ASP:HB2	1:K:309:LEU:HD11	1.88	0.55
1:U:180:VAL:HG11	1:U:308:TYR:OH	2.06	0.55
1:A:152:GLY:HA2	1:A:158:VAL:CG1	2.37	0.55
1:E:77:GLN:CG	1:E:97:VAL:HG11	3.93	0.55
1:G:204:ILE:HD12	1:O:302:ARG:NE	2.21	0.55
1:R:110:ALA:HB2	1:R:149:PHE:CD2	2.41	0.55
1:C:212:ARG:O	1:C:216:VAL:HG23	2.32	0.55
1:F:60:ALA:HB2	1:F:312:PRO:HG3	2.19	0.55
1:R:79:PHE:O	1:R:83:LEU:HG	2.06	0.55
1:T:139:LEU:O	1:T:143:MET:HG3	2.07	0.55
1:A:105:PHE:HB2	1:A:305:THR:CG2	2.39	0.55
1:G:301:PRO:HD2	1:G:302:ARG:HD2	1.89	0.55
1:N:64:ARG:HH21	1:N:99:ASP:HB3	1.71	0.55
1:T:79:PHE:O	1:T:83:LEU:HG	2.06	0.55
1:X:124:TYR:OH	1:X:167:GLU:HG3	2.07	0.55
1:Y:70:LEU:HD11	1:Y:98:MET:HB3	1.88	0.55
1:F:64:ARG:HA	1:F:102:TYR:HB2	1.89	0.54
1:I:122:THR:HG23	1:I:124:TYR:HB3	1.89	0.54
1:R:224:ARG:HG2	1:R:228:ILE:HD11	1.89	0.54
1:A:230:GLN:OE1	1:B:274:ALA:HB1	2.07	0.54
1:D:316:VAL:HG23	1:D:317:LYS:HG3	7.67	0.54
1:F:214:GLU:OE2	1:F:283:TYR:OH	2.63	0.54
1:M:122:THR:HG23	1:M:124:TYR:HB3	1.88	0.54
1:P:141:ASP:HA	1:P:144:ILE:HD12	1.89	0.54
1:C:126:LYS:HA	1:C:129:MET:HG3	2.60	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:216:VAL:HG13	1:D:284:ASP:HB3	2.11	0.54
1:E:227:SER:HB2	1:F:275:VAL:HG23	2.54	0.54
1:F:73:TYR:CE1	1:F:191:LEU:HB3	2.42	0.54
1:I:61:ILE:HB	1:I:310:ARG:HB3	1.90	0.54
1:P:207:LYS:CE	1:P:294:ASN:HD21	2.20	0.54
1:S:122:THR:HG22	1:S:125:TYR:H	1.70	0.54
1:R:141:ASP:HA	1:R:144:ILE:HD12	1.88	0.54
1:S:122:THR:CG2	1:S:125:TYR:H	2.20	0.54
1:D:110:ALA:O	1:D:115:ARG:NH2	3.04	0.54
1:H:152:GLY:N	1:H:160:ASP:OD2	2.30	0.54
1:J:64:ARG:HD3	1:J:99:ASP:CA	2.30	0.54
1:M:83:LEU:HD21	1:M:289:MET:CE	2.38	0.54
1:O:300:ASP:OD1	1:O:302:ARG:NH1	2.30	0.54
1:R:56:TRP:HE3	1:R:315:PRO:HG2	1.72	0.54
1:X:125:TYR:O	1:X:129:MET:N	2.40	0.54
1:Z:78:GLN:HG2	1:Z:97:VAL:HG21	1.89	0.54
1:A:153:ASP:H	1:A:158:VAL:HG12	1.73	0.54
1:F:104:GLU:HG2	1:F:191:LEU:HG	1.90	0.54
1:Q:213:GLN:HE22	1:Q:283:TYR:HA	1.71	0.54
1:C:98:MET:N	1:C:98:MET:SD	3.61	0.54
1:D:225:MET:HE3	1:D:273:GLN:HG3	1.89	0.54
1:F:128:ARG:CB	1:F:139:LEU:HD21	2.38	0.54
1:I:122:THR:O	1:I:126:LYS:HG3	2.08	0.54
1:S:74:TYR:HD1	1:S:97:VAL:CG2	2.20	0.54
1:W:116:ARG:HG3	1:W:140:LEU:HD21	1.90	0.54
1:X:122:THR:CG2	1:X:125:TYR:H	2.20	0.54
1:B:68:ASN:HD22	1:B:68:ASN:H	1.56	0.54
1:E:57:SER:CB	1:E:163:LYS:HE2	2.58	0.54
1:F:119:TRP:CE3	1:F:122:THR:HG21	2.43	0.54
1:G:187:ALA:CB	1:G:305:THR:HG21	2.38	0.54
1:H:213:GLN:NE2	1:H:286:ASN:HD22	2.04	0.54
1:K:226:ASN:O	1:K:230:GLN:HG3	2.08	0.54
1:G:200:ALA:HB1	1:O:302:ARG:NH1	2.22	0.54
1:T:200:ALA:O	1:T:204:ILE:HG12	2.07	0.54
1:B:302:ARG:HH22	1:T:292:THR:HG22	177.13	0.54
1:U:128:ARG:HB3	1:U:139:LEU:HD21	1.90	0.54
1:X:67:VAL:HG22	1:X:98:MET:HE1	1.89	0.54
1:I:310:ARG:HB2	1:P:112:TRP:HB3	1.89	0.54
1:N:122:THR:CG2	1:N:125:TYR:H	2.21	0.54
1:T:300:ASP:OD1	1:T:302:ARG:HB2	2.07	0.54
1:A:104:GLU:CD	1:B:307:ARG:HH22	3.53	0.54
1:E:169:ALA:HB3	1:E:170:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:108:GLN:HG3	1:F:187:ALA:HB2	1.90	0.54
1:H:56:TRP:CE3	1:H:169:ALA:HB2	2.43	0.54
1:T:199:TRP:NE1	1:T:296:GLY:HA2	2.23	0.54
1:C:122:THR:CG2	1:C:125:TYR:H	2.19	0.53
1:H:119:TRP:CD2	1:H:143:MET:HB3	2.43	0.53
1:K:169:ALA:HB3	1:K:170:PRO:HD3	1.90	0.53
1:L:66:THR:OG1	1:L:69:MET:HG3	2.08	0.53
1:M:126:LYS:HA	1:M:129:MET:HG3	1.89	0.53
1:T:76:GLN:NE2	1:T:298:THR:O	2.41	0.53
1:V:61:ILE:HB	1:V:310:ARG:HB3	1.89	0.53
1:E:283:TYR:OH	1:E:287:ARG:NH1	3.93	0.53
1:E:112:TRP:HB3	1:F:310:ARG:HB2	2.73	0.53
1:I:83:LEU:HB3	1:I:202:ARG:HH11	1.74	0.53
1:K:80:LEU:HD23	1:K:83:LEU:HD12	1.90	0.53
1:T:202:ARG:HH21	1:T:205:GLN:NE2	2.06	0.53
1:U:227:SER:HB2	1:V:275:VAL:HG23	1.90	0.53
1:Z:185:GLN:NE2	1:Z:301:PRO:O	2.35	0.53
1:A:112:TRP:HB3	1:B:310:ARG:HB2	2.31	0.53
1:B:72:GLY:C	1:B:76:GLN:HE21	2.11	0.53
1:G:119:TRP:O	1:G:125:TYR:HB3	2.08	0.53
1:K:210:VAL:HG13	1:K:283:TYR:CE1	2.42	0.53
1:L:106:VAL:HG13	1:L:149:PHE:CZ	2.44	0.53
1:L:288:ALA:O	1:L:291:ASN:HB2	2.08	0.53
1:P:206:MET:SD	1:P:289:MET:HG3	2.48	0.53
1:Z:80:LEU:HD23	1:Z:83:LEU:HD12	1.90	0.53
1:A:124:TYR:OH	1:A:167:GLU:HG3	2.08	0.53
1:A:226:ASN:OD1	1:A:230:GLN:NE2	2.40	0.53
1:E:122:THR:O	1:E:126:LYS:HG3	2.24	0.53
1:E:57:SER:HB2	1:E:163:LYS:HE2	2.27	0.53
1:F:184:SER:HA	1:F:305:THR:HG22	1.89	0.53
1:L:96:SER:HB3	1:L:99:ASP:OD2	2.09	0.53
1:U:76:GLN:HE22	1:U:297:PRO:HA	1.72	0.53
1:W:57:SER:CB	1:W:163:LYS:HE2	2.39	0.53
1:X:288:ALA:O	1:X:292:THR:OG1	2.26	0.53
1:D:64:ARG:O	1:D:307:ARG:HG2	2.19	0.53
1:F:96:SER:O	1:F:100:GLU:HG2	2.08	0.53
1:P:163:LYS:HE3	1:P:165:ILE:HD12	1.91	0.53
1:Q:143:MET:HA	1:Q:146:ASN:HB2	1.91	0.53
1:U:169:ALA:HB3	1:U:170:PRO:HD3	1.91	0.53
1:W:119:TRP:CE2	1:W:143:MET:HB3	2.43	0.53
1:W:300:ASP:OD1	1:W:302:ARG:HD3	2.09	0.53
1:G:143:MET:HA	1:G:146:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:152:GLY:HA2	1:Q:158:VAL:HG12	1.90	0.53
1:U:61:ILE:HB	1:U:310:ARG:HB3	1.91	0.53
1:W:122:THR:HG22	1:W:125:TYR:H	1.72	0.53
1:F:266:GLN:HE21	1:F:269:LEU:HD23	1.72	0.53
1:U:120:LEU:HD23	1:U:125:TYR:CE2	2.43	0.53
1:W:108:GLN:HG3	1:W:187:ALA:HB2	1.90	0.53
1:X:124:TYR:OH	1:X:167:GLU:N	2.39	0.53
1:A:283:TYR:CZ	1:A:287:ARG:HD3	2.78	0.53
1:B:57:SER:CB	1:B:163:LYS:HE2	2.39	0.53
1:C:199:TRP:CD1	1:C:297:PRO:HD3	2.43	0.53
1:F:105:PHE:CZ	1:F:109:LEU:HD13	2.44	0.53
1:F:122:THR:CG2	1:F:125:TYR:H	2.25	0.53
1:L:64:ARG:NE	1:L:99:ASP:OD1	2.42	0.53
1:I:275:VAL:HG23	1:P:227:SER:HB2	1.91	0.53
1:B:81:ARG:NH1	1:B:95:PRO:O	2.82	0.53
1:F:212:ARG:O	1:F:216:VAL:HG23	2.09	0.53
1:S:73:TYR:CZ	1:S:191:LEU:HB3	2.43	0.53
1:U:122:THR:CG2	1:U:124:TYR:HB3	2.39	0.53
1:C:83:LEU:HB3	1:C:202:ARG:HH11	3.11	0.52
1:K:56:TRP:CD1	1:K:168:THR:HA	2.43	0.52
1:Q:300:ASP:OD1	1:Q:302:ARG:HD3	2.09	0.52
1:S:194:GLU:HA	1:S:194:GLU:OE2	2.09	0.52
1:V:152:GLY:HA2	1:V:158:VAL:HG12	1.90	0.52
1:D:119:TRP:NE1	1:D:143:MET:O	3.08	0.52
1:E:122:THR:CG2	1:E:125:TYR:H	2.52	0.52
1:F:69:MET:O	1:F:303:PHE:HB2	2.11	0.52
1:P:202:ARG:HH21	1:P:205:GLN:NE2	2.07	0.52
1:S:122:THR:CG2	1:S:124:TYR:HB3	2.39	0.52
1:T:104:GLU:CD	1:U:307:ARG:HH22	2.12	0.52
1:U:202:ARG:NH2	1:U:205:GLN:OE1	2.42	0.52
1:F:194:GLU:OE2	1:F:194:GLU:HA	2.48	0.52
1:M:140:LEU:O	1:M:144:ILE:HG13	2.08	0.52
1:U:119:TRP:CE2	1:U:143:MET:HB3	2.43	0.52
1:X:152:GLY:HA2	1:X:158:VAL:HG12	1.91	0.52
1:A:55:GLU:O	1:A:319:ASP:N	2.70	0.52
1:C:194:GLU:OE2	1:D:67:VAL:HG23	2.36	0.52
1:K:155:THR:HB	1:K:156:ARG:HD2	1.90	0.52
1:R:125:TYR:HD1	1:R:143:MET:SD	2.32	0.52
1:T:207:LYS:CE	1:T:294:ASN:HD21	2.20	0.52
1:A:221:TYR:CE1	1:A:272:LEU:HG	2.45	0.52
1:C:73:TYR:CZ	1:C:191:LEU:HB3	2.44	0.52
1:J:187:ALA:HB3	1:J:305:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:66:THR:HG21	1:X:190:HIS:NE2	2.23	0.52
1:S:275:VAL:HG13	1:S:276:GLY:O	2.09	0.52
1:W:115:ARG:HD2	1:W:144:ILE:O	2.10	0.52
1:Z:199:TRP:O	1:Z:203:THR:OG1	2.27	0.52
1:A:168:THR:OG1	1:A:171:ASP:OD2	3.94	0.52
1:A:307:ARG:NH2	1:H:104:GLU:OE1	2.43	0.52
1:D:266:GLN:HG2	1:D:269:LEU:HB3	1.92	0.52
1:L:280:ASP:OD2	1:L:282:ASP:HB3	2.09	0.52
1:L:76:GLN:OE1	1:L:298:THR:N	2.24	0.52
1:A:224:ARG:HA	1:A:227:SER:HG	1.75	0.52
1:B:108:GLN:HG3	1:B:187:ALA:HB2	1.90	0.52
1:B:141:ASP:HB2	1:C:316:VAL:HG11	4.89	0.52
1:D:169:ALA:HB1	1:D:314:GLU:HG2	3.87	0.52
1:I:203:THR:HA	1:I:293:LEU:HD23	1.92	0.52
1:U:63:ASP:OD1	1:U:64:ARG:N	2.35	0.52
1:W:212:ARG:O	1:W:216:VAL:HG23	2.10	0.52
1:Y:57:SER:HA	1:Y:164:LEU:O	2.10	0.52
1:B:207:LYS:HE3	1:B:290:LEU:HD21	3.17	0.52
1:I:122:THR:CG2	1:I:124:TYR:HB3	2.40	0.52
1:J:119:TRP:NE1	1:J:147:ILE:HD11	2.25	0.52
1:M:275:VAL:HG13	1:M:276:GLY:N	2.24	0.52
1:N:168:THR:OG1	1:N:171:ASP:OD2	2.25	0.52
1:N:213:GLN:NE2	1:N:286:ASN:HD22	2.08	0.52
1:Q:199:TRP:CE2	1:Q:293:LEU:HD12	2.45	0.52
1:V:164:LEU:HD13	1:V:176:LEU:HA	1.91	0.52
1:A:206:MET:HA	1:A:206:MET:HE2	4.61	0.52
1:C:83:LEU:O	1:C:202:ARG:NH1	3.44	0.52
1:D:122:THR:HG22	1:D:125:TYR:H	1.75	0.52
1:E:77:GLN:HG2	1:E:97:VAL:CG1	3.40	0.52
1:F:122:THR:CG2	1:F:124:TYR:HB3	2.40	0.52
1:J:121:GLN:O	1:J:121:GLN:HG2	2.10	0.52
1:S:182:PHE:CE2	1:S:186:ARG:HD2	2.45	0.52
1:U:209:GLN:HA	1:U:212:ARG:NH2	2.25	0.52
1:X:57:SER:HA	1:X:164:LEU:O	2.10	0.52
1:Z:214:GLU:HA	1:Z:279:PHE:HE2	1.75	0.52
1:C:55:GLU:O	1:C:318:ARG:HG2	4.63	0.52
1:F:147:ILE:HG12	1:F:164:LEU:HD12	1.92	0.52
1:F:194:GLU:OE2	1:Y:66:THR:HB	176.08	0.52
1:F:64:ARG:HD3	1:F:99:ASP:OD1	2.10	0.52
1:G:272:LEU:HA	1:G:275:VAL:HG12	1.91	0.52
1:H:122:THR:CG2	1:H:125:TYR:H	2.22	0.52
1:L:223:ARG:CZ	1:M:279:PHE:HB2	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:184:SER:HB2	1:P:306:TYR:CE1	2.45	0.52
1:H:61:ILE:HG22	1:H:309:LEU:HB2	1.92	0.51
1:J:57:SER:HB2	1:J:163:LYS:HE2	1.92	0.51
1:S:194:GLU:OE2	1:T:66:THR:HB	2.10	0.51
1:W:55:GLU:O	1:W:318:ARG:HB2	2.09	0.51
1:Y:221:TYR:CE1	1:Y:272:LEU:HG	2.44	0.51
1:C:283:TYR:CZ	1:C:287:ARG:HD3	2.45	0.51
1:C:63:ASP:HB2	1:C:309:LEU:HD11	2.59	0.51
1:O:80:LEU:HD12	1:O:195:LEU:HD12	1.93	0.51
1:U:96:SER:HG	1:U:98:MET:HG2	1.75	0.51
1:V:169:ALA:HB3	1:V:170:PRO:HD3	1.91	0.51
1:Q:66:THR:HB	1:X:194:GLU:CD	2.31	0.51
1:E:187:ALA:HB1	1:E:305:THR:HG21	2.50	0.51
1:G:116:ARG:HG3	1:G:140:LEU:HD21	1.92	0.51
1:G:295:VAL:HA	1:N:204:ILE:HD11	1.92	0.51
1:H:119:TRP:NE1	1:H:143:MET:O	2.43	0.51
1:H:196:LYS:HD2	1:H:299:LEU:CD1	2.40	0.51
1:Q:196:LYS:HD2	1:Q:299:LEU:HD21	1.91	0.51
1:S:187:ALA:CB	1:S:305:THR:HG21	2.39	0.51
1:F:269:LEU:O	1:F:273:GLN:HB2	3.26	0.51
1:F:105:PHE:CG	1:F:306:TYR:HB3	2.46	0.51
1:K:119:TRP:HA	1:K:122:THR:HB	1.92	0.51
1:R:122:THR:HG23	1:R:124:TYR:HB3	1.92	0.51
1:X:70:LEU:HD11	1:X:98:MET:HB3	1.90	0.51
1:Y:301:PRO:HD2	1:Y:302:ARG:HH11	1.75	0.51
1:A:129:MET:HG2	1:A:136:ASP:CG	3.50	0.51
1:B:187:ALA:CB	1:B:305:THR:HG21	2.40	0.51
1:B:72:GLY:O	1:B:76:GLN:HG3	2.22	0.51
1:Q:122:THR:O	1:Q:126:LYS:HG3	2.10	0.51
1:V:199:TRP:NE1	1:V:293:LEU:O	2.40	0.51
1:C:289:MET:HA	1:C:292:THR:OG1	2.11	0.51
1:D:164:LEU:HB2	1:D:176:LEU:HD13	1.92	0.51
1:E:141:ASP:HA	1:E:144:ILE:HD12	2.30	0.51
1:I:128:ARG:HE	1:I:167:GLU:CD	2.14	0.51
1:B:72:GLY:O	1:B:76:GLN:NE2	2.29	0.51
1:F:119:TRP:HA	1:F:122:THR:HB	1.92	0.51
1:F:288:ALA:O	1:F:291:ASN:HB2	2.29	0.51
1:L:119:TRP:CD2	1:L:143:MET:HB3	2.45	0.51
1:R:81:ARG:NH2	1:R:95:PRO:O	2.40	0.51
1:S:168:THR:OG1	1:S:171:ASP:OD2	2.23	0.51
1:Y:63:ASP:OD2	1:Y:64:ARG:HG2	2.11	0.51
1:E:151:PRO:HG3	1:F:157:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:207:LYS:HG3	1:F:290:LEU:HD21	1.92	0.51
1:N:182:PHE:CE2	1:N:186:ARG:HD2	2.46	0.51
1:Y:271:ASN:O	1:Y:275:VAL:HB	2.11	0.51
1:Z:225:MET:HE1	1:Z:273:GLN:HA	1.93	0.51
1:Z:70:LEU:HD11	1:Z:98:MET:CB	2.41	0.51
1:C:125:TYR:HD1	1:C:143:MET:SD	2.33	0.51
1:L:182:PHE:CE2	1:L:186:ARG:HD2	2.46	0.51
1:A:199:TRP:NE1	1:A:296:GLY:HA2	2.54	0.51
1:D:120:LEU:HD21	1:D:140:LEU:HD22	2.56	0.51
1:D:134:LYS:HZ3	1:E:316:VAL:HB	2.44	0.51
1:F:202:ARG:HE	1:F:205:GLN:HE21	4.59	0.51
1:F:83:LEU:HB3	1:F:202:ARG:NH1	3.28	0.51
1:L:73:TYR:CD1	1:L:195:LEU:HD22	2.46	0.51
1:R:107:MET:CE	1:S:309:LEU:HD22	2.41	0.51
1:S:122:THR:HG23	1:S:124:TYR:HB3	1.92	0.51
1:U:125:TYR:CE2	1:U:129:MET:SD	3.04	0.51
1:B:169:ALA:HB3	1:B:170:PRO:HD3	2.07	0.50
1:D:213:GLN:HE22	1:D:286:ASN:HD22	1.59	0.50
1:D:81:ARG:NH2	1:D:95:PRO:O	2.43	0.50
1:E:115:ARG:HB2	1:E:144:ILE:HG23	3.09	0.50
1:R:120:LEU:HG	1:R:140:LEU:HD11	1.93	0.50
1:R:283:TYR:CZ	1:R:287:ARG:HD3	2.46	0.50
1:S:74:TYR:CD1	1:S:97:VAL:CG2	2.94	0.50
1:V:122:THR:HG22	1:V:125:TYR:H	1.75	0.50
1:W:58:SER:OG	1:W:172:ALA:C	2.50	0.50
1:W:207:LYS:HZ2	1:W:294:ASN:HD21	1.57	0.50
1:C:169:ALA:HB3	1:C:170:PRO:HD3	1.93	0.50
1:G:58:SER:OG	1:G:313:GLU:O	2.29	0.50
1:W:169:ALA:C	1:W:314:GLU:HG2	2.31	0.50
1:I:288:ALA:O	1:I:291:ASN:HB2	2.11	0.50
1:V:203:THR:O	1:V:207:LYS:HB2	2.12	0.50
1:V:210:VAL:HG13	1:V:283:TYR:CE1	2.46	0.50
1:E:105:PHE:HB2	1:E:305:THR:CG2	2.38	0.50
1:P:202:ARG:NH2	1:P:205:GLN:HE21	2.09	0.50
1:S:105:PHE:HB2	1:S:305:THR:CG2	2.37	0.50
1:S:198:ALA:HB2	1:T:67:VAL:HG21	1.93	0.50
1:Y:122:THR:O	1:Y:126:LYS:HG3	2.11	0.50
1:E:143:MET:O	1:E:146:ASN:HB2	2.12	0.50
1:E:134:LYS:NZ	1:F:316:VAL:O	3.11	0.50
1:G:229:GLU:HG2	1:G:269:LEU:HD11	1.92	0.50
1:H:196:LYS:HD2	1:H:299:LEU:HD11	1.94	0.50
1:L:177:ARG:NH2	1:L:312:PRO:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:299:LEU:HD12	1:O:121:GLN:HE21	1.77	0.50
1:R:139:LEU:O	1:R:143:MET:HG3	2.11	0.50
1:W:74:TYR:CZ	1:W:78:GLN:HG3	2.46	0.50
1:W:97:VAL:HB	1:W:98:MET:CE	2.41	0.50
1:X:77:GLN:HG3	1:X:97:VAL:HG22	1.94	0.50
1:B:230:GLN:HE21	1:C:274:ALA:HB1	4.28	0.50
1:C:122:THR:HG23	1:C:124:TYR:H	1.77	0.50
1:B:138:ALA:HB2	1:C:316:VAL:HG11	1.93	0.50
1:E:123:ASP:HB3	1:E:127:GLN:NE2	2.27	0.50
1:E:76:GLN:NE2	1:E:298:THR:H	2.10	0.50
1:M:124:TYR:CE1	1:M:143:MET:HE2	2.47	0.50
1:W:119:TRP:O	1:W:125:TYR:HB3	2.12	0.50
1:L:196:LYS:HA	1:L:297:PRO:HG3	1.94	0.50
1:M:83:LEU:HD21	1:M:289:MET:HE3	1.94	0.50
1:Q:122:THR:HG22	1:Q:125:TYR:H	1.76	0.50
1:S:124:TYR:O	1:S:128:ARG:NH1	2.40	0.50
1:Z:122:THR:CG2	1:Z:125:TYR:H	2.25	0.50
1:A:57:SER:HA	1:A:164:LEU:O	2.12	0.50
1:C:104:GLU:O	1:C:108:GLN:HG2	2.47	0.50
1:C:225:MET:O	1:C:229:GLU:HG3	2.12	0.50
1:C:76:GLN:HE22	1:C:297:PRO:HA	2.11	0.50
1:D:63:ASP:OD1	1:D:64:ARG:HG2	3.27	0.50
1:D:64:ARG:NE	1:D:99:ASP:OD1	2.45	0.50
1:F:69:MET:HB3	1:F:304:GLN:HB3	1.94	0.50
1:Q:64:ARG:HA	1:Q:102:TYR:CD1	2.47	0.50
1:Q:116:ARG:HG3	1:Q:140:LEU:HD21	1.94	0.50
1:U:112:TRP:CE2	1:U:144:ILE:HG21	2.47	0.50
1:A:63:ASP:OD2	1:A:64:ARG:N	2.40	0.50
1:B:120:LEU:HD21	1:B:140:LEU:HD22	1.94	0.50
1:H:57:SER:HA	1:H:164:LEU:O	2.11	0.50
1:Q:70:LEU:HD11	1:Q:98:MET:HB3	1.93	0.50
1:R:138:ALA:N	1:S:316:VAL:HG11	2.27	0.50
1:R:56:TRP:CD1	1:R:168:THR:HA	2.47	0.50
1:B:118:PHE:CG	1:B:179:TYR:HD1	2.28	0.49
1:K:119:TRP:CE3	1:K:122:THR:HG21	2.47	0.49
1:M:122:THR:CG2	1:M:124:TYR:HB3	2.42	0.49
1:N:56:TRP:CE3	1:N:169:ALA:HB2	2.47	0.49
1:P:199:TRP:NE1	1:P:296:GLY:HA2	2.26	0.49
1:S:56:TRP:CE3	1:S:169:ALA:HB2	2.47	0.49
1:Z:141:ASP:HA	1:Z:144:ILE:HD12	1.92	0.49
1:A:69:MET:HE1	1:A:307:ARG:HB3	1.93	0.49
1:F:61:ILE:HB	1:F:310:ARG:HB3	2.15	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:122:THR:CG2	1:I:125:TYR:H	2.26	0.49
1:M:148:GLN:HE21	1:M:148:GLN:N	2.09	0.49
1:Q:141:ASP:HA	1:Q:144:ILE:HD12	1.94	0.49
1:R:122:THR:CG2	1:R:125:TYR:H	2.24	0.49
1:T:271:ASN:O	1:T:275:VAL:HB	2.12	0.49
1:B:101:ALA:HA	1:B:191:LEU:HD21	1.94	0.49
1:D:103:LYS:O	1:D:107:MET:HG3	2.11	0.49
1:G:65:PRO:CB	1:G:69:MET:HG2	2.41	0.49
1:K:226:ASN:OD1	1:K:230:GLN:NE2	2.45	0.49
1:N:213:GLN:HE22	1:N:286:ASN:HD22	1.60	0.49
1:A:83:LEU:HB3	1:A:202:ARG:NH1	2.68	0.49
1:A:285:GLN:HA	1:Z:216:VAL:CG2	148.12	0.49
1:B:141:ASP:O	1:B:145:ASN:ND2	2.46	0.49
1:H:132:ASN:HB3	1:H:135:ALA:HB3	1.95	0.49
1:O:61:ILE:HB	1:O:310:ARG:HB3	1.95	0.49
1:Q:125:TYR:OH	1:Q:136:ASP:O	2.22	0.49
1:S:61:ILE:HB	1:S:310:ARG:HB3	1.93	0.49
1:S:74:TYR:CD1	1:S:97:VAL:HG21	2.47	0.49
1:T:169:ALA:HB3	1:T:170:PRO:HD3	1.93	0.49
1:B:302:ARG:NH2	1:T:292:THR:HG22	176.48	0.49
1:W:119:TRP:CZ3	1:W:175:LEU:HD22	2.47	0.49
1:A:61:ILE:CG1	1:A:310:ARG:HB3	2.34	0.49
1:C:60:ALA:HB2	1:C:312:PRO:HG3	1.94	0.49
1:I:168:THR:OG1	1:I:171:ASP:OD2	2.19	0.49
1:J:152:GLY:HA2	1:J:158:VAL:HG12	1.94	0.49
1:K:267:ALA:O	1:K:271:ASN:ND2	2.45	0.49
1:U:122:THR:HG23	1:U:124:TYR:HB3	1.94	0.49
1:A:69:MET:CE	1:A:307:ARG:HB3	2.42	0.49
1:D:70:LEU:HA	1:D:303:PHE:CD1	2.48	0.49
1:F:64:ARG:HA	1:F:102:TYR:CD1	2.67	0.49
1:H:207:LYS:CE	1:H:294:ASN:HD21	2.23	0.49
1:P:119:TRP:CD2	1:P:143:MET:HB2	2.47	0.49
1:P:203:THR:HA	1:P:293:LEU:HD23	1.95	0.49
1:T:114:THR:HG22	1:T:179:TYR:CE1	2.47	0.49
1:U:213:GLN:NE2	1:U:286:ASN:HD22	2.11	0.49
1:Z:60:ALA:HB2	1:Z:312:PRO:HG3	1.94	0.49
1:C:76:GLN:HE22	1:C:298:THR:H	1.60	0.49
1:D:70:LEU:O	1:D:73:TYR:HB3	2.13	0.49
1:F:77:GLN:HG2	1:F:97:VAL:HG13	2.51	0.49
1:G:199:TRP:CE2	1:G:297:PRO:HD3	2.48	0.49
1:O:169:ALA:HB3	1:O:170:PRO:HD3	1.94	0.49
1:Q:57:SER:HA	1:Q:164:LEU:O	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:56:TRP:CD1	1:Q:168:THR:HA	2.48	0.49
1:T:83:LEU:HB3	1:T:202:ARG:NH1	2.26	0.49
1:U:76:GLN:NE2	1:U:297:PRO:HA	2.27	0.49
1:Y:218:LYS:HE2	1:Y:222:ASP:OD2	2.12	0.49
1:Z:74:TYR:CE1	1:Z:98:MET:SD	3.06	0.49
1:A:199:TRP:CD1	1:A:297:PRO:HD3	2.84	0.49
1:C:230:GLN:OE1	1:D:274:ALA:HB1	2.13	0.49
1:F:79:PHE:O	1:F:83:LEU:HG	3.68	0.49
1:F:83:LEU:C	1:F:85:VAL:H	2.15	0.49
1:J:169:ALA:HB3	1:J:170:PRO:HD3	1.94	0.49
1:N:57:SER:CB	1:N:163:LYS:HE2	2.41	0.49
1:U:55:GLU:N	1:U:166:ALA:O	2.45	0.49
1:A:104:GLU:OE2	1:B:307:ARG:NH1	4.15	0.49
1:C:304:GLN:HG2	1:C:306:TYR:CE1	2.91	0.49
1:D:169:ALA:HB3	1:D:170:PRO:HD3	2.05	0.49
1:S:74:TYR:HD1	1:S:97:VAL:HG21	1.78	0.49
1:U:61:ILE:HG12	1:U:161:SER:HB3	1.95	0.49
1:B:122:THR:CG2	1:B:125:TYR:H	2.26	0.49
1:B:190:HIS:CE1	1:C:66:THR:HG21	2.74	0.49
1:D:184:SER:HB2	1:D:306:TYR:CE1	2.47	0.49
1:E:216:VAL:CG2	1:F:285:GLN:HA	2.43	0.49
1:J:119:TRP:O	1:J:122:THR:HG22	2.13	0.49
1:J:212:ARG:O	1:J:216:VAL:HG23	2.13	0.49
1:K:301:PRO:HD2	1:K:302:ARG:HH11	1.78	0.49
1:L:104:GLU:CD	1:M:307:ARG:HH22	2.16	0.49
1:S:164:LEU:HD13	1:S:176:LEU:HA	1.95	0.49
1:V:228:ILE:HD12	1:V:272:LEU:HD22	1.95	0.49
1:A:207:LYS:HG3	1:A:290:LEU:HD21	3.15	0.48
1:B:55:GLU:O	1:B:318:ARG:HG2	2.13	0.48
1:C:227:SER:HB2	1:D:275:VAL:HG23	2.69	0.48
1:H:84:ASP:OD1	1:H:85:VAL:HG12	2.13	0.48
1:I:57:SER:CB	1:I:163:LYS:HE2	2.43	0.48
1:V:98:MET:H	1:V:98:MET:HG2	1.46	0.48
1:X:283:TYR:OH	1:X:287:ARG:HD3	2.13	0.48
1:Z:119:TRP:CE2	1:Z:143:MET:HB3	2.48	0.48
1:Z:77:GLN:HG2	1:Z:97:VAL:HG13	1.94	0.48
1:B:61:ILE:HB	1:B:310:ARG:CB	2.44	0.48
1:E:211:LYS:CE	1:E:211:LYS:HA	2.29	0.48
1:E:300:ASP:HA	1:E:302:ARG:HH11	1.78	0.48
1:F:201:ALA:O	1:F:205:GLN:HB3	3.28	0.48
1:F:81:ARG:NH1	1:F:95:PRO:O	2.63	0.48
1:G:169:ALA:HB3	1:G:170:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:120:LEU:HD21	1:H:140:LEU:HD22	1.95	0.48
1:K:168:THR:OG1	1:K:171:ASP:OD2	2.27	0.48
1:K:288:ALA:O	1:K:291:ASN:HB2	2.13	0.48
1:M:209:GLN:HA	1:M:212:ARG:NH2	2.28	0.48
1:P:101:ALA:HA	1:P:191:LEU:HD11	1.95	0.48
1:Q:80:LEU:HD23	1:Q:83:LEU:HD12	1.95	0.48
1:S:225:MET:CE	1:S:273:GLN:HG3	2.43	0.48
1:S:300:ASP:OD1	1:S:302:ARG:HD3	2.13	0.48
1:I:224:ARG:O	1:I:228:ILE:HG13	2.14	0.48
1:I:64:ARG:NE	1:I:99:ASP:OD1	2.46	0.48
1:J:113:ASP:OD2	1:K:311:THR:OG1	2.28	0.48
1:T:202:ARG:NH2	1:T:205:GLN:NE2	2.61	0.48
1:W:118:PHE:O	1:W:122:THR:OG1	2.14	0.48
1:A:153:ASP:N	1:A:158:VAL:HG12	2.29	0.48
1:A:275:VAL:HG13	1:A:276:GLY:O	2.14	0.48
1:D:126:LYS:HA	1:D:129:MET:HG3	3.60	0.48
1:F:226:ASN:OD1	1:F:230:GLN:NE2	4.16	0.48
1:G:124:TYR:CG	1:G:175:LEU:HD11	2.48	0.48
1:I:124:TYR:OH	1:I:167:GLU:HG3	2.13	0.48
1:L:57:SER:CB	1:L:163:LYS:HE3	2.40	0.48
1:P:122:THR:CG2	1:P:125:TYR:H	2.26	0.48
1:P:285:GLN:O	1:P:289:MET:HB2	2.13	0.48
1:U:122:THR:O	1:U:126:LYS:HG3	2.13	0.48
1:V:214:GLU:HG3	1:V:283:TYR:CE1	2.48	0.48
1:B:81:ARG:HH12	1:B:96:SER:HA	1.77	0.48
1:G:125:TYR:HA	1:G:143:MET:HE3	1.94	0.48
1:H:81:ARG:NH2	1:H:95:PRO:O	2.34	0.48
1:H:74:TYR:CE1	1:H:98:MET:HE1	2.48	0.48
1:I:169:ALA:HB3	1:I:170:PRO:HD3	1.95	0.48
1:K:126:LYS:HA	1:K:129:MET:HG3	1.95	0.48
1:N:58:SER:OG	1:N:313:GLU:O	2.28	0.48
1:R:108:GLN:OE1	1:R:114:THR:OG1	2.30	0.48
1:S:81:ARG:HA	1:S:84:ASP:OD2	2.14	0.48
1:U:152:GLY:N	1:U:160:ASP:OD2	2.37	0.48
1:D:153:ASP:H	1:D:158:VAL:HB	1.79	0.48
1:G:200:ALA:C	1:O:302:ARG:NH2	2.63	0.48
1:N:272:LEU:HA	1:N:275:VAL:HG12	1.95	0.48
1:P:199:TRP:CD1	1:P:297:PRO:HD3	2.49	0.48
1:W:122:THR:O	1:W:126:LYS:HG3	2.13	0.48
1:Z:214:GLU:HG2	1:Z:279:PHE:CZ	2.49	0.48
1:B:56:TRP:CD1	1:B:168:THR:HA	2.51	0.48
1:B:185:GLN:HE22	1:B:301:PRO:HB2	2.67	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:ILE:HD13	1:B:61:ILE:HG21	1.65	0.48
1:C:57:SER:CB	1:C:163:LYS:HE2	5.44	0.48
1:E:70:LEU:HD11	1:E:98:MET:HB3	2.04	0.48
1:N:105:PHE:HB2	1:N:305:THR:HG23	1.95	0.48
1:Q:69:MET:HE1	1:Q:307:ARG:HB3	1.95	0.48
1:S:300:ASP:OD1	1:S:302:ARG:HB2	2.13	0.48
1:F:197:GLY:HA3	1:Y:68:ASN:OD1	176.14	0.48
1:Z:121:GLN:HG2	1:Z:121:GLN:O	2.14	0.48
1:A:285:GLN:HG2	1:Z:216:VAL:HG21	148.94	0.48
1:C:77:GLN:HG2	1:C:97:VAL:CG1	2.43	0.48
1:D:78:GLN:HE21	1:D:97:VAL:HG23	4.54	0.48
1:F:119:TRP:O	1:F:125:TYR:HB3	2.14	0.48
1:F:300:ASP:OD2	1:F:302:ARG:NH2	2.47	0.48
1:P:180:VAL:HG11	1:P:308:TYR:CE1	2.49	0.48
1:R:109:LEU:HD23	1:R:149:PHE:CE1	2.48	0.48
1:T:134:LYS:NZ	1:U:316:VAL:HB	2.29	0.48
1:T:73:TYR:CZ	1:T:191:LEU:HB3	2.48	0.48
1:U:194:GLU:OE2	1:V:67:VAL:HG23	2.14	0.48
1:V:268:ARG:HD2	1:V:268:ARG:HA	1.62	0.48
1:Y:316:VAL:HG23	1:Y:317:LYS:HD3	1.96	0.48
1:A:194:GLU:OE2	1:A:194:GLU:HA	2.32	0.48
1:A:69:MET:HB3	1:A:304:GLN:HB3	3.56	0.48
1:E:153:ASP:H	1:E:158:VAL:HB	1.79	0.48
1:F:63:ASP:HB2	1:F:309:LEU:HD11	1.95	0.48
1:G:187:ALA:HB1	1:G:305:THR:HG21	1.96	0.48
1:H:205:GLN:HG3	1:H:206:MET:N	2.29	0.48
1:A:130:VAL:HG23	1:A:132:ASN:H	1.81	0.48
1:B:103:LYS:O	1:B:107:MET:HB2	2.13	0.48
1:B:190:HIS:O	1:B:193:ASP:HB2	2.14	0.48
1:B:74:TYR:CZ	1:B:78:GLN:HG3	2.49	0.48
1:C:213:GLN:NE2	1:C:286:ASN:HD22	2.11	0.48
1:A:292:THR:CG2	1:H:212:ARG:HD3	2.43	0.48
1:L:169:ALA:HB3	1:L:170:PRO:HD3	1.96	0.48
1:M:119:TRP:CE3	1:M:122:THR:HG21	2.48	0.48
1:S:223:ARG:O	1:S:227:SER:OG	2.31	0.48
1:A:119:TRP:CE2	1:A:143:MET:HG2	2.49	0.47
1:B:275:VAL:HG13	1:B:276:GLY:O	4.22	0.47
1:D:141:ASP:O	1:D:145:ASN:ND2	2.73	0.47
1:D:270:GLU:HA	1:D:273:GLN:HB2	2.31	0.47
1:E:213:GLN:HE22	1:E:286:ASN:HD22	1.90	0.47
1:H:55:GLU:HG3	1:H:167:GLU:HA	1.95	0.47
1:H:199:TRP:CG	1:H:297:PRO:HD3	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:74:TYR:HD1	1:K:97:VAL:HG21	1.79	0.47
1:N:120:LEU:O	1:N:126:LYS:HE3	2.14	0.47
1:O:168:THR:OG1	1:O:171:ASP:OD2	2.25	0.47
1:P:168:THR:OG1	1:P:171:ASP:OD2	2.29	0.47
1:P:203:THR:CG2	1:P:207:LYS:HE3	2.42	0.47
1:T:199:TRP:CE2	1:T:293:LEU:HD12	2.49	0.47
1:A:227:SER:CB	1:B:275:VAL:HG22	2.42	0.47
1:A:287:ARG:NH2	1:U:302:ARG:HH22	153.56	0.47
1:C:101:ALA:HA	1:C:191:LEU:HD21	1.96	0.47
1:C:210:VAL:HG13	1:C:283:TYR:HE1	1.79	0.47
1:F:105:PHE:CE2	1:F:109:LEU:HD22	2.49	0.47
1:R:210:VAL:HA	1:R:213:GLN:HE21	1.79	0.47
1:U:119:TRP:CD2	1:U:143:MET:HB3	2.49	0.47
1:E:116:ARG:HA	1:E:144:ILE:HG12	2.70	0.47
1:H:61:ILE:O	1:H:309:LEU:N	2.33	0.47
1:M:228:ILE:HD11	1:M:272:LEU:HD22	1.95	0.47
1:O:122:THR:O	1:O:126:LYS:CG	2.63	0.47
1:R:122:THR:CG2	1:R:124:TYR:HB3	2.44	0.47
1:V:130:VAL:HG23	1:V:132:ASN:H	1.79	0.47
1:W:77:GLN:HG2	1:W:97:VAL:HG13	1.96	0.47
1:N:124:TYR:CD2	1:N:175:LEU:HD11	2.48	0.47
1:T:206:MET:HB3	1:T:290:LEU:HG	1.97	0.47
1:Y:119:TRP:CD2	1:Y:143:MET:HB3	2.49	0.47
1:A:215:GLU:OE2	1:A:215:GLU:HA	2.14	0.47
1:F:65:PRO:HD2	1:F:102:TYR:HB2	2.24	0.47
1:M:122:THR:HG22	1:M:125:TYR:HB3	1.96	0.47
1:M:266:GLN:HG2	1:M:266:GLN:O	2.14	0.47
1:O:118:PHE:CG	1:O:179:TYR:HD1	2.32	0.47
1:P:122:THR:HG22	1:P:125:TYR:H	1.78	0.47
1:Q:63:ASP:OD2	1:Q:64:ARG:HG2	2.15	0.47
1:T:293:LEU:HA	1:T:293:LEU:HD12	1.70	0.47
1:V:63:ASP:HB2	1:V:309:LEU:HD11	1.95	0.47
1:C:194:GLU:OE2	1:C:194:GLU:HA	2.87	0.47
1:F:156:ARG:HG3	1:F:158:VAL:HG23	1.95	0.47
1:F:206:MET:CE	1:F:289:MET:HG2	2.84	0.47
1:H:128:ARG:HE	1:H:167:GLU:CD	2.18	0.47
1:O:76:GLN:HE21	1:O:298:THR:HG23	1.79	0.47
1:P:126:LYS:HA	1:P:129:MET:HG3	1.96	0.47
1:R:57:SER:HB3	1:R:319:ASP:OD2	2.14	0.47
1:S:202:ARG:NH2	1:S:205:GLN:OE1	2.44	0.47
1:Y:66:THR:OG1	1:Y:69:MET:HG3	2.14	0.47
1:A:198:ALA:HB2	1:B:67:VAL:HG21	3.25	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:224:ARG:HD2	1:B:224:ARG:HA	4.20	0.47
1:C:286:ASN:O	1:C:290:LEU:HB2	2.14	0.47
1:E:98:MET:HG2	1:E:98:MET:H	3.55	0.47
1:V:61:ILE:HG22	1:V:309:LEU:HB2	1.97	0.47
1:A:147:ILE:HG12	1:A:164:LEU:HD12	2.37	0.47
1:C:77:GLN:OE1	1:C:195:LEU:HD13	3.35	0.47
1:D:280:ASP:OD1	1:D:283:TYR:N	5.40	0.47
1:K:187:ALA:HB3	1:K:305:THR:HG21	1.96	0.47
1:L:229:GLU:HG3	1:L:269:LEU:HD11	1.97	0.47
1:Q:120:LEU:HD21	1:Q:140:LEU:HD22	1.95	0.47
1:R:109:LEU:HD23	1:R:149:PHE:CD1	2.50	0.47
1:W:124:TYR:OH	1:W:167:GLU:HG3	2.14	0.47
1:W:216:VAL:HG13	1:X:284:ASP:HB2	1.97	0.47
1:A:112:TRP:CD1	1:B:310:ARG:HG3	2.49	0.47
1:F:272:LEU:HA	1:F:275:VAL:HG12	1.96	0.47
1:F:56:TRP:HE3	1:F:315:PRO:HG2	1.79	0.47
1:G:292:THR:O	1:G:295:VAL:HG22	2.15	0.47
1:L:96:SER:HG	1:L:98:MET:HG2	1.79	0.47
1:O:124:TYR:OH	1:O:167:GLU:HG3	2.15	0.47
1:P:199:TRP:CG	1:P:297:PRO:HD3	2.48	0.47
1:Q:64:ARG:HE	1:Q:99:ASP:HA	1.80	0.47
1:S:118:PHE:CG	1:S:179:TYR:HD1	2.33	0.47
1:S:60:ALA:HB2	1:S:312:PRO:HG3	1.96	0.47
1:B:300:ASP:OD2	1:T:295:VAL:HG11	173.67	0.47
1:X:122:THR:CG2	1:X:124:TYR:HB3	2.44	0.47
1:F:216:VAL:HG21	1:Y:285:GLN:HG2	157.80	0.47
1:F:286:ASN:O	1:F:290:LEU:HB2	2.15	0.47
1:H:122:THR:HG23	1:H:124:TYR:HB3	1.97	0.47
1:L:66:THR:O	1:L:69:MET:HB2	2.14	0.47
1:Q:108:GLN:OE1	1:Q:186:ARG:NE	2.39	0.47
1:Q:57:SER:CB	1:Q:163:LYS:HE2	2.45	0.47
1:T:56:TRP:CE3	1:T:169:ALA:HB2	2.50	0.47
1:V:61:ILE:O	1:V:309:LEU:N	2.33	0.47
1:C:76:GLN:NE2	1:C:298:THR:H	2.13	0.47
1:D:69:MET:O	1:D:304:GLN:N	2.48	0.47
1:M:60:ALA:HB2	1:M:312:PRO:HG3	1.97	0.47
1:O:130:VAL:HG23	1:O:132:ASN:H	1.80	0.47
1:R:119:TRP:NE1	1:R:143:MET:O	2.48	0.47
1:X:122:THR:HG23	1:X:124:TYR:HB3	1.96	0.47
1:A:56:TRP:CE3	1:A:169:ALA:HB2	2.87	0.46
1:B:120:LEU:HD11	1:B:140:LEU:HD21	1.97	0.46
1:F:206:MET:HG3	1:F:290:LEU:HG	2.39	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:124:TYR:HE1	1:G:143:MET:SD	2.38	0.46
1:I:211:LYS:HA	1:I:211:LYS:HE3	1.97	0.46
1:K:130:VAL:HG23	1:K:132:ASN:H	1.80	0.46
1:R:60:ALA:HB2	1:R:312:PRO:HG3	1.97	0.46
1:S:226:ASN:O	1:S:230:GLN:HG3	2.15	0.46
1:T:100:GLU:OE1	1:T:103:LYS:HD3	2.14	0.46
1:A:96:SER:HB3	1:A:99:ASP:OD2	2.22	0.46
1:D:124:TYR:HE1	1:D:143:MET:SD	2.86	0.46
1:D:66:THR:OG1	1:D:69:MET:HG3	2.14	0.46
1:F:58:SER:OG	1:F:173:ASN:HA	2.68	0.46
1:G:81:ARG:NH1	1:G:95:PRO:O	2.42	0.46
1:B:61:ILE:CG2	1:B:309:LEU:HB2	2.45	0.46
1:B:76:GLN:O	1:B:79:PHE:HB3	2.50	0.46
1:E:121:GLN:HG2	1:E:121:GLN:O	2.39	0.46
1:J:206:MET:CE	1:J:289:MET:HG2	2.46	0.46
1:M:114:THR:HG23	1:M:186:ARG:CD	2.43	0.46
1:P:63:ASP:HB2	1:P:309:LEU:HD11	1.97	0.46
1:S:120:LEU:HD21	1:S:140:LEU:HD22	1.97	0.46
1:V:122:THR:CG2	1:V:124:TYR:HB3	2.46	0.46
1:X:121:GLN:O	1:X:121:GLN:HG2	2.15	0.46
1:X:79:PHE:O	1:X:83:LEU:HG	2.16	0.46
1:A:96:SER:OG	1:A:98:MET:HG2	4.33	0.46
1:B:164:LEU:HB2	1:B:176:LEU:HD13	1.98	0.46
1:C:199:TRP:CE2	1:C:293:LEU:HD12	2.90	0.46
1:D:210:VAL:HA	1:D:213:GLN:HE21	2.35	0.46
1:F:184:SER:HA	1:F:305:THR:CG2	2.46	0.46
1:F:77:GLN:HA	1:F:77:GLN:OE1	2.64	0.46
1:Q:124:TYR:OH	1:Q:167:GLU:HG3	2.16	0.46
1:S:124:TYR:OH	1:S:167:GLU:HG3	2.16	0.46
1:U:132:ASN:HD21	1:U:134:LYS:HB3	1.80	0.46
1:T:194:GLU:OE2	1:U:66:THR:HB	2.15	0.46
1:A:74:TYR:CE1	1:A:98:MET:CE	3.15	0.46
1:B:122:THR:HG22	1:B:125:TYR:H	1.81	0.46
1:C:126:LYS:O	1:C:129:MET:HG3	3.56	0.46
1:D:132:ASN:HB3	1:D:135:ALA:HB3	2.77	0.46
1:E:228:ILE:HD13	1:E:228:ILE:HG21	2.09	0.46
1:E:61:ILE:HG21	1:E:61:ILE:HD13	1.67	0.46
1:O:64:ARG:HA	1:O:102:TYR:CD1	2.50	0.46
1:P:119:TRP:CE2	1:P:143:MET:HB2	2.50	0.46
1:B:121:GLN:O	1:B:121:GLN:HG2	4.24	0.46
1:C:214:GLU:HG3	1:C:283:TYR:CE1	3.06	0.46
1:K:188:ALA:HA	1:K:303:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:210:VAL:HG13	1:L:283:TYR:CE1	2.51	0.46
1:L:298:THR:O	1:L:298:THR:OG1	2.33	0.46
1:M:216:VAL:HG22	1:N:285:GLN:HA	1.97	0.46
1:P:149:PHE:HE1	1:P:160:ASP:HB3	1.81	0.46
1:P:169:ALA:HB3	1:P:170:PRO:HD3	1.98	0.46
1:W:216:VAL:HG13	1:X:284:ASP:CB	2.46	0.46
1:W:216:VAL:HG22	1:X:284:ASP:C	2.35	0.46
1:W:198:ALA:HA	1:X:67:VAL:HG11	1.98	0.46
1:A:112:TRP:CE2	1:A:144:ILE:HG21	3.38	0.46
1:B:96:SER:HB3	1:B:99:ASP:OD2	3.08	0.46
1:C:289:MET:HA	1:C:292:THR:HG1	1.79	0.46
1:D:268:ARG:HD2	1:D:268:ARG:HA	2.00	0.46
1:E:275:VAL:HG13	1:E:276:GLY:N	2.21	0.46
1:G:199:TRP:CZ2	1:G:293:LEU:HA	2.51	0.46
1:J:64:ARG:HG2	1:J:102:TYR:HB2	1.97	0.46
1:L:191:LEU:O	1:L:194:GLU:HB2	2.16	0.46
1:N:164:LEU:HB2	1:N:176:LEU:HD13	1.96	0.46
1:P:289:MET:O	1:P:293:LEU:HB2	2.16	0.46
1:U:280:ASP:OD2	1:U:283:TYR:N	2.47	0.46
1:V:214:GLU:OE2	1:V:283:TYR:OH	2.17	0.46
1:Y:97:VAL:O	1:Y:100:GLU:HB2	2.15	0.46
1:C:122:THR:HG23	1:C:124:TYR:N	2.31	0.46
1:E:101:ALA:HA	1:E:191:LEU:HD11	2.42	0.46
1:F:122:THR:HG23	1:F:124:TYR:HB3	1.98	0.46
1:I:202:ARG:NH2	1:I:205:GLN:OE1	2.48	0.46
1:K:185:GLN:HA	1:K:185:GLN:OE1	2.16	0.46
1:T:201:ALA:O	1:T:205:GLN:HB3	2.16	0.46
1:W:266:GLN:O	1:W:266:GLN:HG2	2.16	0.46
1:Z:57:SER:CB	1:Z:163:LYS:HE2	2.46	0.46
1:A:122:THR:O	1:A:126:LYS:HG3	2.15	0.46
1:D:98:MET:HG3	1:D:98:MET:H	3.20	0.46
1:E:184:SER:HB2	1:E:306:TYR:CE1	2.67	0.46
1:I:57:SER:HB2	1:I:163:LYS:HE2	1.98	0.46
1:L:101:ALA:HA	1:L:191:LEU:HD11	1.98	0.46
1:M:216:VAL:CG2	1:N:285:GLN:HA	2.45	0.46
1:Q:64:ARG:HA	1:Q:102:TYR:CG	2.51	0.46
1:V:96:SER:OG	1:V:98:MET:HG2	2.15	0.46
1:E:128:ARG:HB3	1:E:139:LEU:HD21	2.13	0.46
1:F:64:ARG:CZ	1:F:102:TYR:HD2	2.28	0.46
1:G:304:GLN:OE1	1:G:306:TYR:CZ	2.68	0.46
1:G:96:SER:HB3	1:G:99:ASP:OD2	2.15	0.46
1:H:60:ALA:HA	1:H:310:ARG:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:213:GLN:NE2	1:J:286:ASN:HD22	2.13	0.46
1:J:63:ASP:CG	1:J:64:ARG:H	2.20	0.46
1:L:168:THR:OG1	1:L:171:ASP:OD2	2.27	0.46
1:P:63:ASP:OD1	1:P:64:ARG:HG2	2.16	0.46
1:R:209:GLN:HA	1:R:212:ARG:NH2	2.31	0.46
1:U:301:PRO:HD2	1:U:302:ARG:CD	2.46	0.46
1:U:57:SER:OG	1:U:319:ASP:OD1	2.32	0.46
1:V:214:GLU:HA	1:V:279:PHE:HE2	1.81	0.46
1:W:141:ASP:O	1:W:145:ASN:ND2	2.49	0.46
1:Z:169:ALA:HB3	1:Z:170:PRO:HD3	1.98	0.46
1:Z:96:SER:HB3	1:Z:99:ASP:OD2	2.16	0.46
1:C:226:ASN:CG	1:C:230:GLN:HE22	3.10	0.45
1:D:81:ARG:NH1	1:D:95:PRO:O	2.63	0.45
1:E:64:ARG:H	1:E:64:ARG:HG2	1.59	0.45
1:L:300:ASP:O	1:L:303:PHE:HD2	1.99	0.45
1:P:185:GLN:HA	1:P:185:GLN:OE1	2.16	0.45
1:Q:214:GLU:HA	1:Q:279:PHE:HE2	1.81	0.45
1:Q:69:MET:CE	1:Q:307:ARG:HB3	2.46	0.45
1:U:187:ALA:HB3	1:U:305:THR:HG21	1.97	0.45
1:W:119:TRP:CH2	1:W:175:LEU:HD13	2.50	0.45
1:Y:169:ALA:HB3	1:Y:170:PRO:HD3	1.98	0.45
1:Y:286:ASN:O	1:Y:290:LEU:HB2	2.16	0.45
1:B:66:THR:O	1:B:70:LEU:HG	2.16	0.45
1:D:212:ARG:HD3	1:E:292:THR:HG21	2.99	0.45
1:G:109:LEU:HD23	1:G:149:PHE:CE1	2.51	0.45
1:N:124:TYR:CG	1:N:175:LEU:HD11	2.50	0.45
1:N:192:ASN:HB3	1:N:299:LEU:HD22	1.97	0.45
1:T:199:TRP:O	1:T:203:THR:OG1	2.23	0.45
1:W:177:ARG:NH2	1:W:312:PRO:O	2.49	0.45
1:A:199:TRP:CE2	1:A:293:LEU:HD12	2.51	0.45
1:A:288:ALA:O	1:A:291:ASN:HB2	2.16	0.45
1:D:122:THR:CG2	1:D:125:TYR:H	2.29	0.45
1:D:206:MET:HG3	1:D:290:LEU:HG	1.97	0.45
1:D:180:VAL:HG11	1:D:308:TYR:OH	3.51	0.45
1:D:67:VAL:HG22	1:D:98:MET:CE	2.46	0.45
1:F:220:ILE:HG13	1:F:220:ILE:H	2.21	0.45
1:E:212:ARG:HH11	1:F:292:THR:HG21	1.91	0.45
1:J:117:GLU:OE1	1:J:186:ARG:NH1	2.38	0.45
1:O:152:GLY:HA2	1:O:158:VAL:HG12	1.98	0.45
1:O:301:PRO:HD2	1:O:302:ARG:HD2	1.96	0.45
1:P:269:LEU:O	1:P:273:GLN:HB2	2.15	0.45
1:R:109:LEU:HD21	1:R:162:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:156:ARG:HD2	1:T:156:ARG:HA	1.33	0.45
1:X:120:LEU:HD23	1:X:125:TYR:CE2	2.51	0.45
1:Y:148:GLN:HE21	1:Y:148:GLN:HB2	1.53	0.45
1:A:304:GLN:NE2	1:A:306:TYR:O	2.50	0.45
1:B:64:ARG:HA	1:B:102:TYR:CD1	2.51	0.45
1:D:199:TRP:CE2	1:D:297:PRO:HD3	2.52	0.45
1:J:122:THR:O	1:J:126:LYS:HG3	2.15	0.45
1:K:106:VAL:HG13	1:K:149:PHE:CZ	2.51	0.45
1:P:61:ILE:HG13	1:P:161:SER:HB3	1.97	0.45
1:Q:79:PHE:O	1:Q:83:LEU:HG	2.15	0.45
1:X:56:TRP:CE3	1:X:169:ALA:HB2	2.51	0.45
1:B:58:SER:HB2	1:B:176:LEU:CD2	3.86	0.45
1:E:216:VAL:HG21	1:F:285:GLN:HG3	1.98	0.45
1:J:106:VAL:HG13	1:J:149:PHE:CZ	2.52	0.45
1:M:96:SER:HB3	1:M:99:ASP:OD2	2.17	0.45
1:U:101:ALA:HA	1:U:191:LEU:HD11	1.99	0.45
1:V:119:TRP:NE1	1:V:143:MET:O	2.50	0.45
1:W:124:TYR:CE2	1:W:171:ASP:HB3	2.51	0.45
1:W:115:ARG:HG2	1:W:147:ILE:HD12	1.98	0.45
1:X:270:GLU:O	1:X:273:GLN:HB2	2.17	0.45
1:F:104:GLU:CD	1:Y:307:ARG:HH22	182.35	0.45
1:Z:74:TYR:HE1	1:Z:98:MET:SD	2.38	0.45
1:C:77:GLN:HG2	1:C:97:VAL:HG13	1.98	0.45
1:D:77:GLN:HG3	1:D:97:VAL:HG22	2.30	0.45
1:F:120:LEU:HD23	1:F:125:TYR:CE2	2.51	0.45
1:T:202:ARG:HE	1:T:205:GLN:CG	2.25	0.45
1:U:177:ARG:NH2	1:U:312:PRO:O	2.49	0.45
1:Z:105:PHE:HB2	1:Z:305:THR:CG2	2.39	0.45
1:Z:67:VAL:HG13	1:Z:74:TYR:CD2	2.52	0.45
1:A:307:ARG:HH22	1:Z:104:GLU:CD	146.25	0.45
1:D:228:ILE:HG22	1:D:269:LEU:HD13	1.98	0.45
1:F:153:ASP:O	1:F:158:VAL:HG23	3.65	0.45
1:F:169:ALA:HB3	1:F:170:PRO:HD3	2.03	0.45
1:F:221:TYR:CE1	1:F:272:LEU:HG	2.75	0.45
1:E:216:VAL:HG13	1:F:284:ASP:HB3	2.52	0.45
1:H:125:TYR:OH	1:H:140:LEU:HB2	2.15	0.45
1:J:109:LEU:HD23	1:J:149:PHE:CD1	2.52	0.45
1:L:64:ARG:HA	1:L:102:TYR:HB2	1.98	0.45
1:M:202:ARG:HH21	1:M:205:GLN:CD	2.18	0.45
1:O:60:ALA:HB2	1:O:312:PRO:HG3	1.99	0.45
1:T:196:LYS:HG3	1:T:299:LEU:CD2	2.27	0.45
1:X:125:TYR:OH	1:X:136:ASP:HB3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:105:PHE:HB2	1:X:305:THR:CG2	2.46	0.45
1:D:120:LEU:HD23	1:D:120:LEU:HA	2.42	0.45
1:D:268:ARG:HA	1:D:271:ASN:HB3	1.99	0.45
1:F:101:ALA:HA	1:F:191:LEU:HD21	1.99	0.45
1:L:100:GLU:OE1	1:L:103:LYS:HD3	2.17	0.45
1:S:77:GLN:HG2	1:S:97:VAL:HG12	1.99	0.45
1:W:305:THR:HG22	1:W:305:THR:O	2.16	0.45
1:W:74:TYR:HE1	1:W:98:MET:HE1	1.80	0.45
1:Z:122:THR:O	1:Z:126:LYS:HG3	2.16	0.45
1:A:182:PHE:CE2	1:A:186:ARG:HD2	2.62	0.45
1:B:300:ASP:O	1:B:303:PHE:HD2	1.99	0.45
1:C:69:MET:O	1:C:303:PHE:HB2	2.44	0.45
1:F:123:ASP:O	1:F:127:GLN:HB2	2.17	0.45
1:E:216:VAL:HG22	1:F:285:GLN:HA	1.98	0.45
1:H:286:ASN:O	1:H:290:LEU:HB2	2.16	0.45
1:N:308:TYR:CE1	1:N:312:PRO:HD3	2.51	0.45
1:T:266:GLN:HE21	1:T:269:LEU:HD22	1.81	0.45
1:V:64:ARG:HD3	1:V:99:ASP:OD1	2.17	0.45
1:Z:66:THR:H	1:Z:69:MET:HB2	1.81	0.45
1:A:141:ASP:O	1:A:145:ASN:ND2	2.50	0.45
1:D:272:LEU:HA	1:D:275:VAL:HG12	2.29	0.45
1:G:199:TRP:CD2	1:G:297:PRO:HD3	2.51	0.45
1:H:192:ASN:HA	1:H:192:ASN:HD22	1.64	0.45
1:I:290:LEU:HD23	1:I:290:LEU:HA	1.81	0.45
1:J:199:TRP:CD1	1:J:297:PRO:HD3	2.52	0.45
1:P:122:THR:CG2	1:P:124:TYR:HB3	2.47	0.45
1:U:126:LYS:O	1:U:129:MET:HB2	2.17	0.45
1:A:116:ARG:HG3	1:A:140:LEU:HD21	1.99	0.44
1:A:293:LEU:HA	1:A:293:LEU:HD12	2.10	0.44
1:A:66:THR:HB	1:H:194:GLU:OE2	2.16	0.44
1:B:215:GLU:OE1	1:B:218:LYS:HG2	2.17	0.44
1:E:300:ASP:HA	1:E:302:ARG:NH1	2.32	0.44
1:Q:65:PRO:CD	1:Q:102:TYR:HB2	2.46	0.44
1:Q:124:TYR:CD2	1:Q:175:LEU:HD11	2.52	0.44
1:Q:169:ALA:HB3	1:Q:170:PRO:HD3	1.99	0.44
1:X:120:LEU:HG	1:X:140:LEU:HD11	1.99	0.44
1:Y:301:PRO:HD2	1:Y:302:ARG:HD3	1.99	0.44
1:B:298:THR:HA	1:T:291:ASN:HD22	176.63	0.44
1:C:268:ARG:HA	1:C:268:ARG:HD2	1.92	0.44
1:F:57:SER:N	1:F:315:PRO:HG3	2.92	0.44
1:H:156:ARG:HG3	1:H:158:VAL:HG23	1.99	0.44
1:K:117:GLU:OE1	1:K:186:ARG:NH1	2.40	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:130:VAL:N	1:K:136:ASP:OD1	2.42	0.44
1:N:218:LYS:HG3	1:N:218:LYS:O	2.17	0.44
1:H:299:LEU:HD12	1:O:121:GLN:NE2	2.33	0.44
1:O:300:ASP:OD1	1:O:302:ARG:HD3	2.17	0.44
1:S:228:ILE:HG21	1:S:228:ILE:HD13	1.61	0.44
1:S:66:THR:O	1:S:70:LEU:HG	2.16	0.44
1:V:213:GLN:HE22	1:V:283:TYR:HA	1.81	0.44
1:X:81:ARG:HH21	1:X:100:GLU:HG3	1.82	0.44
1:B:156:ARG:HA	1:B:156:ARG:HD2	4.45	0.44
1:C:119:TRP:CE2	1:C:143:MET:HB3	3.07	0.44
1:E:119:TRP:CE2	1:E:143:MET:HB3	2.66	0.44
1:P:164:LEU:HB2	1:P:176:LEU:HD13	1.99	0.44
1:P:206:MET:HG2	1:P:290:LEU:HG	2.00	0.44
1:R:152:GLY:HA2	1:R:158:VAL:HG12	2.00	0.44
1:R:169:ALA:HB3	1:R:170:PRO:HD3	1.99	0.44
1:U:289:MET:O	1:U:293:LEU:HB2	2.17	0.44
1:B:116:ARG:HG3	1:B:144:ILE:HD11	1.99	0.44
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.83	0.44
1:B:56:TRP:CE3	1:B:169:ALA:HB2	2.52	0.44
1:D:146:ASN:O	1:D:164:LEU:HA	2.18	0.44
1:F:164:LEU:HD13	1:F:176:LEU:N	3.01	0.44
1:F:184:SER:HB2	1:F:306:TYR:CD1	2.52	0.44
1:V:56:TRP:CE3	1:V:315:PRO:HG2	2.50	0.44
1:X:269:LEU:O	1:X:273:GLN:HG3	2.18	0.44
1:Z:61:ILE:HB	1:Z:310:ARG:HB3	2.00	0.44
1:B:139:LEU:O	1:B:143:MET:HG3	2.18	0.44
1:E:148:GLN:HE21	1:E:148:GLN:HB2	3.02	0.44
1:G:66:THR:O	1:G:69:MET:HB3	2.18	0.44
1:K:105:PHE:HB2	1:K:305:THR:CG2	2.39	0.44
1:M:118:PHE:CG	1:M:179:TYR:HD1	2.35	0.44
1:Q:68:ASN:ND2	1:X:194:GLU:OE2	2.49	0.44
1:A:268:ARG:O	1:A:272:LEU:HD23	4.74	0.44
1:E:122:THR:HG23	1:E:124:TYR:HB3	2.19	0.44
1:H:105:PHE:CE2	1:H:109:LEU:HD22	2.52	0.44
1:H:207:LYS:HG2	1:H:290:LEU:HD11	1.98	0.44
1:P:105:PHE:HB2	1:P:305:THR:CG2	2.33	0.44
1:P:202:ARG:NH2	1:P:205:GLN:NE2	2.65	0.44
1:W:83:LEU:C	1:W:85:VAL:H	2.21	0.44
1:X:119:TRP:CD2	1:X:143:MET:HB3	2.52	0.44
1:X:169:ALA:HB3	1:X:170:PRO:HD3	2.00	0.44
1:Y:128:ARG:HE	1:Y:167:GLU:CD	2.20	0.44
1:A:206:MET:HG2	1:A:290:LEU:HA	3.67	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:193:ASP:O	1:D:196:LYS:HB3	3.19	0.44
1:D:289:MET:O	1:D:293:LEU:HB2	2.53	0.44
1:E:84:ASP:C	1:E:84:ASP:OD1	2.56	0.44
1:F:184:SER:HB2	1:F:306:TYR:HE1	1.82	0.44
1:J:98:MET:SD	1:J:98:MET:N	2.89	0.44
1:O:194:GLU:HA	1:O:194:GLU:OE2	2.18	0.44
1:O:212:ARG:O	1:O:216:VAL:HG23	2.18	0.44
1:O:221:TYR:HB2	1:O:277:PRO:HA	2.00	0.44
1:Q:272:LEU:HA	1:Q:275:VAL:HG12	2.00	0.44
1:U:96:SER:OG	1:U:97:VAL:N	2.49	0.44
1:A:128:ARG:HE	1:A:167:GLU:CD	2.21	0.44
1:A:64:ARG:HE	1:A:99:ASP:HA	1.83	0.44
1:C:221:TYR:CE1	1:C:272:LEU:HG	4.47	0.44
1:C:275:VAL:HG13	1:C:276:GLY:O	2.46	0.44
1:D:129:MET:HA	1:D:136:ASP:OD1	2.18	0.44
1:G:105:PHE:HB2	1:G:305:THR:CG2	2.48	0.44
1:H:122:THR:HG22	1:H:125:TYR:H	1.82	0.44
1:H:76:GLN:O	1:H:79:PHE:HB3	2.18	0.44
1:T:56:TRP:CD1	1:T:168:THR:HA	2.52	0.44
1:U:83:LEU:HB3	1:U:202:ARG:NH1	2.29	0.44
1:V:217:ALA:HB1	1:V:277:PRO:HB2	2.00	0.44
1:Y:202:ARG:NH2	1:Y:205:GLN:OE1	2.51	0.44
1:Y:77:GLN:HB3	1:Y:97:VAL:HG11	1.99	0.44
1:Z:64:ARG:HG2	1:Z:102:TYR:CB	2.48	0.44
1:D:80:LEU:HD12	1:D:195:LEU:HD12	2.00	0.44
1:D:212:ARG:HH11	1:E:292:THR:HG21	1.82	0.44
1:D:76:GLN:NE2	1:D:195:LEU:HD21	3.64	0.44
1:K:115:ARG:HD3	1:K:147:ILE:CG2	2.47	0.44
1:M:55:GLU:O	1:M:318:ARG:HG2	2.18	0.44
1:P:229:GLU:HG3	1:P:269:LEU:HD11	2.00	0.44
1:Q:56:TRP:CE3	1:Q:169:ALA:HB2	2.52	0.44
1:U:152:GLY:HA2	1:U:158:VAL:HG12	1.99	0.44
1:U:194:GLU:OE2	1:U:194:GLU:HA	2.18	0.44
1:V:124:TYR:OH	1:V:167:GLU:N	2.42	0.44
1:V:266:GLN:HE21	1:V:269:LEU:CD2	2.30	0.44
1:F:212:ARG:HD3	1:Y:292:THR:HG21	159.34	0.44
1:B:120:LEU:HG	1:B:140:LEU:HD11	2.00	0.43
1:B:58:SER:HB2	1:B:176:LEU:HD22	3.55	0.43
1:B:202:ARG:HH21	1:B:205:GLN:CD	2.22	0.43
1:F:72:GLY:O	1:F:76:GLN:HG3	2.17	0.43
1:J:57:SER:CB	1:J:163:LYS:HE2	2.47	0.43
1:K:98:MET:HG2	1:K:98:MET:H	1.11	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:96:SER:HB3	1:N:99:ASP:OD2	2.18	0.43
1:O:122:THR:HG23	1:O:124:TYR:HB3	2.00	0.43
1:R:62:THR:HG1	1:R:102:TYR:HH	1.56	0.43
1:V:122:THR:HG23	1:V:124:TYR:HB3	1.99	0.43
1:A:61:ILE:HG23	1:A:160:ASP:O	2.30	0.43
1:B:61:ILE:O	1:B:309:LEU:N	2.36	0.43
1:D:81:ARG:O	1:D:85:VAL:HG12	2.18	0.43
1:H:210:VAL:HG22	1:H:286:ASN:CB	2.46	0.43
1:K:228:ILE:HD12	1:K:272:LEU:CD2	2.48	0.43
1:L:83:LEU:HB3	1:L:202:ARG:HD3	2.00	0.43
1:M:304:GLN:HG2	1:M:306:TYR:CE1	2.53	0.43
1:Q:300:ASP:OD1	1:Q:302:ARG:HB2	2.18	0.43
1:S:67:VAL:HG13	1:S:74:TYR:CD2	2.53	0.43
1:X:290:LEU:HD23	1:X:290:LEU:HA	1.79	0.43
1:Y:55:GLU:O	1:Y:318:ARG:HG2	2.18	0.43
1:A:68:ASN:OD1	1:Z:194:GLU:OE2	146.68	0.43
1:B:221:TYR:CE1	1:B:272:LEU:HG	2.81	0.43
1:B:80:LEU:HD23	1:B:83:LEU:HD12	2.88	0.43
1:G:103:LYS:O	1:G:107:MET:HB2	2.18	0.43
1:H:206:MET:HB2	1:H:206:MET:HE2	1.88	0.43
1:S:280:ASP:O	1:S:283:TYR:HB3	2.18	0.43
1:S:198:ALA:CA	1:T:67:VAL:HG11	2.49	0.43
1:U:202:ARG:HH21	1:U:205:GLN:CD	2.22	0.43
1:U:210:VAL:HG13	1:U:283:TYR:CE1	2.53	0.43
1:Z:218:LYS:HE3	1:Z:218:LYS:HB2	1.72	0.43
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.81	0.43
1:B:216:VAL:O	1:B:220:ILE:HG13	2.19	0.43
1:D:64:ARG:HD3	1:D:99:ASP:OD1	2.87	0.43
1:F:266:GLN:O	1:F:269:LEU:HB3	2.18	0.43
1:H:63:ASP:CG	1:H:64:ARG:H	2.22	0.43
1:I:300:ASP:OD1	1:I:302:ARG:HB2	2.19	0.43
1:L:64:ARG:HG2	1:L:64:ARG:H	1.58	0.43
1:B:298:THR:HA	1:T:291:ASN:ND2	177.05	0.43
1:T:64:ARG:NE	1:T:99:ASP:OD1	2.50	0.43
1:W:152:GLY:HA2	1:W:158:VAL:HG12	2.00	0.43
1:X:177:ARG:NH2	1:X:312:PRO:O	2.52	0.43
1:Y:293:LEU:HD12	1:Y:293:LEU:HA	1.84	0.43
1:Z:214:GLU:HG3	1:Z:283:TYR:CE1	2.53	0.43
1:A:223:ARG:O	1:A:227:SER:HB3	3.25	0.43
1:D:150:ILE:HA	1:D:151:PRO:HD2	1.91	0.43
1:F:105:PHE:HA	1:F:187:ALA:HB2	2.28	0.43
1:G:266:GLN:O	1:G:269:LEU:N	2.45	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:114:THR:HG22	1:Q:179:TYR:CE1	2.53	0.43
1:R:227:SER:HB2	1:S:275:VAL:CG2	2.48	0.43
1:S:169:ALA:HB3	1:S:170:PRO:HD3	2.00	0.43
1:V:83:LEU:C	1:V:85:VAL:H	2.21	0.43
1:W:169:ALA:HB3	1:W:170:PRO:HD3	1.99	0.43
1:B:203:THR:OG1	1:B:293:LEU:HD11	2.19	0.43
1:B:67:VAL:HG13	1:B:74:TYR:CG	2.53	0.43
1:B:98:MET:HG2	1:B:98:MET:H	2.36	0.43
1:F:169:ALA:C	1:F:314:GLU:HG2	3.97	0.43
1:G:141:ASP:HB2	1:H:316:VAL:HG11	1.99	0.43
1:J:132:ASN:HB3	1:J:135:ALA:HB3	2.00	0.43
1:L:293:LEU:HD12	1:L:293:LEU:HA	1.80	0.43
1:R:118:PHE:CG	1:R:179:TYR:HD1	2.36	0.43
1:U:212:ARG:O	1:U:216:VAL:HG23	2.18	0.43
1:W:130:VAL:HG23	1:W:132:ASN:H	1.83	0.43
1:X:174:ASN:HB3	1:X:178:GLN:NE2	2.33	0.43
1:B:58:SER:HB3	1:B:312:PRO:HB3	2.00	0.43
1:C:169:ALA:HB1	1:C:314:GLU:HG2	3.68	0.43
1:C:80:LEU:HD11	1:C:199:TRP:HB2	2.27	0.43
1:D:122:THR:HG23	1:D:124:TYR:N	2.34	0.43
1:D:194:GLU:CD	1:E:66:THR:HB	2.58	0.43
1:J:207:LYS:HA	1:J:290:LEU:HD11	2.00	0.43
1:N:128:ARG:HB3	1:N:139:LEU:HD21	2.01	0.43
1:N:156:ARG:O	1:N:157:ALA:HB3	2.18	0.43
1:G:204:ILE:HB	1:O:302:ARG:HH21	1.84	0.43
1:O:169:ALA:HA	1:O:315:PRO:HG2	2.00	0.43
1:P:116:ARG:HA	1:P:144:ILE:HG12	2.00	0.43
1:O:107:MET:CE	1:P:63:ASP:OD2	2.66	0.43
1:W:61:ILE:HG21	1:W:61:ILE:HD13	1.59	0.43
1:B:162:VAL:HG13	1:B:176:LEU:HD11	2.01	0.43
1:B:302:ARG:HH12	1:T:292:THR:CG2	177.81	0.43
1:F:199:TRP:CZ2	1:F:293:LEU:HA	3.78	0.43
1:F:199:TRP:CD1	1:F:297:PRO:HD3	2.66	0.43
1:H:269:LEU:O	1:H:273:GLN:HG3	2.18	0.43
1:I:104:GLU:CD	1:J:307:ARG:HH22	2.21	0.43
1:I:170:PRO:O	1:I:174:ASN:ND2	2.52	0.43
1:L:141:ASP:OD2	1:L:145:ASN:ND2	2.49	0.43
1:L:61:ILE:HB	1:L:310:ARG:HB3	2.01	0.43
1:M:280:ASP:OD2	1:M:283:TYR:N	2.48	0.43
1:M:61:ILE:HB	1:M:310:ARG:HB3	2.00	0.43
1:W:119:TRP:CD2	1:W:143:MET:HB3	2.53	0.43
1:W:81:ARG:NE	1:W:97:VAL:HG22	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:115:ARG:HD3	1:X:147:ILE:HB	2.01	0.43
1:F:122:THR:HG23	1:F:124:TYR:H	1.84	0.43
1:F:61:ILE:N	1:F:310:ARG:HB3	2.34	0.43
1:N:102:TYR:O	1:N:106:VAL:HG23	2.18	0.43
1:G:196:LYS:CE	1:O:298:THR:HG22	2.46	0.43
1:S:228:ILE:HD13	1:S:268:ARG:HG3	2.01	0.43
1:Y:211:LYS:HE3	1:Y:211:LYS:HA	2.01	0.43
1:A:285:GLN:HA	1:Z:216:VAL:HG22	148.10	0.43
1:B:153:ASP:H	1:B:158:VAL:HB	1.84	0.43
1:D:125:TYR:HA	1:D:143:MET:HE1	3.69	0.43
1:E:57:SER:HA	1:E:164:LEU:O	2.18	0.43
1:G:204:ILE:HB	1:O:302:ARG:NH2	2.34	0.43
1:L:141:ASP:HA	1:L:144:ILE:HD12	2.00	0.43
1:M:98:MET:H	1:M:98:MET:HG2	1.50	0.43
1:P:122:THR:O	1:P:126:LYS:HG3	2.19	0.43
1:S:98:MET:N	1:S:98:MET:SD	2.79	0.43
1:T:207:LYS:NZ	1:T:294:ASN:HD21	2.17	0.43
1:U:73:TYR:CZ	1:U:191:LEU:HB3	2.54	0.43
1:V:56:TRP:CD1	1:V:168:THR:HA	2.53	0.43
1:W:122:THR:CG2	1:W:124:TYR:HB3	2.48	0.43
1:Z:122:THR:CG2	1:Z:124:TYR:HB3	2.48	0.43
1:A:214:GLU:OE2	1:A:283:TYR:OH	2.62	0.42
1:A:64:ARG:HA	1:A:102:TYR:CG	2.54	0.42
1:C:124:TYR:O	1:C:128:ARG:HD2	2.19	0.42
1:C:211:LYS:HE3	1:C:211:LYS:HA	3.37	0.42
1:D:275:VAL:HG13	1:D:276:GLY:O	2.53	0.42
1:E:268:ARG:NH1	1:E:268:ARG:CG	3.11	0.42
1:M:126:LYS:O	1:M:129:MET:HE2	2.19	0.42
1:V:213:GLN:NE2	1:V:283:TYR:HA	2.34	0.42
1:W:103:LYS:O	1:W:107:MET:HB2	2.18	0.42
1:Z:73:TYR:CE1	1:Z:191:LEU:HB3	2.54	0.42
1:B:300:ASP:HB2	1:T:295:VAL:HG22	173.98	0.42
1:D:64:ARG:HA	1:D:102:TYR:HB2	2.01	0.42
1:F:120:LEU:HD21	1:F:140:LEU:HD22	2.10	0.42
1:F:58:SER:CB	1:F:173:ASN:HA	3.31	0.42
1:G:153:ASP:H	1:G:158:VAL:HB	1.84	0.42
1:H:153:ASP:H	1:H:158:VAL:HB	1.84	0.42
1:H:58:SER:O	1:H:163:LYS:HG3	2.18	0.42
1:K:294:ASN:HA	1:K:294:ASN:HD22	1.63	0.42
1:O:229:GLU:HG3	1:O:269:LEU:CD1	2.48	0.42
1:Q:280:ASP:O	1:Q:283:TYR:HB3	2.19	0.42
1:R:105:PHE:CE2	1:R:109:LEU:HD22	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:293:LEU:HD12	1:R:293:LEU:HA	1.81	0.42
1:V:105:PHE:HB2	1:V:305:THR:HG23	2.00	0.42
1:Y:125:TYR:HD1	1:Y:143:MET:CE	2.32	0.42
1:Y:76:GLN:NE2	1:Y:297:PRO:HA	2.34	0.42
1:Z:300:ASP:OD1	1:Z:302:ARG:HB2	2.18	0.42
1:A:112:TRP:CZ2	1:A:144:ILE:HG21	3.55	0.42
1:B:203:THR:HA	1:B:293:LEU:HG	2.01	0.42
1:F:280:ASP:OD1	1:F:283:TYR:N	2.35	0.42
1:H:56:TRP:O	1:H:165:ILE:HA	2.20	0.42
1:M:125:TYR:HB2	1:M:143:MET:SD	2.59	0.42
1:N:210:VAL:HG13	1:N:283:TYR:CE1	2.53	0.42
1:P:104:GLU:O	1:P:108:GLN:HG2	2.19	0.42
1:V:187:ALA:HB3	1:V:305:THR:HG21	2.01	0.42
1:A:301:PRO:HD2	1:A:302:ARG:HH11	1.84	0.42
1:B:268:ARG:HA	1:B:268:ARG:HD2	1.76	0.42
1:F:150:ILE:HA	1:F:151:PRO:HD2	1.87	0.42
1:F:61:ILE:HG23	1:F:160:ASP:O	2.19	0.42
1:H:96:SER:O	1:H:99:ASP:HB2	2.19	0.42
1:I:118:PHE:CG	1:I:179:TYR:HD1	2.37	0.42
1:I:223:ARG:HH12	1:J:284:ASP:CG	2.20	0.42
1:M:268:ARG:HD3	1:M:268:ARG:HA	1.91	0.42
1:S:57:SER:CB	1:S:163:LYS:HE2	2.49	0.42
1:R:107:MET:HE3	1:S:309:LEU:HD22	2.00	0.42
1:T:148:GLN:HE21	1:T:148:GLN:HB2	1.61	0.42
1:T:63:ASP:OD1	1:T:64:ARG:N	2.44	0.42
1:Z:79:PHE:CE2	1:Z:83:LEU:HD11	2.54	0.42
1:D:290:LEU:HD23	1:D:290:LEU:HA	1.92	0.42
1:E:294:ASN:HA	1:E:294:ASN:HD22	1.81	0.42
1:F:57:SER:O	1:F:315:PRO:HB3	2.99	0.42
1:G:128:ARG:CB	1:G:139:LEU:HD21	2.50	0.42
1:G:203:THR:HA	1:G:293:LEU:HD23	2.01	0.42
1:G:267:ALA:O	1:G:271:ASN:HB2	2.19	0.42
1:L:266:GLN:HE21	1:L:269:LEU:HD22	1.83	0.42
1:N:169:ALA:HB3	1:N:170:PRO:HD3	2.01	0.42
1:N:210:VAL:HG13	1:N:283:TYR:HE1	1.83	0.42
1:R:62:THR:OG1	1:R:102:TYR:OH	2.27	0.42
1:Y:177:ARG:HG3	1:Y:312:PRO:HB2	2.01	0.42
1:Y:194:GLU:HA	1:Y:194:GLU:OE2	2.20	0.42
1:B:64:ARG:H	1:B:64:ARG:HG2	3.29	0.42
1:D:73:TYR:OH	1:D:191:LEU:HD22	2.20	0.42
1:E:152:GLY:N	1:E:160:ASP:OD2	2.36	0.42
1:F:126:LYS:HG2	1:F:129:MET:HE2	3.29	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:185:GLN:HE22	1:F:301:PRO:HB2	1.83	0.42
1:I:194:GLU:OE2	1:I:194:GLU:HA	2.20	0.42
1:J:229:GLU:HG3	1:J:269:LEU:HD11	2.01	0.42
1:L:69:MET:O	1:L:304:GLN:N	2.52	0.42
1:M:202:ARG:NH2	1:M:205:GLN:OE1	2.46	0.42
1:R:177:ARG:HG3	1:R:312:PRO:HB2	2.02	0.42
1:A:119:TRP:CH2	1:A:143:MET:HG2	2.55	0.42
1:B:180:VAL:HG11	1:B:308:TYR:OH	2.49	0.42
1:C:272:LEU:HA	1:C:275:VAL:HG12	2.16	0.42
1:F:164:LEU:HD13	1:F:175:LEU:C	3.26	0.42
1:I:216:VAL:HG13	1:J:284:ASP:HB3	2.01	0.42
1:N:280:ASP:OD1	1:N:283:TYR:N	2.50	0.42
1:O:141:ASP:O	1:O:145:ASN:ND2	2.53	0.42
1:P:268:ARG:HD2	1:P:268:ARG:HA	1.60	0.42
1:P:64:ARG:H	1:P:64:ARG:HG2	1.51	0.42
1:Q:60:ALA:HB2	1:Q:312:PRO:HG3	2.02	0.42
1:R:137:ALA:C	1:S:316:VAL:HG11	2.40	0.42
1:W:115:ARG:HB3	1:W:144:ILE:HA	2.01	0.42
1:W:194:GLU:OE2	1:W:194:GLU:HA	2.20	0.42
1:W:60:ALA:HB2	1:W:312:PRO:HG3	2.01	0.42
1:D:130:VAL:HG23	1:D:132:ASN:H	2.41	0.42
1:E:228:ILE:HG22	1:E:269:LEU:HD13	2.01	0.42
1:L:300:ASP:O	1:L:303:PHE:CD2	2.73	0.42
1:P:202:ARG:CZ	1:P:205:GLN:HE21	2.33	0.42
1:U:291:ASN:O	1:U:294:ASN:HB2	2.20	0.42
1:U:57:SER:CB	1:U:163:LYS:HE2	2.49	0.42
1:W:105:PHE:HB2	1:W:305:THR:CG2	2.43	0.42
1:Y:56:TRP:CD1	1:Y:168:THR:HA	2.54	0.42
1:A:58:SER:O	1:A:163:LYS:HA	2.19	0.42
1:C:102:TYR:HA	1:C:105:PHE:HB3	2.29	0.42
1:C:216:VAL:HG13	1:D:284:ASP:CB	2.74	0.42
1:D:275:VAL:HG13	1:D:276:GLY:N	2.34	0.42
1:D:96:SER:HB3	1:D:99:ASP:OD2	2.98	0.42
1:G:210:VAL:HA	1:G:213:GLN:NE2	2.31	0.42
1:G:217:ALA:HB1	1:G:277:PRO:HB3	2.02	0.42
1:H:266:GLN:HG2	1:H:266:GLN:O	2.19	0.42
1:O:63:ASP:HB2	1:O:309:LEU:HD11	2.01	0.42
1:O:58:SER:HB2	1:O:172:ALA:C	2.40	0.42
1:Y:65:PRO:HD2	1:Y:102:TYR:HB2	2.02	0.42
1:C:132:ASN:HB3	1:C:135:ALA:HB3	2.02	0.42
1:C:73:TYR:CE1	1:C:191:LEU:HB3	2.55	0.42
1:D:148:GLN:HE21	1:D:148:GLN:HB2	3.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:224:ARG:HA	1:D:227:SER:OG	2.20	0.42
1:I:152:GLY:HA2	1:I:158:VAL:HG12	2.02	0.42
1:M:216:VAL:HG21	1:N:285:GLN:HG2	2.02	0.42
1:N:126:LYS:O	1:N:129:MET:CG	2.67	0.42
1:N:268:ARG:HD2	1:N:268:ARG:HA	1.59	0.42
1:Q:109:LEU:HD23	1:Q:149:PHE:CE1	2.54	0.42
1:S:153:ASP:OD2	1:S:156:ARG:HD2	2.19	0.42
1:S:66:THR:OG1	1:S:69:MET:SD	2.73	0.42
1:T:70:LEU:HB2	1:T:74:TYR:HB2	2.01	0.42
1:U:148:GLN:HB2	1:U:148:GLN:HE21	1.61	0.42
1:U:57:SER:HA	1:U:164:LEU:O	2.20	0.42
1:A:74:TYR:HA	1:A:97:VAL:HG11	2.66	0.41
1:D:280:ASP:O	1:D:283:TYR:HB3	2.43	0.41
1:E:77:GLN:OE1	1:E:77:GLN:HA	2.96	0.41
1:F:67:VAL:HG12	1:F:98:MET:CE	2.50	0.41
1:G:122:THR:CG2	1:G:124:TYR:HB3	2.50	0.41
1:H:56:TRP:CD1	1:H:168:THR:HA	2.55	0.41
1:H:74:TYR:CZ	1:H:78:GLN:HG3	2.55	0.41
1:L:209:GLN:HA	1:L:212:ARG:NH2	2.35	0.41
1:L:294:ASN:HD22	1:L:294:ASN:HA	1.66	0.41
1:M:102:TYR:OH	1:M:160:ASP:OD1	2.35	0.41
1:N:226:ASN:OD1	1:N:230:GLN:NE2	2.48	0.41
1:P:184:SER:HB2	1:P:306:TYR:CD1	2.55	0.41
1:P:207:LYS:O	1:P:211:LYS:HB2	2.20	0.41
1:Q:293:LEU:HA	1:Q:293:LEU:HD12	1.91	0.41
1:S:188:ALA:HA	1:S:303:PHE:CZ	2.55	0.41
1:S:198:ALA:HA	1:T:67:VAL:HG11	2.01	0.41
1:X:112:TRP:CD2	1:X:144:ILE:HG21	2.55	0.41
1:B:224:ARG:HB3	1:B:272:LEU:CD2	4.11	0.41
1:D:55:GLU:O	1:D:319:ASP:N	2.39	0.41
1:D:68:ASN:ND2	1:D:68:ASN:H	2.18	0.41
1:D:223:ARG:NH1	1:E:284:ASP:OD2	2.53	0.41
1:J:130:VAL:HG23	1:J:132:ASN:H	1.86	0.41
1:K:182:PHE:CE2	1:K:186:ARG:HD2	2.55	0.41
1:L:126:LYS:O	1:L:129:MET:HE2	2.20	0.41
1:L:156:ARG:HA	1:L:156:ARG:HE	1.85	0.41
1:M:211:LYS:HA	1:M:211:LYS:HE3	2.01	0.41
1:N:98:MET:HG2	1:N:98:MET:H	1.00	0.41
1:Q:101:ALA:HA	1:Q:191:LEU:HD11	2.02	0.41
1:S:268:ARG:HD2	1:S:268:ARG:HA	1.76	0.41
1:S:63:ASP:OD1	1:S:64:ARG:N	2.48	0.41
1:V:121:GLN:HG2	1:V:121:GLN:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:119:TRP:NE1	1:X:143:MET:O	2.53	0.41
1:Y:69:MET:CE	1:Y:304:GLN:HB3	2.50	0.41
1:Y:63:ASP:OD2	1:Y:64:ARG:N	2.44	0.41
1:A:77:GLN:HA	1:A:77:GLN:OE1	2.20	0.41
1:D:293:LEU:HA	1:D:293:LEU:HD12	1.78	0.41
1:D:60:ALA:HB2	1:D:312:PRO:HG3	2.02	0.41
1:E:74:TYR:HE1	1:E:98:MET:HE1	1.85	0.41
1:F:162:VAL:HG13	1:F:176:LEU:HD11	2.72	0.41
1:F:223:ARG:O	1:F:227:SER:HB3	2.78	0.41
1:I:293:LEU:HD12	1:I:293:LEU:HA	1.88	0.41
1:L:63:ASP:OD1	1:L:64:ARG:HG2	2.20	0.41
1:N:173:ASN:HB2	1:N:314:GLU:HA	2.01	0.41
1:Q:194:GLU:OE2	1:Q:194:GLU:HA	2.21	0.41
1:R:124:TYR:HH	1:R:167:GLU:H	1.60	0.41
1:U:281:LEU:O	1:U:285:GLN:HG3	2.20	0.41
1:W:57:SER:OG	1:W:163:LYS:HE2	2.20	0.41
1:X:101:ALA:HA	1:X:191:LEU:HD11	2.01	0.41
1:B:199:TRP:CG	1:B:297:PRO:HD3	2.58	0.41
1:E:304:GLN:HG2	1:E:306:TYR:O	2.20	0.41
1:M:156:ARG:O	1:M:157:ALA:HB3	2.20	0.41
1:M:56:TRP:CD1	1:M:168:THR:HA	2.56	0.41
1:N:203:THR:O	1:N:207:LYS:HB2	2.20	0.41
1:O:194:GLU:OE2	1:P:66:THR:HB	2.20	0.41
1:P:179:TYR:O	1:P:182:PHE:HB3	2.20	0.41
1:Q:65:PRO:HA	1:Q:69:MET:HE1	2.03	0.41
1:R:56:TRP:CE3	1:R:315:PRO:HG2	2.53	0.41
1:U:73:TYR:OH	1:U:191:LEU:HB3	2.20	0.41
1:X:74:TYR:OH	1:X:78:GLN:NE2	2.46	0.41
1:Z:61:ILE:HG22	1:Z:309:LEU:HB2	2.03	0.41
1:A:125:TYR:OH	1:A:136:ASP:HB3	2.20	0.41
1:A:180:VAL:HG11	1:A:308:TYR:OH	2.33	0.41
1:C:56:TRP:CE3	1:C:169:ALA:HB2	2.55	0.41
1:C:291:ASN:O	1:C:295:VAL:HG23	2.21	0.41
1:C:187:ALA:CB	1:C:305:THR:HG21	2.48	0.41
1:F:203:THR:O	1:F:207:LYS:HG2	5.19	0.41
1:F:289:MET:O	1:F:293:LEU:HB2	2.27	0.41
1:J:225:MET:CE	1:J:273:GLN:HG2	2.50	0.41
1:J:188:ALA:HB1	1:J:303:PHE:CE2	2.55	0.41
1:K:115:ARG:HG3	1:K:179:TYR:OH	2.20	0.41
1:K:177:ARG:NH2	1:K:312:PRO:O	2.54	0.41
1:M:57:SER:HA	1:M:164:LEU:O	2.20	0.41
1:B:302:ARG:CZ	1:T:292:THR:HG22	176.60	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:301:PRO:HD2	1:U:302:ARG:HD3	2.02	0.41
1:W:63:ASP:OD1	1:W:64:ARG:HG2	2.20	0.41
1:A:122:THR:HG22	1:A:125:TYR:H	1.85	0.41
1:B:300:ASP:OD1	1:B:302:ARG:HB2	3.72	0.41
1:B:55:GLU:HG2	1:B:167:GLU:HA	2.02	0.41
1:A:198:ALA:HA	1:B:67:VAL:HG11	3.16	0.41
1:B:223:ARG:NH2	1:C:284:ASP:OD1	2.90	0.41
1:C:74:TYR:CE2	1:C:78:GLN:HG3	2.55	0.41
1:D:180:VAL:HG23	1:D:181:ALA:N	2.36	0.41
1:D:80:LEU:HA	1:D:83:LEU:HD12	2.01	0.41
1:F:64:ARG:HA	1:F:102:TYR:CG	2.56	0.41
1:F:73:TYR:OH	1:F:191:LEU:HD22	2.21	0.41
1:G:65:PRO:HB2	1:G:69:MET:HG2	2.02	0.41
1:H:122:THR:O	1:H:126:LYS:HE3	2.21	0.41
1:K:225:MET:CB	1:K:272:LEU:HD11	2.44	0.41
1:N:64:ARG:NE	1:N:99:ASP:OD1	2.53	0.41
1:O:119:TRP:HE3	1:O:122:THR:HG21	1.80	0.41
1:R:124:TYR:OH	1:R:167:GLU:HG3	2.20	0.41
1:T:184:SER:HB2	1:T:306:TYR:CD1	2.56	0.41
1:V:294:ASN:HD22	1:V:294:ASN:HA	1.64	0.41
1:Y:56:TRP:O	1:Y:165:ILE:HA	2.20	0.41
1:B:214:GLU:OE2	1:B:283:TYR:OH	2.31	0.41
1:B:68:ASN:H	1:B:68:ASN:ND2	2.18	0.41
1:D:147:ILE:HA	1:D:163:LYS:O	2.20	0.41
1:D:182:PHE:CE2	1:D:186:ARG:HD2	2.56	0.41
1:D:225:MET:HE1	1:D:273:GLN:HA	2.03	0.41
1:E:74:TYR:HE1	1:E:98:MET:CE	2.33	0.41
1:F:96:SER:OG	1:F:98:MET:SD	2.68	0.41
1:J:182:PHE:CE2	1:J:186:ARG:HD2	2.55	0.41
1:J:206:MET:HG3	1:J:206:MET:O	2.21	0.41
1:O:176:LEU:HA	1:O:176:LEU:HD12	1.85	0.41
1:P:202:ARG:HH21	1:P:205:GLN:HE21	1.68	0.41
1:R:127:GLN:HB2	1:R:127:GLN:HE21	1.77	0.41
1:W:221:TYR:HB2	1:W:277:PRO:HB3	2.03	0.41
1:X:177:ARG:HG3	1:X:312:PRO:HB2	2.03	0.41
1:W:198:ALA:CA	1:X:67:VAL:HG11	2.51	0.41
1:Z:168:THR:OG1	1:Z:171:ASP:OD2	2.31	0.41
1:A:104:GLU:OE1	1:B:307:ARG:NH2	3.78	0.41
1:D:266:GLN:NE2	1:D:269:LEU:HD23	2.36	0.41
1:E:293:LEU:HD12	1:E:293:LEU:HA	1.73	0.41
1:E:291:ASN:O	1:E:294:ASN:HB2	2.21	0.41
1:E:64:ARG:HA	1:E:102:TYR:CG	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:125:TYR:CD1	1:G:143:MET:HE2	2.52	0.41
1:I:63:ASP:OD2	1:I:159:ASN:ND2	2.54	0.41
1:J:202:ARG:CZ	1:J:205:GLN:HG2	2.51	0.41
1:L:76:GLN:CB	1:L:195:LEU:HD11	2.51	0.41
1:P:288:ALA:O	1:P:291:ASN:HB2	2.21	0.41
1:P:180:VAL:HG11	1:P:308:TYR:CZ	2.56	0.41
1:U:194:GLU:OE2	1:V:66:THR:HB	2.21	0.41
1:U:290:LEU:HA	1:U:290:LEU:HD23	1.84	0.41
1:X:171:ASP:O	1:X:175:LEU:HB2	2.20	0.41
1:X:272:LEU:HA	1:X:275:VAL:HG12	2.02	0.41
1:Y:216:VAL:HG13	1:Z:284:ASP:HB3	2.03	0.41
1:Y:290:LEU:HD23	1:Y:290:LEU:HA	1.92	0.41
1:Z:280:ASP:O	1:Z:283:TYR:HB3	2.20	0.41
1:A:137:ALA:O	1:A:140:LEU:HB3	2.21	0.41
1:B:57:SER:HA	1:B:164:LEU:O	2.21	0.41
1:G:268:ARG:HA	1:G:268:ARG:HD2	1.72	0.41
1:J:294:ASN:HA	1:J:294:ASN:HD22	1.66	0.41
1:J:69:MET:HG2	1:J:304:GLN:HB3	2.03	0.41
1:K:120:LEU:O	1:K:126:LYS:HE3	2.21	0.41
1:K:206:MET:HG2	1:K:290:LEU:HG	2.03	0.41
1:S:61:ILE:HG22	1:S:309:LEU:HD12	2.01	0.41
1:C:283:TYR:OH	1:C:287:ARG:HD3	2.20	0.41
1:C:300:ASP:OD1	1:C:302:ARG:HD3	4.32	0.41
1:D:122:THR:HG23	1:D:124:TYR:H	1.84	0.41
1:D:300:ASP:OD1	1:D:302:ARG:NH1	2.54	0.41
1:E:275:VAL:CG1	1:E:276:GLY:H	2.24	0.41
1:H:73:TYR:CD1	1:H:195:LEU:HD22	2.56	0.41
1:I:67:VAL:O	1:I:70:LEU:HB2	2.21	0.41
1:J:61:ILE:HB	1:J:310:ARG:HB3	2.03	0.41
1:L:97:VAL:HB	1:L:98:MET:HE2	2.03	0.41
1:N:77:GLN:OE1	1:N:77:GLN:HA	2.21	0.41
1:O:128:ARG:HE	1:O:167:GLU:CD	2.24	0.41
1:O:209:GLN:HA	1:O:212:ARG:NH2	2.36	0.41
1:O:272:LEU:HA	1:O:275:VAL:HG12	2.02	0.41
1:Q:146:ASN:HA	1:Q:146:ASN:HD22	1.68	0.41
1:R:213:GLN:NE2	1:R:286:ASN:HD22	2.18	0.41
1:S:74:TYR:CD1	1:S:97:VAL:HG22	2.56	0.41
1:T:122:THR:CG2	1:T:125:TYR:H	2.34	0.41
1:T:70:LEU:HA	1:T:303:PHE:HD1	1.86	0.41
1:X:141:ASP:HA	1:X:144:ILE:HD12	2.03	0.41
1:Y:122:THR:CG2	1:Y:124:TYR:HB3	2.51	0.41
1:Y:305:THR:O	1:Y:305:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:MET:HG3	1:B:304:GLN:HB3	4.29	0.41
1:B:67:VAL:HG13	1:B:74:TYR:CD1	2.56	0.41
1:C:147:ILE:HG12	1:C:164:LEU:HD12	2.45	0.41
1:D:305:THR:O	1:D:305:THR:HG23	2.33	0.41
1:E:119:TRP:CG	1:E:143:MET:HB3	3.41	0.41
1:F:207:LYS:NZ	1:F:294:ASN:HD21	4.23	0.41
1:H:118:PHE:HE1	1:H:178:GLN:HB3	1.86	0.41
1:I:300:ASP:OD1	1:I:302:ARG:HD3	2.21	0.41
1:K:280:ASP:OD1	1:K:282:ASP:HB2	2.21	0.41
1:P:280:ASP:O	1:P:283:TYR:HB3	2.21	0.41
1:Q:61:ILE:O	1:Q:309:LEU:N	2.33	0.41
1:U:60:ALA:HB2	1:U:312:PRO:HG3	2.03	0.41
1:V:124:TYR:OH	1:V:167:GLU:HG3	2.21	0.41
1:B:74:TYR:OH	1:B:78:GLN:NE2	2.53	0.40
1:C:70:LEU:HA	1:C:303:PHE:HD1	1.86	0.40
1:D:177:ARG:NH2	1:D:312:PRO:O	2.54	0.40
1:F:268:ARG:HA	1:F:268:ARG:HD2	2.14	0.40
1:F:59:THR:O	1:F:312:PRO:HA	2.93	0.40
1:G:76:GLN:HE21	1:G:298:THR:H	1.68	0.40
1:G:80:LEU:HD23	1:G:80:LEU:HA	1.80	0.40
1:H:139:LEU:HD11	1:H:143:MET:CE	2.51	0.40
1:H:119:TRP:CE2	1:H:143:MET:HB3	2.56	0.40
1:J:141:ASP:O	1:J:145:ASN:ND2	2.54	0.40
1:M:104:GLU:OE1	1:N:307:ARG:NH2	2.46	0.40
1:P:228:ILE:HG22	1:P:269:LEU:HD12	2.03	0.40
1:S:198:ALA:N	1:T:67:VAL:HG11	2.36	0.40
1:Z:74:TYR:CD1	1:Z:97:VAL:HB	2.56	0.40
1:A:122:THR:CG2	1:A:125:TYR:H	2.34	0.40
1:A:227:SER:HB2	1:B:275:VAL:HG23	3.60	0.40
1:C:124:TYR:CD2	1:C:175:LEU:HD11	2.83	0.40
1:E:188:ALA:HB1	1:E:303:PHE:CE2	2.66	0.40
1:F:122:THR:HG23	1:F:124:TYR:N	2.37	0.40
1:F:119:TRP:CE2	1:F:143:MET:HB3	2.63	0.40
1:F:125:TYR:HB2	1:F:143:MET:SD	2.61	0.40
1:F:221:TYR:HE1	1:F:272:LEU:O	2.08	0.40
1:Q:105:PHE:HA	1:Q:187:ALA:HB2	2.03	0.40
1:U:203:THR:HA	1:U:293:LEU:HG	2.04	0.40
1:U:209:GLN:O	1:U:213:GLN:HG3	2.21	0.40
1:W:119:TRP:NE1	1:W:143:MET:O	2.54	0.40
1:W:76:GLN:NE2	1:W:297:PRO:HA	2.36	0.40
1:Y:162:VAL:HG13	1:Y:176:LEU:HD11	2.02	0.40
1:C:150:ILE:HA	1:C:151:PRO:HD2	1.91	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:147:ILE:HG12	1:D:164:LEU:HD12	2.14	0.40
1:D:199:TRP:CG	1:D:297:PRO:HD3	2.56	0.40
1:E:80:LEU:HA	1:E:80:LEU:HD23	1.90	0.40
1:F:188:ALA:HB1	1:F:303:PHE:CE2	2.77	0.40
1:G:128:ARG:HB3	1:G:139:LEU:HD21	2.04	0.40
1:G:125:TYR:OH	1:G:140:LEU:HB2	2.22	0.40
1:L:216:VAL:O	1:L:220:ILE:HG13	2.22	0.40
1:R:210:VAL:O	1:R:213:GLN:HB2	2.21	0.40
1:S:212:ARG:HG2	1:T:288:ALA:CB	2.48	0.40
1:V:286:ASN:O	1:V:290:LEU:HB2	2.21	0.40
1:W:294:ASN:HA	1:W:294:ASN:HD22	1.60	0.40
1:X:137:ALA:O	1:X:140:LEU:HB3	2.21	0.40
1:X:146:ASN:HB3	1:X:165:ILE:HB	2.04	0.40
1:A:59:THR:HA	1:A:162:VAL:O	2.30	0.40
1:A:98:MET:HG2	1:A:98:MET:H	3.58	0.40
1:B:126:LYS:HA	1:B:129:MET:SD	3.79	0.40
1:C:169:ALA:CB	1:C:314:GLU:HG2	4.30	0.40
1:C:199:TRP:NE1	1:C:293:LEU:O	2.68	0.40
1:D:191:LEU:O	1:D:194:GLU:HB2	2.88	0.40
1:F:56:TRP:CE3	1:F:169:ALA:HB2	2.56	0.40
1:G:123:ASP:O	1:G:127:GLN:HG3	2.22	0.40
1:I:61:ILE:HG22	1:I:309:LEU:HB2	2.02	0.40
1:N:57:SER:O	1:N:315:PRO:HB3	2.22	0.40
1:O:180:VAL:HG11	1:O:308:TYR:CE1	2.57	0.40
1:O:77:GLN:HA	1:O:77:GLN:OE1	2.21	0.40
1:P:122:THR:HG23	1:P:124:TYR:HB3	2.02	0.40
1:P:143:MET:HB3	1:P:143:MET:HE2	1.97	0.40
1:R:148:GLN:HE21	1:R:148:GLN:HB2	1.55	0.40
1:U:132:ASN:ND2	1:U:134:LYS:HB3	2.37	0.40
1:V:122:THR:CG2	1:V:125:TYR:H	2.34	0.40
1:V:210:VAL:HA	1:V:213:GLN:HE21	1.86	0.40
1:V:213:GLN:NE2	1:V:286:ASN:HD22	2.19	0.40
1:W:124:TYR:OH	1:W:167:GLU:N	2.42	0.40
1:A:148:GLN:HB2	1:A:148:GLN:HE21	1.57	0.40
1:A:81:ARG:O	1:A:85:VAL:HG22	2.76	0.40
1:B:194:GLU:CD	1:C:66:THR:HB	2.42	0.40
1:D:61:ILE:HG13	1:D:161:SER:HB3	3.56	0.40
1:E:77:GLN:OE1	1:E:195:LEU:HD13	2.21	0.40
1:F:70:LEU:HD11	1:F:98:MET:HA	2.04	0.40
1:H:206:MET:HE1	1:H:289:MET:HG2	2.03	0.40
1:M:119:TRP:HE3	1:M:122:THR:HG21	1.85	0.40
1:P:79:PHE:O	1:P:83:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:308:TYR:CE2	1:S:311:THR:HG23	2.57	0.40
1:W:109:LEU:HA	1:W:109:LEU:HD12	1.96	0.40
1:Z:64:ARG:O	1:Z:307:ARG:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:196:LYS:NZ	1:L:296:GLY:O[2_546]	1.93	0.27

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	B	215/356 (60%)	212 (99%)	3 (1%)	0	100	100
1	C	215/356 (60%)	213 (99%)	2 (1%)	0	100	100
1	D	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	E	215/356 (60%)	212 (99%)	2 (1%)	1 (0%)	38	88
1	F	215/356 (60%)	210 (98%)	4 (2%)	1 (0%)	38	88
1	G	215/356 (60%)	211 (98%)	3 (1%)	1 (0%)	38	88
1	H	215/356 (60%)	211 (98%)	3 (1%)	1 (0%)	38	88
1	I	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	J	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	K	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	L	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	M	215/356 (60%)	207 (96%)	8 (4%)	0	100	100
1	N	215/356 (60%)	208 (97%)	7 (3%)	0	100	100
1	O	215/356 (60%)	210 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	Q	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	R	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	S	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	T	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	U	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	V	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	W	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	X	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	Y	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	Z	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	a	215/356 (60%)	208 (97%)	7 (3%)	0	100	100
1	b	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	c	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	d	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	e	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	f	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
All	All	6880/11392 (60%)	6715 (98%)	161 (2%)	4 (0%)	59	95

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	275	VAL
1	H	303	PHE
1	F	318	ARG
1	G	269	LEU

### 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	190/296 (64%)	165 (87%)	25 (13%)	6	35
1	B	190/296 (64%)	174 (92%)	16 (8%)	16	60
1	C	190/296 (64%)	169 (89%)	21 (11%)	9	45
1	D	190/296 (64%)	173 (91%)	17 (9%)	14	56
1	E	190/296 (64%)	166 (87%)	24 (13%)	7	38
1	F	190/296 (64%)	175 (92%)	15 (8%)	18	62
1	G	190/296 (64%)	175 (92%)	15 (8%)	18	62
1	H	190/296 (64%)	167 (88%)	23 (12%)	7	40
1	I	190/296 (64%)	165 (87%)	25 (13%)	6	35
1	J	190/296 (64%)	169 (89%)	21 (11%)	9	45
1	K	190/296 (64%)	167 (88%)	23 (12%)	7	40
1	L	190/296 (64%)	164 (86%)	26 (14%)	5	33
1	M	190/296 (64%)	162 (85%)	28 (15%)	4	30
1	N	190/296 (64%)	174 (92%)	16 (8%)	16	60
1	O	190/296 (64%)	172 (90%)	18 (10%)	12	52
1	P	190/296 (64%)	166 (87%)	24 (13%)	7	38
1	Q	190/296 (64%)	172 (90%)	18 (10%)	12	52
1	R	190/296 (64%)	170 (90%)	20 (10%)	10	47
1	S	190/296 (64%)	167 (88%)	23 (12%)	7	40
1	T	190/296 (64%)	171 (90%)	19 (10%)	11	50
1	U	190/296 (64%)	165 (87%)	25 (13%)	6	35
1	V	190/296 (64%)	172 (90%)	18 (10%)	12	52
1	W	190/296 (64%)	173 (91%)	17 (9%)	14	56
1	X	190/296 (64%)	171 (90%)	19 (10%)	11	50
1	Y	190/296 (64%)	161 (85%)	29 (15%)	4	28
1	Z	190/296 (64%)	166 (87%)	24 (13%)	7	38
1	a	190/296 (64%)	168 (88%)	22 (12%)	8	42
1	b	190/296 (64%)	167 (88%)	23 (12%)	7	40
1	c	190/296 (64%)	169 (89%)	21 (11%)	9	45
1	d	190/296 (64%)	171 (90%)	19 (10%)	11	50
1	e	190/296 (64%)	168 (88%)	22 (12%)	8	42
1	f	190/296 (64%)	169 (89%)	21 (11%)	9	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6080/9472 (64%)	5403 (89%)	677 (11%)	9 45

All (677) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	61	ILE
1	A	67	VAL
1	A	68	ASN
1	A	96	SER
1	A	98	MET
1	A	106	VAL
1	A	121	GLN
1	A	122	THR
1	A	148	GLN
1	A	150	ILE
1	A	155	THR
1	A	158	VAL
1	A	202	ARG
1	A	206	MET
1	A	211	LYS
1	A	282	ASP
1	A	289	MET
1	A	290	LEU
1	A	292	THR
1	A	293	LEU
1	A	299	LEU
1	A	302	ARG
1	A	305	THR
1	A	317	LYS
1	B	62	THR
1	B	84	ASP
1	B	85	VAL
1	B	98	MET
1	B	121	GLN
1	B	133	SER
1	B	148	GLN
1	B	153	ASP
1	B	189	SER
1	B	211	LYS
1	B	218	LYS
1	B	268	ARG

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Mol	Chain	Res	Type
1	B	287	ARG
1	B	293	LEU
1	B	305	THR
1	B	316	VAL
1	C	55	GLU
1	C	68	ASN
1	C	97	VAL
1	C	98	MET
1	C	107	MET
1	C	114	THR
1	C	121	GLN
1	C	122	THR
1	C	133	SER
1	C	206	MET
1	C	211	LYS
1	C	225	MET
1	C	272	LEU
1	C	273	GLN
1	C	282	ASP
1	C	290	LEU
1	C	292	THR
1	C	293	LEU
1	C	305	THR
1	C	316	VAL
1	C	318	ARG
1	D	58	SER
1	D	64	ARG
1	D	98	MET
1	D	122	THR
1	D	130	VAL
1	D	148	GLN
1	D	158	VAL
1	D	204	ILE
1	D	205	GLN
1	D	268	ARG
1	D	273	GLN
1	D	287	ARG
1	D	290	LEU
1	D	293	LEU
1	D	300	ASP
1	D	302	ARG
1	D	305	THR

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Mol	Chain	Res	Type
1	E	64	ARG
1	E	68	ASN
1	E	84	ASP
1	E	98	MET
1	E	111	SER
1	E	121	GLN
1	E	122	THR
1	E	148	GLN
1	E	156	ARG
1	E	185	GLN
1	E	202	ARG
1	E	205	GLN
1	E	211	LYS
1	E	215	GLU
1	E	224	ARG
1	E	266	GLN
1	E	268	ARG
1	E	271	ASN
1	E	282	ASP
1	E	290	LEU
1	E	293	LEU
1	E	299	LEU
1	E	302	ARG
1	E	305	THR
1	F	55	GLU
1	F	59	THR
1	F	84	ASP
1	F	96	SER
1	F	98	MET
1	F	122	THR
1	F	144	ILE
1	F	163	LYS
1	F	207	LYS
1	F	216	VAL
1	F	290	LEU
1	F	298	THR
1	F	302	ARG
1	F	316	VAL
1	F	318	ARG
1	G	58	SER
1	G	64	ARG
1	G	84	ASP

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Mol	Chain	Res	Type
1	G	85	VAL
1	G	98	MET
1	G	111	SER
1	G	121	GLN
1	G	122	THR
1	G	155	THR
1	G	211	LYS
1	G	268	ARG
1	G	282	ASP
1	G	287	ARG
1	G	304	GLN
1	G	305	THR
1	H	55	GLU
1	H	59	THR
1	H	64	ARG
1	H	84	ASP
1	H	85	VAL
1	H	98	MET
1	H	103	LYS
1	H	122	THR
1	H	130	VAL
1	H	133	SER
1	H	134	LYS
1	H	153	ASP
1	H	205	GLN
1	H	206	MET
1	H	210	VAL
1	H	225	MET
1	H	227	SER
1	H	268	ARG
1	H	271	ASN
1	H	287	ARG
1	H	290	LEU
1	H	292	THR
1	H	305	THR
1	I	55	GLU
1	I	58	SER
1	I	59	THR
1	I	66	THR
1	I	68	ASN
1	I	85	VAL
1	I	96	SER

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Mol	Chain	Res	Type
1	I	98	MET
1	I	121	GLN
1	I	122	THR
1	I	147	ILE
1	I	148	GLN
1	I	155	THR
1	I	202	ARG
1	I	211	LYS
1	I	282	ASP
1	I	289	MET
1	I	290	LEU
1	I	292	THR
1	I	293	LEU
1	I	298	THR
1	I	299	LEU
1	I	305	THR
1	I	311	THR
1	I	317	LYS
1	J	66	THR
1	J	68	ASN
1	J	96	SER
1	J	98	MET
1	J	121	GLN
1	J	147	ILE
1	J	148	GLN
1	J	155	THR
1	J	203	THR
1	J	205	GLN
1	J	211	LYS
1	J	224	ARG
1	J	227	SER
1	J	268	ARG
1	J	282	ASP
1	J	290	LEU
1	J	293	LEU
1	J	299	LEU
1	J	302	ARG
1	J	305	THR
1	J	316	VAL
1	K	58	SER
1	K	68	ASN
1	K	78	GLN

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Mol	Chain	Res	Type
1	K	85	VAL
1	K	96	SER
1	K	98	MET
1	K	107	MET
1	K	121	GLN
1	K	122	THR
1	K	202	ARG
1	K	211	LYS
1	K	224	ARG
1	K	225	MET
1	K	227	SER
1	K	272	LEU
1	K	282	ASP
1	K	290	LEU
1	K	293	LEU
1	K	299	LEU
1	K	302	ARG
1	K	305	THR
1	K	316	VAL
1	K	317	LYS
1	L	58	SER
1	L	59	THR
1	L	64	ARG
1	L	66	THR
1	L	68	ASN
1	L	69	MET
1	L	96	SER
1	L	98	MET
1	L	121	GLN
1	L	130	VAL
1	L	148	GLN
1	L	156	ARG
1	L	205	GLN
1	L	211	LYS
1	L	215	GLU
1	L	220	ILE
1	L	225	MET
1	L	227	SER
1	L	271	ASN
1	L	275	VAL
1	L	289	MET
1	L	290	LEU

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Mol	Chain	Res	Type
1	L	293	LEU
1	L	295	VAL
1	L	302	ARG
1	L	305	THR
1	M	58	SER
1	M	66	THR
1	M	96	SER
1	M	97	VAL
1	M	98	MET
1	M	107	MET
1	M	114	THR
1	M	121	GLN
1	M	122	THR
1	M	130	VAL
1	M	144	ILE
1	M	148	GLN
1	M	155	THR
1	M	156	ARG
1	M	202	ARG
1	M	206	MET
1	M	211	LYS
1	M	215	GLU
1	M	220	ILE
1	M	227	SER
1	M	228	ILE
1	M	230	GLN
1	M	282	ASP
1	M	290	LEU
1	M	293	LEU
1	M	299	LEU
1	M	302	ARG
1	M	305	THR
1	N	67	VAL
1	N	68	ASN
1	N	96	SER
1	N	98	MET
1	N	121	GLN
1	N	122	THR
1	N	129	MET
1	N	147	ILE
1	N	148	GLN
1	N	156	ARG

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Mol	Chain	Res	Type
1	N	216	VAL
1	N	290	LEU
1	N	293	LEU
1	N	299	LEU
1	N	305	THR
1	N	317	LYS
1	O	58	SER
1	O	96	SER
1	O	98	MET
1	O	107	MET
1	O	121	GLN
1	O	122	THR
1	O	126	LYS
1	O	144	ILE
1	O	148	GLN
1	O	155	THR
1	O	165	ILE
1	O	227	SER
1	O	282	ASP
1	O	289	MET
1	O	290	LEU
1	O	293	LEU
1	O	299	LEU
1	O	302	ARG
1	P	58	SER
1	P	59	THR
1	P	61	ILE
1	P	68	ASN
1	P	85	VAL
1	P	96	SER
1	P	98	MET
1	P	121	GLN
1	P	122	THR
1	P	134	LYS
1	P	153	ASP
1	P	165	ILE
1	P	202	ARG
1	P	205	GLN
1	P	211	LYS
1	P	220	ILE
1	P	224	ARG
1	P	227	SER

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Mol	Chain	Res	Type
1	P	275	VAL
1	P	289	MET
1	P	290	LEU
1	P	293	LEU
1	P	299	LEU
1	P	305	THR
1	Q	68	ASN
1	Q	85	VAL
1	Q	96	SER
1	Q	98	MET
1	Q	121	GLN
1	Q	148	GLN
1	Q	202	ARG
1	Q	211	LYS
1	Q	220	ILE
1	Q	282	ASP
1	Q	290	LEU
1	Q	292	THR
1	Q	293	LEU
1	Q	298	THR
1	Q	299	LEU
1	Q	302	ARG
1	Q	305	THR
1	Q	317	LYS
1	R	58	SER
1	R	64	ARG
1	R	68	ASN
1	R	96	SER
1	R	98	MET
1	R	107	MET
1	R	121	GLN
1	R	122	THR
1	R	130	VAL
1	R	148	GLN
1	R	202	ARG
1	R	211	LYS
1	R	225	MET
1	R	227	SER
1	R	228	ILE
1	R	268	ARG
1	R	290	LEU
1	R	293	LEU

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Mol	Chain	Res	Type
1	R	305	THR
1	R	317	LYS
1	S	55	GLU
1	S	68	ASN
1	S	69	MET
1	S	85	VAL
1	S	96	SER
1	S	98	MET
1	S	121	GLN
1	S	122	THR
1	S	155	THR
1	S	158	VAL
1	S	202	ARG
1	S	224	ARG
1	S	225	MET
1	S	227	SER
1	S	228	ILE
1	S	272	LEU
1	S	282	ASP
1	S	290	LEU
1	S	293	LEU
1	S	302	ARG
1	S	305	THR
1	S	311	THR
1	S	316	VAL
1	T	55	GLU
1	T	68	ASN
1	T	96	SER
1	T	98	MET
1	T	121	GLN
1	T	148	GLN
1	T	158	VAL
1	T	196	LYS
1	T	203	THR
1	T	215	GLU
1	T	224	ARG
1	T	227	SER
1	T	282	ASP
1	T	290	LEU
1	T	292	THR
1	T	293	LEU
1	T	305	THR

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Mol	Chain	Res	Type
1	T	316	VAL
1	T	317	LYS
1	U	58	SER
1	U	62	THR
1	U	68	ASN
1	U	96	SER
1	U	98	MET
1	U	121	GLN
1	U	122	THR
1	U	134	LYS
1	U	148	GLN
1	U	155	THR
1	U	165	ILE
1	U	168	THR
1	U	180	VAL
1	U	202	ARG
1	U	211	LYS
1	U	215	GLU
1	U	224	ARG
1	U	227	SER
1	U	230	GLN
1	U	282	ASP
1	U	290	LEU
1	U	293	LEU
1	U	299	LEU
1	U	302	ARG
1	U	317	LYS
1	V	68	ASN
1	V	96	SER
1	V	98	MET
1	V	106	VAL
1	V	121	GLN
1	V	122	THR
1	V	127	GLN
1	V	148	GLN
1	V	168	THR
1	V	225	MET
1	V	227	SER
1	V	230	GLN
1	V	290	LEU
1	V	293	LEU
1	V	299	LEU

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Mol	Chain	Res	Type
1	V	302	ARG
1	V	305	THR
1	V	317	LYS
1	W	61	ILE
1	W	67	VAL
1	W	85	VAL
1	W	98	MET
1	W	107	MET
1	W	121	GLN
1	W	148	GLN
1	W	224	ARG
1	W	227	SER
1	W	275	VAL
1	W	282	ASP
1	W	289	MET
1	W	290	LEU
1	W	293	LEU
1	W	302	ARG
1	W	317	LYS
1	W	318	ARG
1	X	58	SER
1	X	62	THR
1	X	68	ASN
1	X	121	GLN
1	X	122	THR
1	X	134	LYS
1	X	155	THR
1	X	205	GLN
1	X	211	LYS
1	X	224	ARG
1	X	227	SER
1	X	289	MET
1	X	290	LEU
1	X	292	THR
1	X	293	LEU
1	X	295	VAL
1	X	299	LEU
1	X	305	THR
1	X	317	LYS
1	Y	55	GLU
1	Y	58	SER
1	Y	61	ILE

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Mol	Chain	Res	Type
1	Y	64	ARG
1	Y	67	VAL
1	Y	68	ASN
1	Y	85	VAL
1	Y	96	SER
1	Y	98	MET
1	Y	103	LYS
1	Y	106	VAL
1	Y	107	MET
1	Y	121	GLN
1	Y	122	THR
1	Y	148	GLN
1	Y	155	THR
1	Y	211	LYS
1	Y	224	ARG
1	Y	225	MET
1	Y	275	VAL
1	Y	282	ASP
1	Y	289	MET
1	Y	290	LEU
1	Y	292	THR
1	Y	293	LEU
1	Y	299	LEU
1	Y	302	ARG
1	Y	305	THR
1	Y	317	LYS
1	Z	58	SER
1	Z	68	ASN
1	Z	96	SER
1	Z	98	MET
1	Z	107	MET
1	Z	121	GLN
1	Z	122	THR
1	Z	129	MET
1	Z	143	MET
1	Z	148	GLN
1	Z	150	ILE
1	Z	153	ASP
1	Z	202	ARG
1	Z	203	THR
1	Z	211	LYS
1	Z	216	VAL

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Mol	Chain	Res	Type
1	Z	224	ARG
1	Z	227	SER
1	Z	282	ASP
1	Z	290	LEU
1	Z	293	LEU
1	Z	302	ARG
1	Z	305	THR
1	Z	317	LYS
1	a	58	SER
1	a	61	ILE
1	a	66	THR
1	a	85	VAL
1	a	96	SER
1	a	98	MET
1	a	107	MET
1	a	121	GLN
1	a	122	THR
1	a	148	GLN
1	a	155	THR
1	a	202	ARG
1	a	206	MET
1	a	227	SER
1	a	272	LEU
1	a	282	ASP
1	a	290	LEU
1	a	293	LEU
1	a	299	LEU
1	a	302	ARG
1	a	305	THR
1	a	316	VAL
1	b	61	ILE
1	b	68	ASN
1	b	69	MET
1	b	96	SER
1	b	98	MET
1	b	103	LYS
1	b	107	MET
1	b	121	GLN
1	b	122	THR
1	b	133	SER
1	b	148	GLN
1	b	155	THR

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Mol	Chain	Res	Type
1	b	205	GLN
1	b	215	GLU
1	b	224	ARG
1	b	227	SER
1	b	282	ASP
1	b	290	LEU
1	b	293	LEU
1	b	299	LEU
1	b	302	ARG
1	b	305	THR
1	b	311	THR
1	c	55	GLU
1	c	59	THR
1	c	96	SER
1	c	98	MET
1	c	107	MET
1	c	121	GLN
1	c	122	THR
1	c	148	GLN
1	c	155	THR
1	c	156	ARG
1	c	158	VAL
1	c	165	ILE
1	c	211	LYS
1	c	227	SER
1	c	282	ASP
1	c	290	LEU
1	c	293	LEU
1	c	299	LEU
1	c	302	ARG
1	c	305	THR
1	c	317	LYS
1	d	59	THR
1	d	61	ILE
1	d	66	THR
1	d	68	ASN
1	d	85	VAL
1	d	96	SER
1	d	121	GLN
1	d	148	GLN
1	d	196	LYS
1	d	207	LYS

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Mol	Chain	Res	Type
1	d	216	VAL
1	d	218	LYS
1	d	227	SER
1	d	230	GLN
1	d	266	GLN
1	d	290	LEU
1	d	293	LEU
1	d	305	THR
1	d	317	LYS
1	e	59	THR
1	e	85	VAL
1	e	96	SER
1	e	97	VAL
1	e	98	MET
1	e	121	GLN
1	e	122	THR
1	e	130	VAL
1	e	144	ILE
1	e	148	GLN
1	e	150	ILE
1	e	211	LYS
1	e	220	ILE
1	e	224	ARG
1	e	227	SER
1	e	268	ARG
1	e	275	VAL
1	e	282	ASP
1	e	290	LEU
1	e	293	LEU
1	e	298	THR
1	e	299	LEU
1	f	62	THR
1	f	68	ASN
1	f	85	VAL
1	f	96	SER
1	f	98	MET
1	f	106	VAL
1	f	107	MET
1	f	121	GLN
1	f	122	THR
1	f	130	VAL
1	f	134	LYS

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Mol	Chain	Res	Type
1	f	155	THR
1	f	158	VAL
1	f	202	ARG
1	f	205	GLN
1	f	220	ILE
1	f	225	MET
1	f	227	SER
1	f	290	LEU
1	f	293	LEU
1	f	299	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (312) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	78	GLN
1	A	82	ASN
1	A	127	GLN
1	A	145	ASN
1	A	146	ASN
1	A	148	GLN
1	A	185	GLN
1	A	192	ASN
1	A	213	GLN
1	A	291	ASN
1	A	294	ASN
1	B	68	ASN
1	B	145	ASN
1	B	146	ASN
1	B	174	ASN
1	B	192	ASN
1	B	205	GLN
1	B	213	GLN
1	B	273	GLN
1	B	286	ASN
1	B	291	ASN
1	B	294	ASN
1	C	76	GLN
1	C	82	ASN
1	C	132	ASN
1	C	145	ASN
1	C	146	ASN

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Mol	Chain	Res	Type
1	C	148	GLN
1	C	192	ASN
1	C	209	GLN
1	C	213	GLN
1	C	273	GLN
1	C	294	ASN
1	D	68	ASN
1	D	82	ASN
1	D	146	ASN
1	D	174	ASN
1	D	192	ASN
1	D	213	GLN
1	D	271	ASN
1	D	273	GLN
1	D	294	ASN
1	E	76	GLN
1	E	82	ASN
1	E	127	GLN
1	E	132	ASN
1	E	146	ASN
1	E	148	GLN
1	E	192	ASN
1	E	213	GLN
1	E	291	ASN
1	E	294	ASN
1	F	78	GLN
1	F	146	ASN
1	F	148	GLN
1	F	159	ASN
1	F	174	ASN
1	F	185	GLN
1	F	192	ASN
1	F	213	GLN
1	F	266	GLN
1	F	291	ASN
1	G	76	GLN
1	G	82	ASN
1	G	121	GLN
1	G	127	GLN
1	G	145	ASN
1	G	146	ASN
1	G	148	GLN

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Mol	Chain	Res	Type
1	G	174	ASN
1	G	192	ASN
1	G	205	GLN
1	G	209	GLN
1	G	213	GLN
1	G	266	GLN
1	G	294	ASN
1	H	68	ASN
1	H	82	ASN
1	H	146	ASN
1	H	148	GLN
1	H	190	HIS
1	H	192	ASN
1	H	213	GLN
1	H	273	GLN
1	H	291	ASN
1	H	294	ASN
1	I	82	ASN
1	I	127	GLN
1	I	145	ASN
1	I	146	ASN
1	I	148	GLN
1	I	159	ASN
1	I	174	ASN
1	I	185	GLN
1	I	192	ASN
1	I	213	GLN
1	I	291	ASN
1	I	294	ASN
1	J	78	GLN
1	J	127	GLN
1	J	145	ASN
1	J	146	ASN
1	J	148	GLN
1	J	192	ASN
1	J	213	GLN
1	J	291	ASN
1	J	294	ASN
1	K	76	GLN
1	K	82	ASN
1	K	127	GLN
1	K	132	ASN

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Mol	Chain	Res	Type
1	K	146	ASN
1	K	192	ASN
1	K	213	GLN
1	K	271	ASN
1	K	294	ASN
1	L	82	ASN
1	L	127	GLN
1	L	146	ASN
1	L	148	GLN
1	L	192	ASN
1	L	213	GLN
1	L	266	GLN
1	L	291	ASN
1	L	294	ASN
1	M	76	GLN
1	M	82	ASN
1	M	127	GLN
1	M	132	ASN
1	M	146	ASN
1	M	148	GLN
1	M	192	ASN
1	M	213	GLN
1	M	291	ASN
1	M	294	ASN
1	N	82	ASN
1	N	127	GLN
1	N	145	ASN
1	N	146	ASN
1	N	148	GLN
1	N	192	ASN
1	N	213	GLN
1	N	273	GLN
1	N	291	ASN
1	N	294	ASN
1	O	68	ASN
1	O	82	ASN
1	O	121	GLN
1	O	127	GLN
1	O	145	ASN
1	O	146	ASN
1	O	148	GLN
1	O	192	ASN

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Mol	Chain	Res	Type
1	O	291	ASN
1	O	294	ASN
1	P	82	ASN
1	P	146	ASN
1	P	192	ASN
1	P	205	GLN
1	P	213	GLN
1	P	273	GLN
1	P	291	ASN
1	P	294	ASN
1	Q	76	GLN
1	Q	82	ASN
1	Q	127	GLN
1	Q	146	ASN
1	Q	148	GLN
1	Q	185	GLN
1	Q	192	ASN
1	Q	213	GLN
1	Q	291	ASN
1	Q	294	ASN
1	R	78	GLN
1	R	82	ASN
1	R	127	GLN
1	R	146	ASN
1	R	148	GLN
1	R	192	ASN
1	R	205	GLN
1	R	213	GLN
1	R	294	ASN
1	S	68	ASN
1	S	76	GLN
1	S	78	GLN
1	S	82	ASN
1	S	146	ASN
1	S	148	GLN
1	S	174	ASN
1	S	192	ASN
1	S	213	GLN
1	S	294	ASN
1	T	82	ASN
1	T	127	GLN
1	T	146	ASN

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Mol	Chain	Res	Type
1	T	148	GLN
1	T	205	GLN
1	T	271	ASN
1	T	291	ASN
1	T	294	ASN
1	U	76	GLN
1	U	82	ASN
1	U	127	GLN
1	U	132	ASN
1	U	146	ASN
1	U	148	GLN
1	U	192	ASN
1	U	213	GLN
1	U	291	ASN
1	U	294	ASN
1	V	78	GLN
1	V	82	ASN
1	V	146	ASN
1	V	174	ASN
1	V	192	ASN
1	V	213	GLN
1	V	266	GLN
1	V	271	ASN
1	V	291	ASN
1	V	294	ASN
1	V	304	GLN
1	W	76	GLN
1	W	82	ASN
1	W	127	GLN
1	W	145	ASN
1	W	146	ASN
1	W	148	GLN
1	W	192	ASN
1	W	294	ASN
1	X	82	ASN
1	X	145	ASN
1	X	146	ASN
1	X	148	GLN
1	X	178	GLN
1	X	192	ASN
1	X	205	GLN
1	X	213	GLN

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Mol	Chain	Res	Type
1	X	273	GLN
1	X	291	ASN
1	X	294	ASN
1	Y	76	GLN
1	Y	82	ASN
1	Y	127	GLN
1	Y	146	ASN
1	Y	148	GLN
1	Y	185	GLN
1	Y	192	ASN
1	Y	291	ASN
1	Y	294	ASN
1	Z	82	ASN
1	Z	146	ASN
1	Z	192	ASN
1	Z	205	GLN
1	Z	213	GLN
1	Z	291	ASN
1	Z	294	ASN
1	a	76	GLN
1	a	82	ASN
1	a	132	ASN
1	a	145	ASN
1	a	146	ASN
1	a	192	ASN
1	a	213	GLN
1	a	294	ASN
1	b	82	ASN
1	b	127	GLN
1	b	145	ASN
1	b	146	ASN
1	b	148	GLN
1	b	185	GLN
1	b	192	ASN
1	b	230	GLN
1	b	294	ASN
1	c	76	GLN
1	c	82	ASN
1	c	127	GLN
1	c	132	ASN
1	c	146	ASN
1	c	148	GLN

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Mol	Chain	Res	Type
1	c	192	ASN
1	c	291	ASN
1	c	294	ASN
1	d	76	GLN
1	d	78	GLN
1	d	127	GLN
1	d	145	ASN
1	d	146	ASN
1	d	148	GLN
1	d	159	ASN
1	d	213	GLN
1	d	266	GLN
1	d	291	ASN
1	d	294	ASN
1	e	82	ASN
1	e	146	ASN
1	e	148	GLN
1	e	213	GLN
1	e	291	ASN
1	e	294	ASN
1	f	82	ASN
1	f	127	GLN
1	f	146	ASN
1	f	148	GLN
1	f	192	ASN
1	f	205	GLN
1	f	213	GLN
1	f	226	ASN
1	f	230	GLN
1	f	271	ASN
1	f	291	ASN
1	f	294	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	221/356 (62%)	0.50	9 (4%) 35 34	232, 286, 334, 403	0
1	B	221/356 (62%)	0.40	3 (1%) 72 60	200, 271, 345, 382	0
1	C	221/356 (62%)	0.72	20 (9%) 10 17	248, 300, 381, 438	0
1	D	221/356 (62%)	0.41	4 (1%) 65 55	223, 281, 331, 361	0
1	E	221/356 (62%)	0.99	39 (17%) 2 7	255, 337, 447, 534	0
1	F	221/356 (62%)	0.54	18 (8%) 12 19	208, 275, 322, 362	0
1	G	221/356 (62%)	0.63	11 (4%) 28 29	229, 279, 337, 357	0
1	H	221/356 (62%)	0.49	5 (2%) 57 48	228, 263, 309, 327	0
1	I	221/356 (62%)	0.58	19 (8%) 11 18	245, 316, 404, 442	0
1	J	221/356 (62%)	0.44	8 (3%) 41 38	244, 286, 351, 372	0
1	K	221/356 (62%)	0.41	8 (3%) 41 38	249, 287, 346, 389	0
1	L	221/356 (62%)	0.54	10 (4%) 32 32	223, 284, 405, 432	0
1	M	221/356 (62%)	0.48	13 (5%) 22 26	205, 265, 333, 351	0
1	N	221/356 (62%)	0.70	23 (10%) 7 15	206, 290, 339, 361	0
1	O	221/356 (62%)	0.59	15 (6%) 17 23	214, 267, 337, 376	0
1	P	221/356 (62%)	0.52	10 (4%) 32 32	245, 283, 320, 341	0
1	Q	221/356 (62%)	0.40	8 (3%) 41 38	204, 276, 333, 350	0
1	R	221/356 (62%)	0.76	28 (12%) 4 11	229, 322, 389, 429	0
1	S	221/356 (62%)	0.34	4 (1%) 65 55	236, 300, 344, 456	0
1	T	221/356 (62%)	0.82	28 (12%) 4 11	205, 313, 404, 456	0
1	U	221/356 (62%)	0.52	14 (6%) 19 25	199, 286, 401, 509	0
1	V	221/356 (62%)	0.54	12 (5%) 25 27	237, 309, 351, 378	0
1	W	221/356 (62%)	0.43	13 (5%) 22 26	211, 301, 375, 398	0
1	X	221/356 (62%)	0.53	15 (6%) 17 23	240, 303, 398, 414	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	221/356 (62%)	0.70	19 (8%)	11	18	236, 326, 449, 465	0
1	Z	221/356 (62%)	0.43	9 (4%)	35	34	228, 310, 395, 408	0
1	a	221/356 (62%)	0.42	6 (2%)	52	45	231, 299, 363, 391	0
1	b	221/356 (62%)	0.74	20 (9%)	10	17	256, 348, 475, 550	0
1	c	221/356 (62%)	0.53	19 (8%)	11	18	256, 314, 369, 399	0
1	d	221/356 (62%)	0.31	6 (2%)	52	45	235, 284, 331, 372	0
1	e	221/356 (62%)	0.43	11 (4%)	28	29	237, 321, 358, 384	0
1	f	221/356 (62%)	0.38	5 (2%)	57	48	214, 289, 334, 393	0
All	All	7072/11392 (62%)	0.54	432 (6%)	21	25	199, 295, 383, 550	0

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	277	PRO	7.8
1	c	266	GLN	6.6
1	X	305	THR	6.4
1	d	229	GLU	6.0
1	b	116	ARG	6.0
1	M	319	ASP	5.7
1	E	314	GLU	5.6
1	G	156	ARG	5.6
1	Y	228	ILE	5.5
1	E	60	ALA	5.5
1	d	230	GLN	5.2
1	J	230	GLN	5.2
1	R	266	GLN	5.1
1	R	74	TYR	4.9
1	X	306	TYR	4.9
1	F	230	GLN	4.8
1	R	206	MET	4.8
1	F	228	ILE	4.6
1	b	109	LEU	4.5
1	Q	62	THR	4.5
1	E	162	VAL	4.5
1	N	270	GLU	4.5
1	Y	278	ALA	4.4
1	E	163	LYS	4.4
1	P	299	LEU	4.4
1	G	299	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	R	98	MET	4.3
1	X	304	GLN	4.3
1	N	73	TYR	4.3
1	U	270	GLU	4.3
1	N	266	GLN	4.3
1	b	119	TRP	4.3
1	F	229	GLU	4.3
1	T	120	LEU	4.3
1	b	120	LEU	4.2
1	R	73	TYR	4.2
1	O	297	PRO	4.2
1	c	308	TYR	4.2
1	T	266	GLN	4.2
1	E	61	ILE	4.1
1	I	224	ARG	4.1
1	E	313	GLU	4.1
1	C	276	GLY	4.1
1	R	129	MET	4.1
1	T	279	PHE	4.1
1	L	277	PRO	4.1
1	I	73	TYR	4.1
1	C	298	THR	4.0
1	E	316	VAL	4.0
1	V	73	TYR	4.0
1	C	277	PRO	4.0
1	C	299	LEU	3.9
1	W	151	PRO	3.9
1	J	228	ILE	3.9
1	U	269	LEU	3.8
1	c	95	PRO	3.8
1	T	268	ARG	3.8
1	D	175	LEU	3.7
1	E	309	LEU	3.7
1	I	195	LEU	3.7
1	O	299	LEU	3.7
1	I	225	MET	3.7
1	G	155	THR	3.7
1	I	298	THR	3.7
1	E	315	PRO	3.7
1	U	273	GLN	3.6
1	C	156	ARG	3.6
1	O	295	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	e	293	LEU	3.6
1	Y	135	ALA	3.6
1	K	275	VAL	3.6
1	f	299	LEU	3.5
1	e	225	MET	3.5
1	T	267	ALA	3.5
1	E	266	GLN	3.5
1	R	267	ALA	3.5
1	C	275	VAL	3.5
1	d	299	LEU	3.4
1	H	109	LEU	3.4
1	I	228	ILE	3.4
1	J	317	LYS	3.4
1	Q	73	TYR	3.4
1	N	207	LYS	3.3
1	T	164	LEU	3.3
1	I	266	GLN	3.3
1	H	134	LYS	3.3
1	F	297	PRO	3.3
1	U	271	ASN	3.3
1	E	112	TRP	3.2
1	A	83	LEU	3.2
1	C	279	PHE	3.2
1	U	268	ARG	3.2
1	O	294	ASN	3.2
1	J	227	SER	3.2
1	Z	147	ILE	3.2
1	C	225	MET	3.2
1	L	164	LEU	3.2
1	Y	134	LYS	3.2
1	S	293	LEU	3.2
1	c	301	PRO	3.2
1	E	270	GLU	3.2
1	C	228	ILE	3.2
1	P	279	PHE	3.1
1	E	202	ARG	3.1
1	Z	162	VAL	3.1
1	T	317	LYS	3.1
1	E	148	GLN	3.1
1	W	228	ILE	3.1
1	C	278	ALA	3.1
1	c	299	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	84	ASP	3.1
1	U	266	GLN	3.1
1	e	266	GLN	3.1
1	Y	279	PHE	3.1
1	M	206	MET	3.1
1	I	299	LEU	3.1
1	T	163	LYS	3.1
1	E	156	ARG	3.1
1	X	191	LEU	3.1
1	R	275	VAL	3.1
1	V	74	TYR	3.0
1	N	267	ALA	3.0
1	Y	276	GLY	3.0
1	R	101	ALA	3.0
1	N	74	TYR	3.0
1	R	269	LEU	3.0
1	b	125	TYR	3.0
1	O	154	PHE	3.0
1	R	289	MET	3.0
1	R	270	GLU	3.0
1	b	277	PRO	3.0
1	E	269	LEU	3.0
1	O	195	LEU	3.0
1	E	179	TYR	3.0
1	a	221	TYR	3.0
1	T	269	LEU	3.0
1	A	74	TYR	3.0
1	c	74	TYR	3.0
1	J	297	PRO	3.0
1	M	317	LYS	3.0
1	Y	132	ASN	3.0
1	X	188	ALA	2.9
1	K	83	LEU	2.9
1	E	59	THR	2.9
1	R	207	LYS	2.9
1	X	156	ARG	2.9
1	W	316	VAL	2.9
1	b	162	VAL	2.9
1	V	195	LEU	2.9
1	I	74	TYR	2.9
1	W	66	THR	2.9
1	M	293	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	308	TYR	2.9
1	I	162	VAL	2.9
1	C	297	PRO	2.9
1	C	230	GLN	2.9
1	d	311	THR	2.9
1	N	206	MET	2.9
1	c	267	ALA	2.9
1	F	80	LEU	2.9
1	L	165	ILE	2.8
1	K	274	ALA	2.8
1	R	83	LEU	2.8
1	M	195	LEU	2.8
1	U	272	LEU	2.8
1	L	276	GLY	2.8
1	E	116	ARG	2.8
1	D	299	LEU	2.8
1	Q	266	GLN	2.8
1	b	118	PHE	2.8
1	T	315	PRO	2.8
1	b	62	THR	2.8
1	E	147	ILE	2.8
1	b	149	PHE	2.7
1	P	120	LEU	2.7
1	L	80	LEU	2.7
1	Z	287	ARG	2.7
1	F	227	SER	2.7
1	Z	164	LEU	2.7
1	X	307	ARG	2.7
1	O	109	LEU	2.7
1	W	156	ARG	2.7
1	T	316	VAL	2.7
1	F	225	MET	2.7
1	C	164	LEU	2.7
1	E	175	LEU	2.7
1	O	290	LEU	2.7
1	N	272	LEU	2.7
1	Z	163	LYS	2.7
1	L	83	LEU	2.7
1	U	60	ALA	2.6
1	U	278	ALA	2.6
1	V	109	LEU	2.6
1	N	129	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	76	GLN	2.6
1	I	70	LEU	2.6
1	N	303	PHE	2.6
1	O	157	ALA	2.6
1	E	317	LYS	2.6
1	W	67	VAL	2.6
1	T	121	GLN	2.6
1	G	298	THR	2.6
1	T	272	LEU	2.6
1	e	289	MET	2.6
1	K	70	LEU	2.6
1	T	119	TRP	2.6
1	G	162	VAL	2.6
1	E	267	ALA	2.6
1	f	109	LEU	2.6
1	I	67	VAL	2.6
1	P	135	ALA	2.6
1	R	190	HIS	2.6
1	V	266	GLN	2.6
1	I	109	LEU	2.6
1	E	62	THR	2.6
1	L	202	ARG	2.5
1	T	277	PRO	2.5
1	L	79	PHE	2.5
1	f	179	TYR	2.5
1	E	83	LEU	2.5
1	Y	268	ARG	2.5
1	R	97	VAL	2.5
1	O	199	TRP	2.5
1	C	155	THR	2.5
1	N	273	GLN	2.5
1	b	179	TYR	2.5
1	b	122	THR	2.5
1	d	228	ILE	2.5
1	T	60	ALA	2.5
1	Y	109	LEU	2.5
1	Z	109	LEU	2.5
1	Y	202	ARG	2.5
1	F	85	VAL	2.5
1	I	77	GLN	2.5
1	Q	195	LEU	2.5
1	V	62	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	Y	191	LEU	2.5
1	W	289	MET	2.5
1	U	279	PHE	2.5
1	N	162	VAL	2.5
1	c	73	TYR	2.5
1	R	299	LEU	2.5
1	b	159	ASN	2.5
1	F	195	LEU	2.5
1	O	287	ARG	2.5
1	E	79	PHE	2.5
1	O	293	LEU	2.4
1	X	187	ALA	2.4
1	R	293	LEU	2.4
1	a	272	LEU	2.4
1	b	301	PRO	2.4
1	M	199	TRP	2.4
1	P	202	ARG	2.4
1	E	206	MET	2.4
1	I	163	LYS	2.4
1	a	60	ALA	2.4
1	R	209	GLN	2.4
1	e	299	LEU	2.4
1	F	79	PHE	2.4
1	E	115	ARG	2.4
1	U	308	TYR	2.4
1	Y	104	GLU	2.4
1	T	273	GLN	2.4
1	e	83	LEU	2.4
1	T	143	MET	2.4
1	I	230	GLN	2.4
1	N	147	ILE	2.4
1	c	311	THR	2.4
1	P	278	ALA	2.4
1	F	299	LEU	2.4
1	f	156	ARG	2.4
1	N	204	ILE	2.4
1	H	302	ARG	2.4
1	R	268	ARG	2.4
1	F	83	LEU	2.4
1	P	109	LEU	2.4
1	G	316	VAL	2.4
1	L	275	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	R	64	ARG	2.4
1	S	74	TYR	2.4
1	S	202	ARG	2.4
1	W	304	GLN	2.3
1	A	79	PHE	2.3
1	K	299	LEU	2.3
1	A	80	LEU	2.3
1	b	83	LEU	2.3
1	K	109	LEU	2.3
1	a	116	ARG	2.3
1	C	229	GLU	2.3
1	C	157	ALA	2.3
1	M	290	LEU	2.3
1	Q	61	ILE	2.3
1	U	267	ALA	2.3
1	X	275	VAL	2.3
1	N	116	ARG	2.3
1	J	226	ASN	2.3
1	T	162	VAL	2.3
1	W	293	LEU	2.3
1	b	143	MET	2.3
1	R	202	ARG	2.3
1	X	266	GLN	2.3
1	E	199	TRP	2.3
1	P	195	LEU	2.3
1	R	217	ALA	2.3
1	V	76	GLN	2.3
1	M	318	ARG	2.3
1	N	191	LEU	2.3
1	T	147	ILE	2.3
1	T	270	GLU	2.3
1	c	180	VAL	2.3
1	e	221	TYR	2.3
1	X	303	PHE	2.3
1	W	152	GLY	2.3
1	G	80	LEU	2.3
1	T	175	LEU	2.3
1	c	309	LEU	2.3
1	V	112	TRP	2.3
1	M	298	THR	2.3
1	W	303	PHE	2.3
1	E	293	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	268	ARG	2.3
1	F	76	GLN	2.3
1	N	79	PHE	2.3
1	e	273	GLN	2.3
1	E	169	ALA	2.3
1	J	109	LEU	2.3
1	T	278	ALA	2.3
1	P	191	LEU	2.3
1	D	101	ALA	2.2
1	b	151	PRO	2.2
1	B	299	LEU	2.2
1	I	272	LEU	2.2
1	b	164	LEU	2.2
1	C	207	LYS	2.2
1	Q	268	ARG	2.2
1	N	195	LEU	2.2
1	T	83	LEU	2.2
1	Y	64	ARG	2.2
1	Y	156	ARG	2.2
1	F	74	TYR	2.2
1	R	125	TYR	2.2
1	O	156	ARG	2.2
1	A	297	PRO	2.2
1	E	297	PRO	2.2
1	Z	284	ASP	2.2
1	c	156	ARG	2.2
1	E	155	THR	2.2
1	M	74	TYR	2.2
1	b	60	ALA	2.2
1	c	97	VAL	2.2
1	E	145	ASN	2.2
1	c	312	PRO	2.2
1	N	269	LEU	2.2
1	c	298	THR	2.2
1	K	271	ASN	2.2
1	I	316	VAL	2.2
1	d	60	ALA	2.2
1	X	270	GLU	2.2
1	Y	305	THR	2.2
1	T	165	ILE	2.2
1	G	101	ALA	2.2
1	G	216	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	206	MET	2.2
1	B	225	MET	2.1
1	Z	206	MET	2.1
1	M	316	VAL	2.1
1	F	59	THR	2.1
1	X	155	THR	2.1
1	F	224	ARG	2.1
1	a	224	ARG	2.1
1	G	76	GLN	2.1
1	R	271	ASN	2.1
1	M	80	LEU	2.1
1	Q	228	ILE	2.1
1	I	297	PRO	2.1
1	R	70	LEU	2.1
1	T	176	LEU	2.1
1	T	116	ARG	2.1
1	Y	188	ALA	2.1
1	E	164	LEU	2.1
1	V	144	ILE	2.1
1	V	116	ARG	2.1
1	D	284	ASP	2.1
1	Y	130	VAL	2.1
1	G	190	HIS	2.1
1	J	73	TYR	2.1
1	A	78	GLN	2.1
1	S	156	ARG	2.1
1	B	220	ILE	2.1
1	O	316	VAL	2.1
1	C	224	ARG	2.1
1	E	170	PRO	2.1
1	N	101	ALA	2.1
1	Z	212	ARG	2.1
1	e	74	TYR	2.1
1	O	70	LEU	2.1
1	U	66	THR	2.1
1	Y	214	GLU	2.1
1	X	62	THR	2.1
1	c	273	GLN	2.1
1	M	76	GLN	2.1
1	a	292	THR	2.1
1	T	283	TYR	2.1
1	A	206	MET	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	145	ASN	2.1
1	C	272	LEU	2.1
1	K	73	TYR	2.1
1	A	155	THR	2.1
1	f	229	GLU	2.1
1	R	292	THR	2.1
1	e	290	LEU	2.1
1	N	271	ASN	2.1
1	N	209	GLN	2.0
1	V	191	LEU	2.0
1	b	117	GLU	2.0
1	c	269	LEU	2.0
1	c	300	ASP	2.0
1	N	83	LEU	2.0
1	E	176	LEU	2.0
1	A	316	VAL	2.0
1	E	312	PRO	2.0
1	R	272	LEU	2.0
1	L	278	ALA	2.0
1	V	97	VAL	2.0
1	U	274	ALA	2.0
1	H	284	ASP	2.0
1	W	230	GLN	2.0
1	e	119	TRP	2.0
1	Q	196	LYS	2.0
1	H	305	THR	2.0
1	W	292	THR	2.0
1	c	175	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.