Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:08 PM GMT

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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

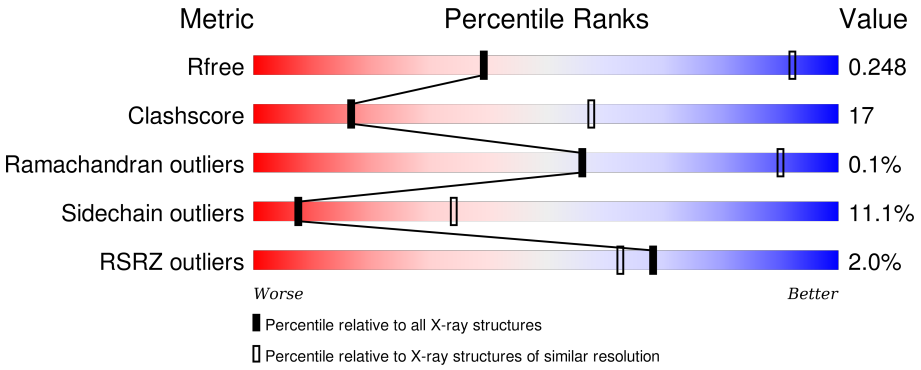
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1002 (8.30-3.66)
Clashscore	102246	1049 (8.20-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	28% 28% 6% • 38%
1	B	356	25% 33% • 38%
1	C	356	3% 32% 26% • • 38%
1	D	356	25% 32% 5% • 38%
1	E	356	5% 33% 24% 5% • 38%

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Mol	Chain	Length	Quality of chain
1	F	356	2% 24% 34% 38%
1	G	356	40% 20% 38%
1	H	356	35% 23% 38%
1	I	356	2% 38% 19% 5% 38%
1	J	356	2% 38% 20% 38%
1	K	356	38% 20% 38%
1	L	356	33% 25% 38%
1	M	356	38% 17% 5% 38%
1	N	356	40% 18% 38%
1	O	356	40% 18% 38%
1	P	356	35% 22% 38%
1	Q	356	37% 21% 38%
1	R	356	3% 39% 19% 38%
1	S	356	38% 18% 38%
1	T	356	3% 38% 18% 5% 38%
1	U	356	2% 35% 22% 5% 38%
1	V	356	41% 17% 38%
1	W	356	37% 21% 38%
1	X	356	2% 36% 22% 38%
1	Y	356	2% 37% 18% 6% 38%
1	Z	356	36% 21% 38%
1	a	356	54% 6% 38%
1	b	356	2% 53% 6% 38%
1	c	356	54% 6% 38%
1	d	356	55% 38%

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Mol	Chain	Length	Quality of chain
1	e	356	
1	f	356	

2 Entry composition (i)

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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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Continued from previous page...

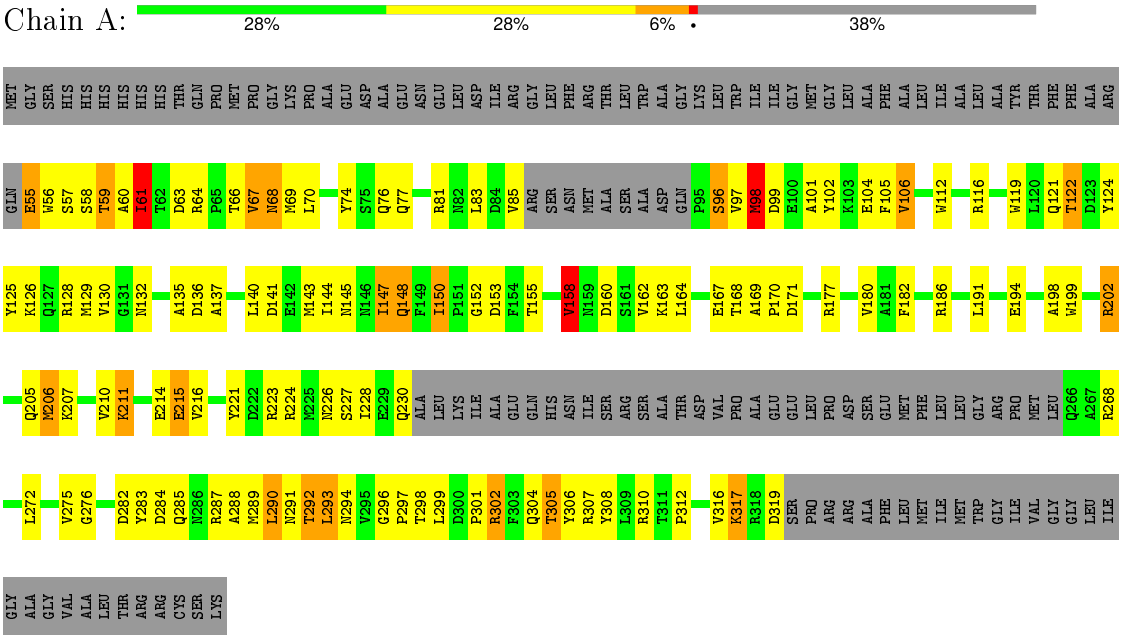
Chain	Residue	Modelled	Actual	Comment	Reference
c	1	HIS	-	expression tag	UNP P0AG01
c	2	HIS	-	expression tag	UNP P0AG01
d	-6	MET	-	initiating methionine	UNP P0AG01
d	-5	GLY	-	expression tag	UNP P0AG01
d	-4	SER	-	expression tag	UNP P0AG01
d	-3	HIS	-	expression tag	UNP P0AG01
d	-2	HIS	-	expression tag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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

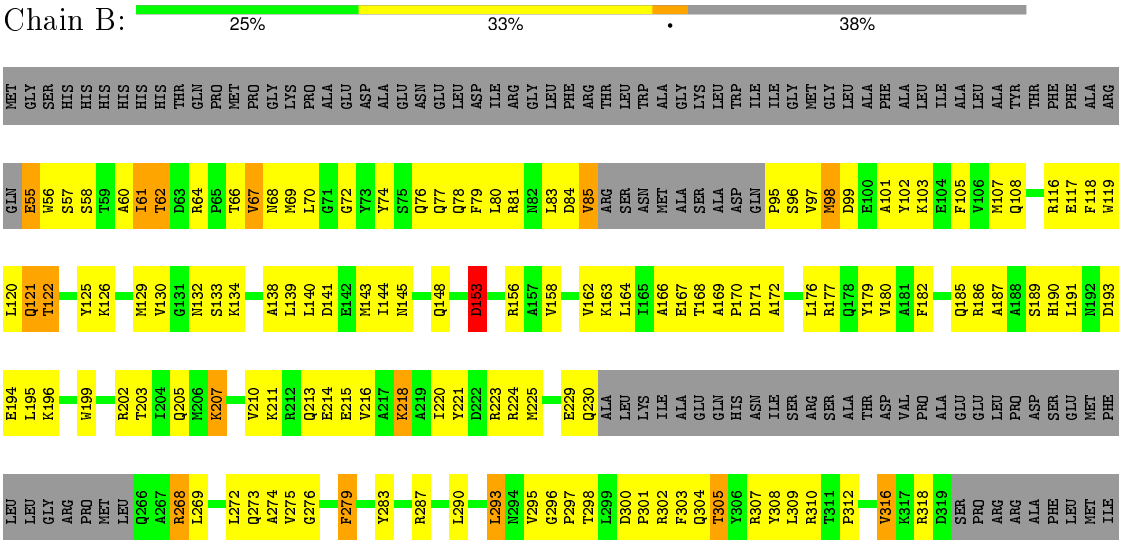
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain A:



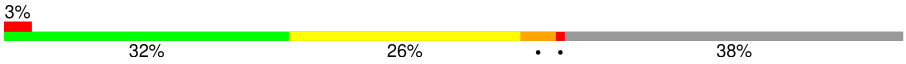
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

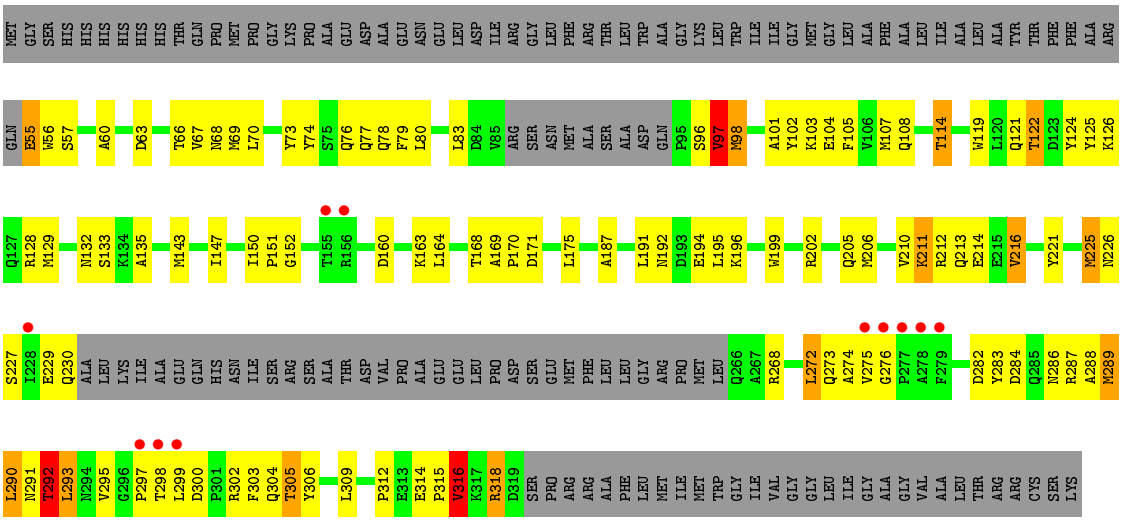
Chain B:



- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

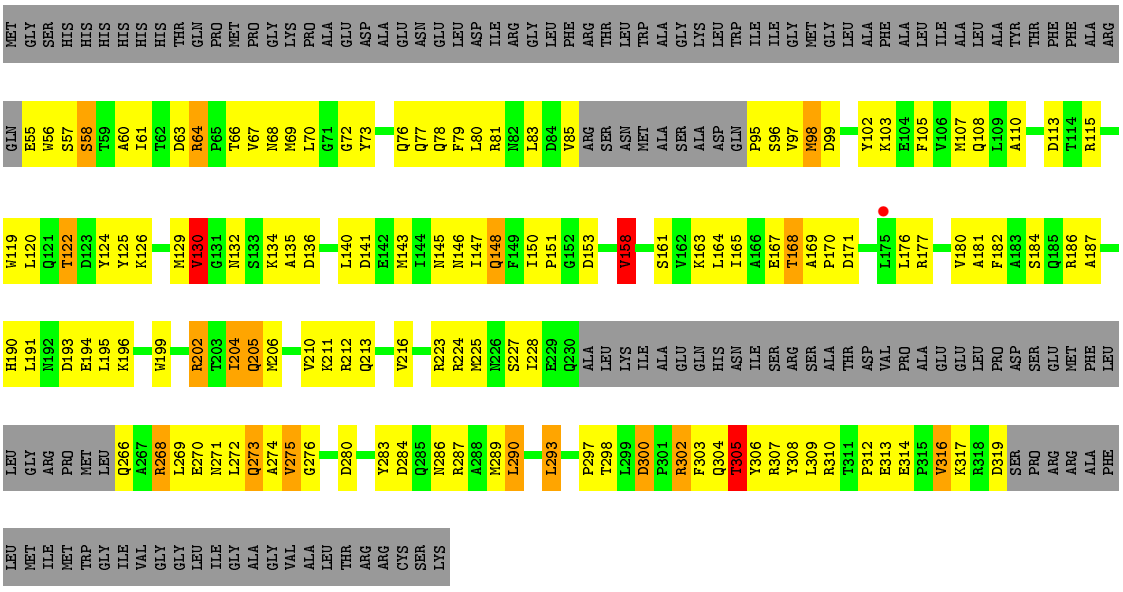
Chain C:





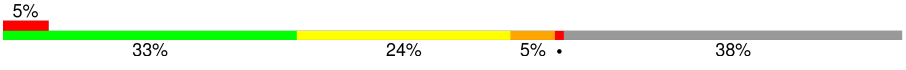
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

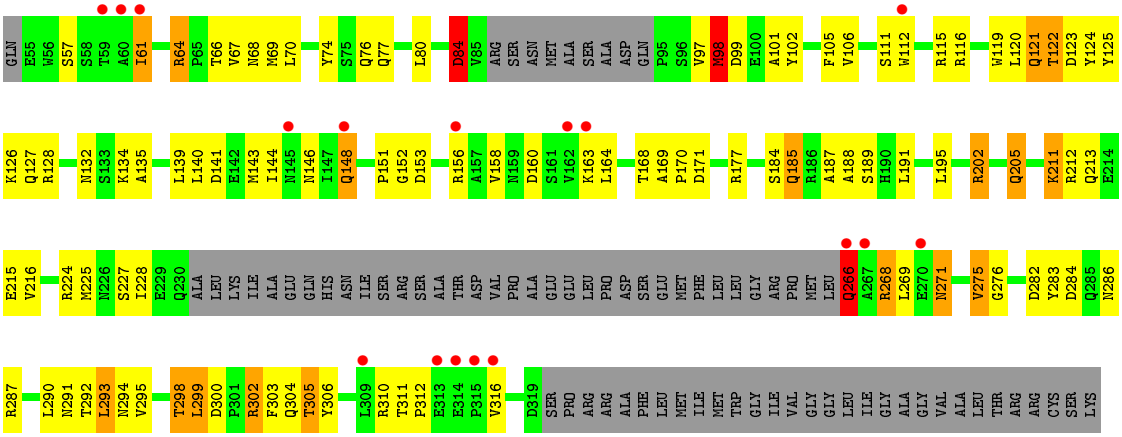
Chain D:



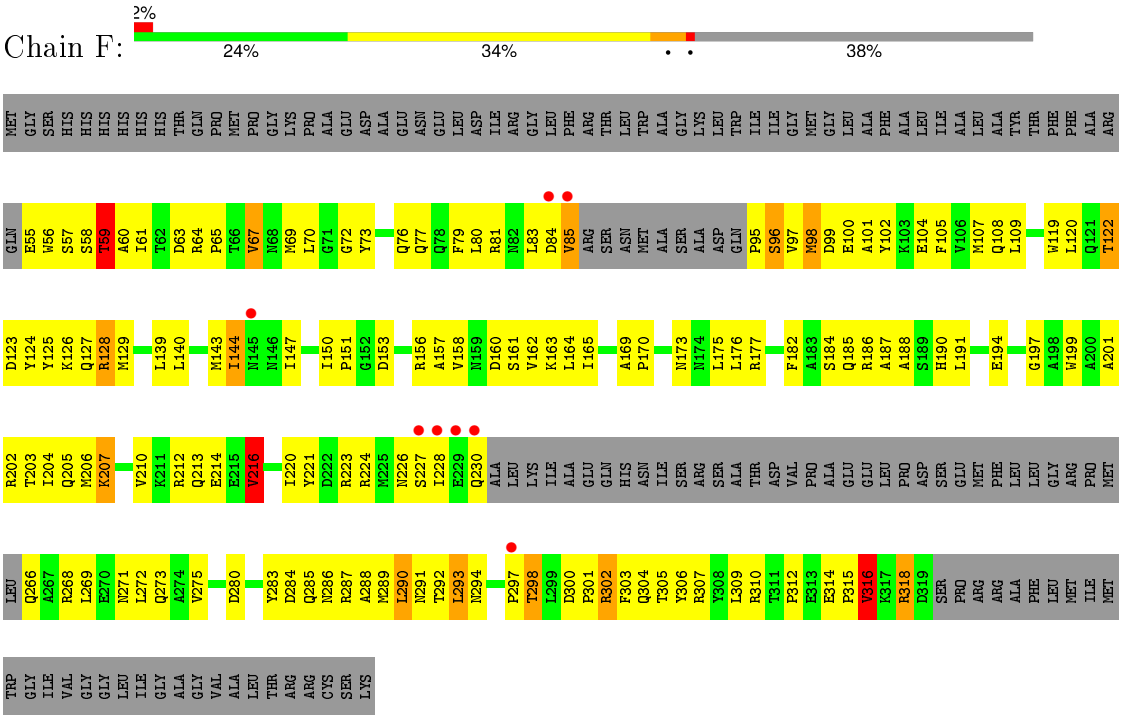
- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain E:

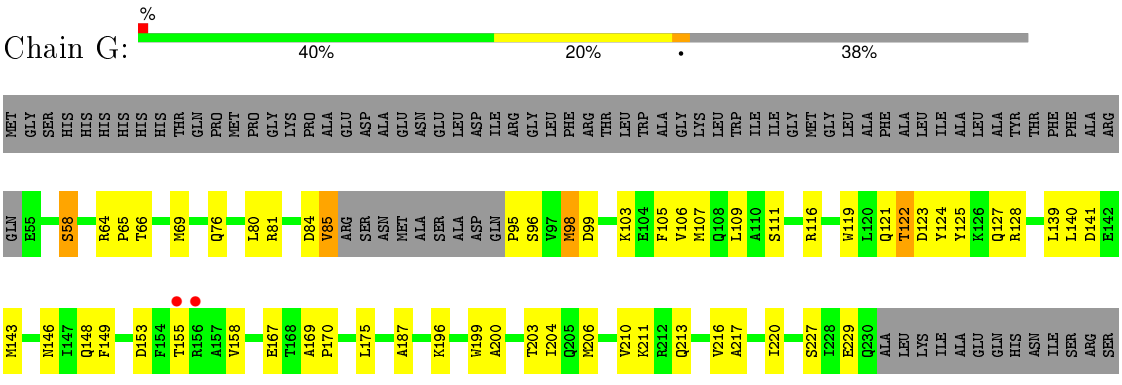


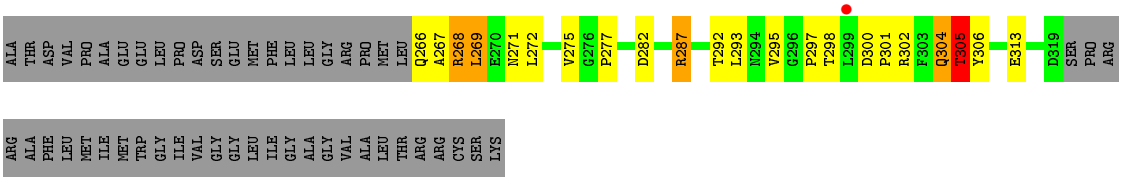


• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE



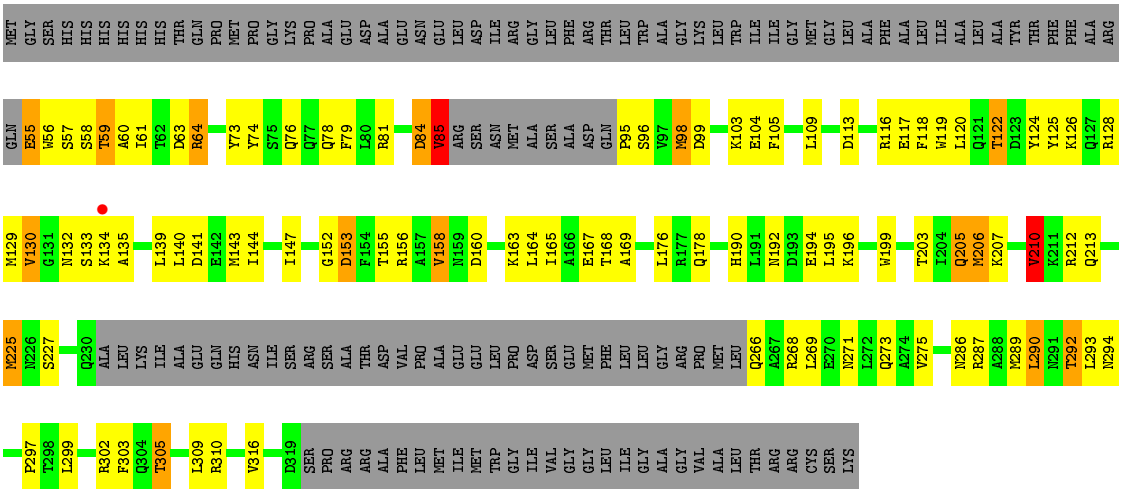
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE





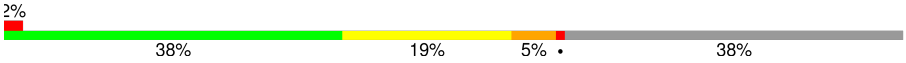
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

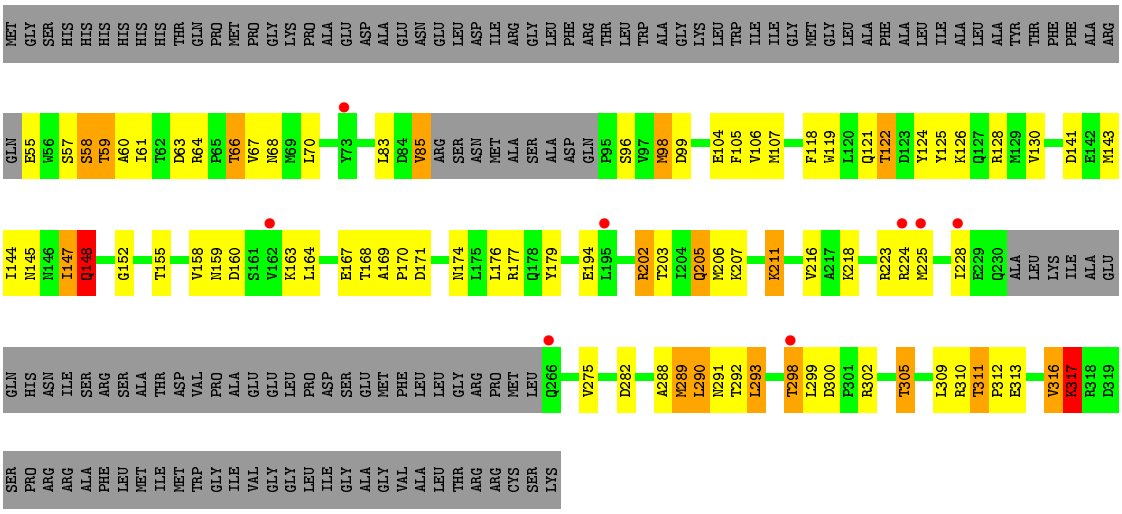
Chain H:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

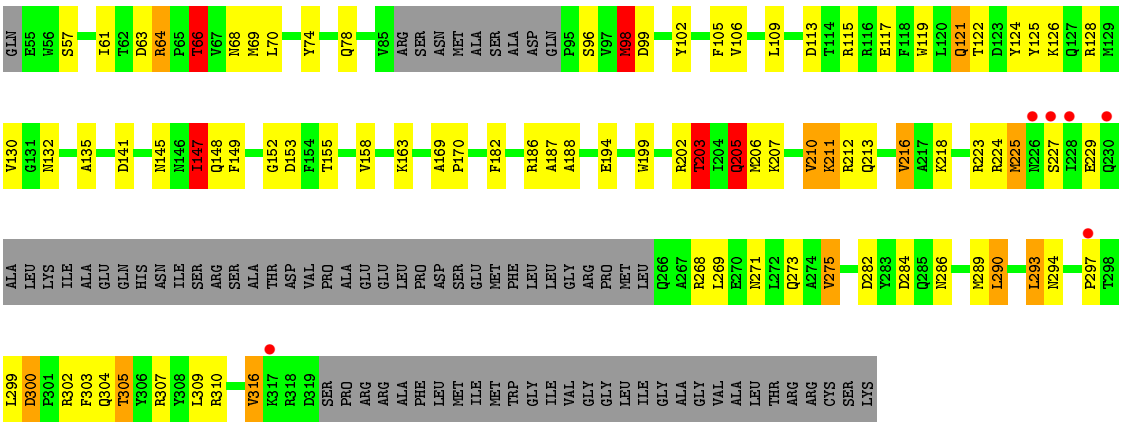
Chain I:





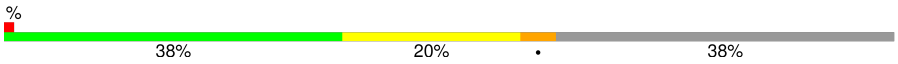
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

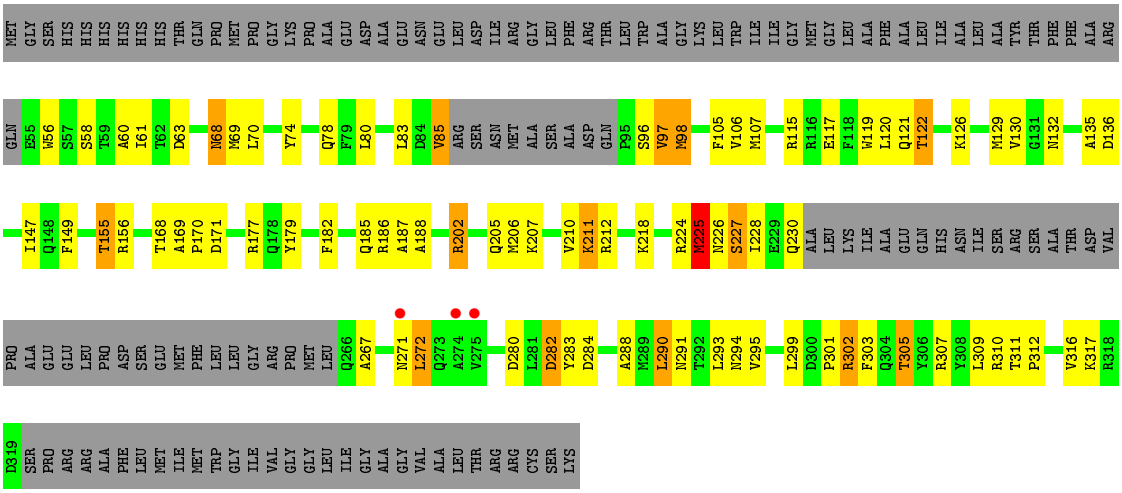
Chain J:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

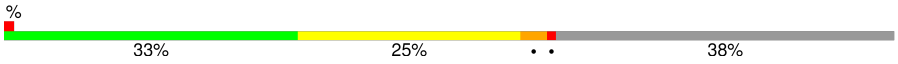
Chain K:

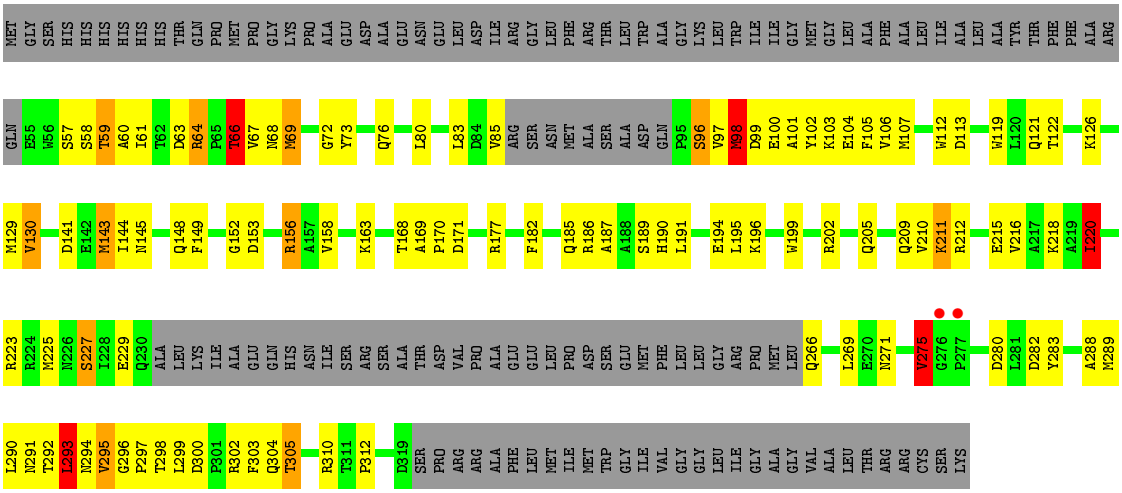




• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

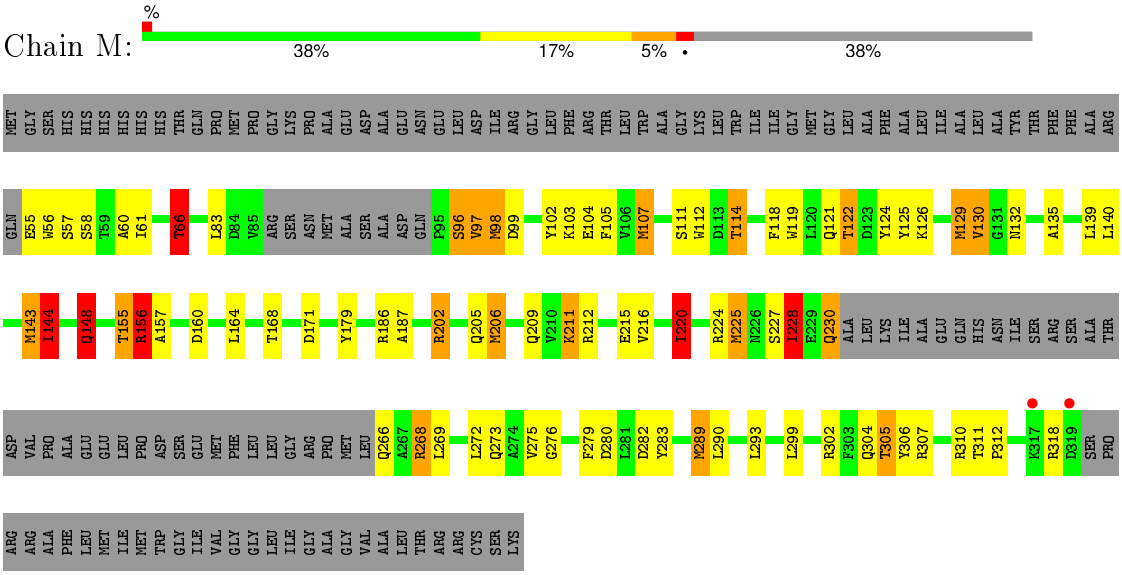
Chain L:





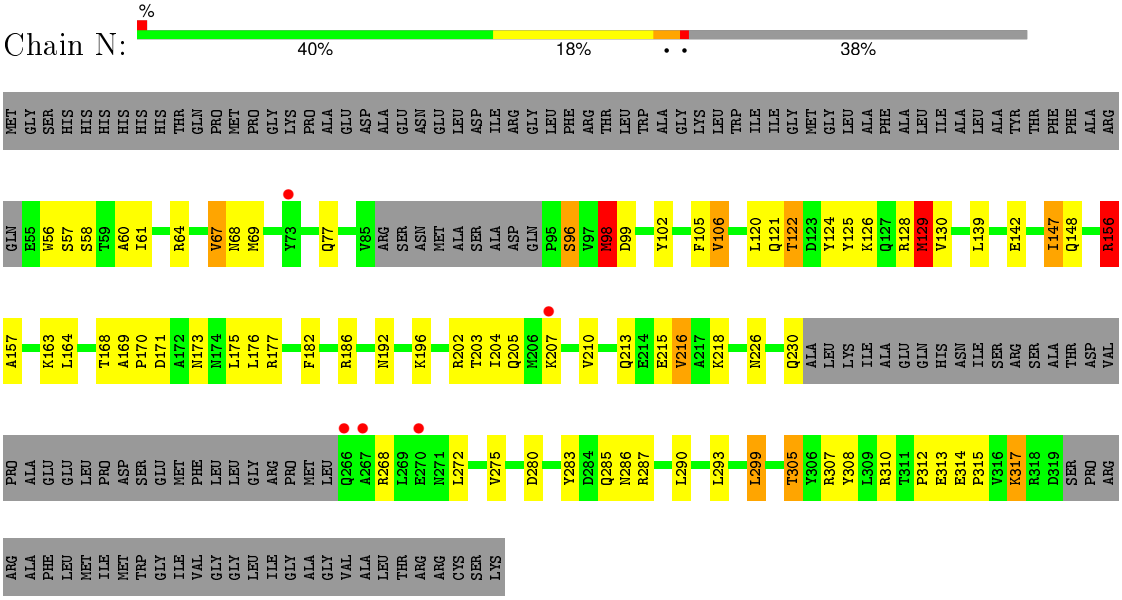
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain M:



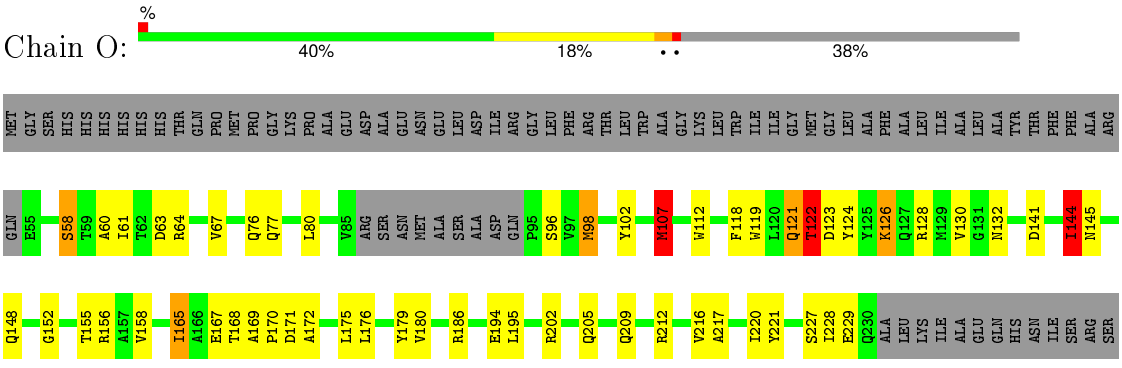
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

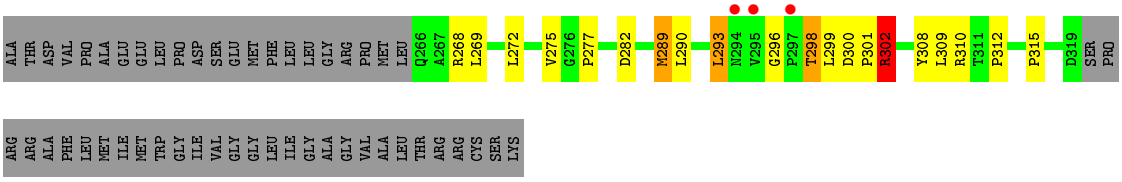
Chain N:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

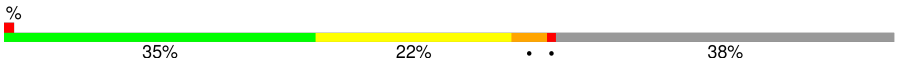
Chain O:

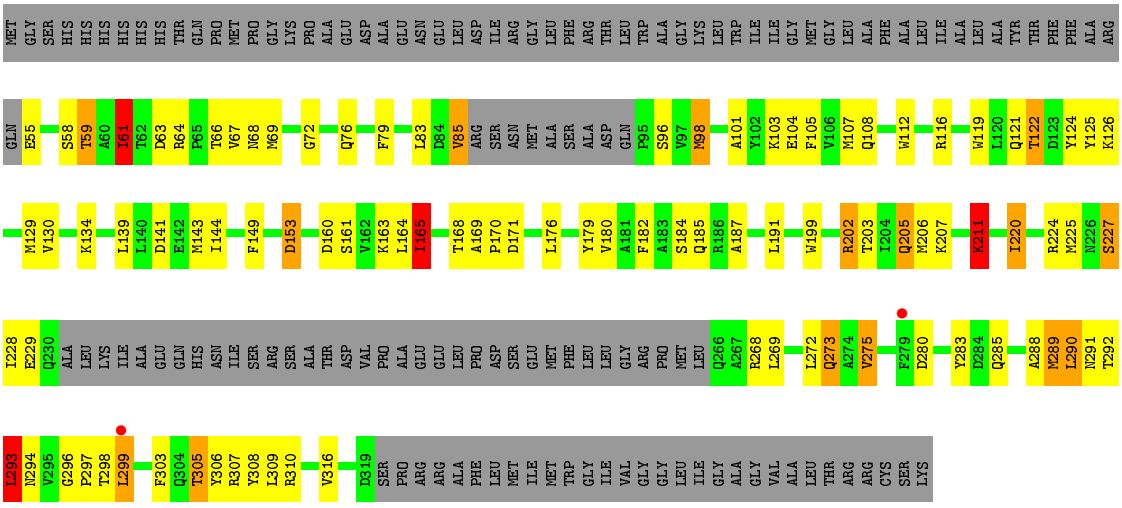




• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

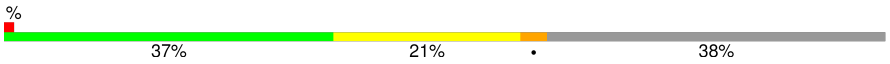
Chain P:

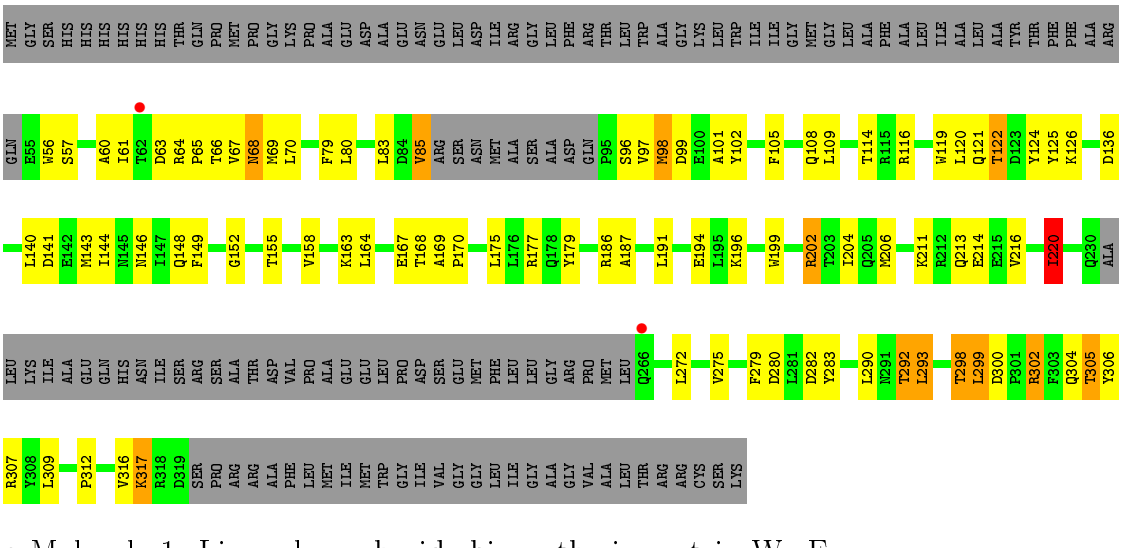




• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

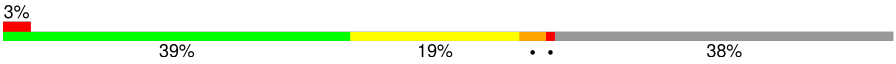
Chain Q:

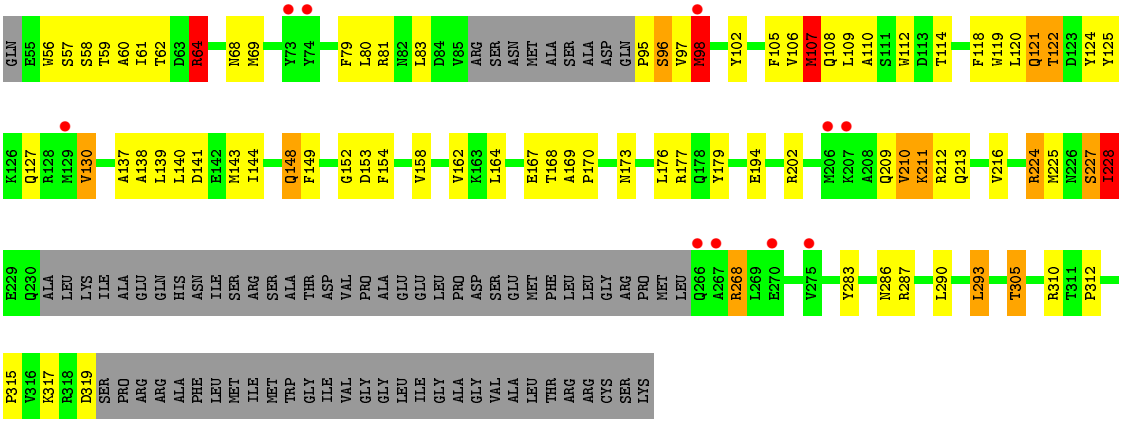




• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

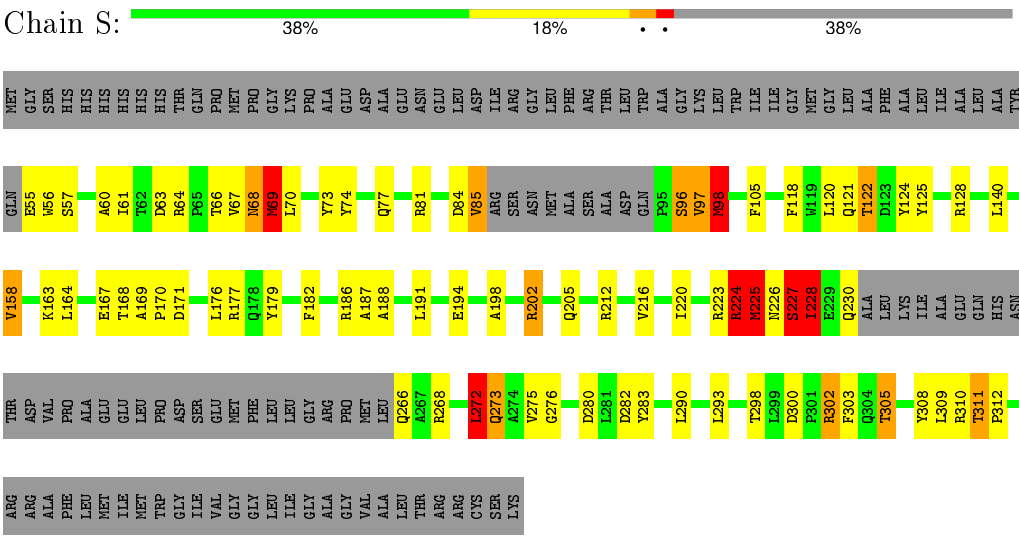
Chain R:





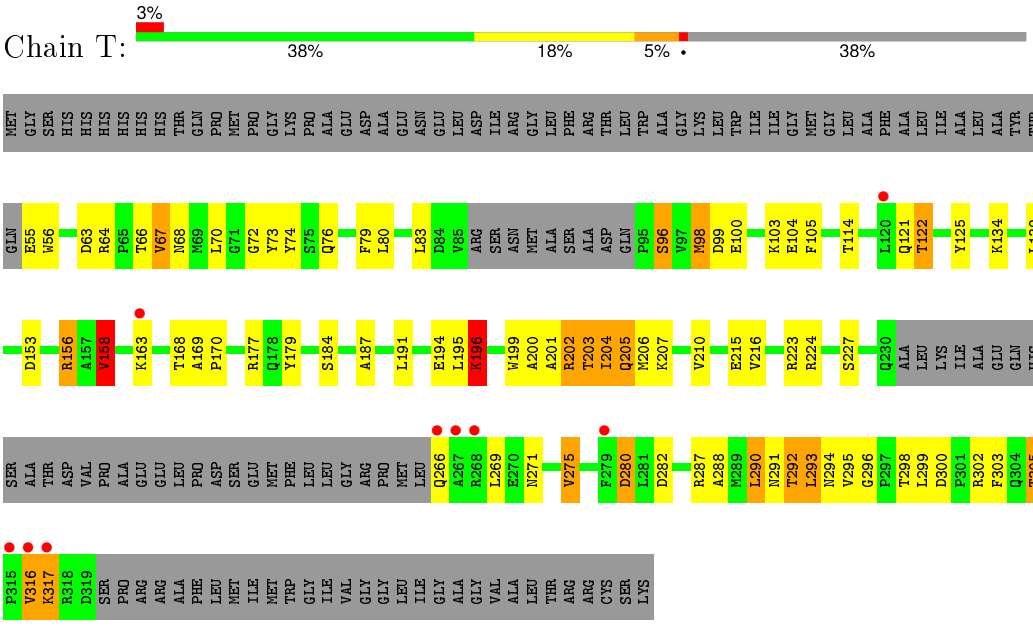
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain S:



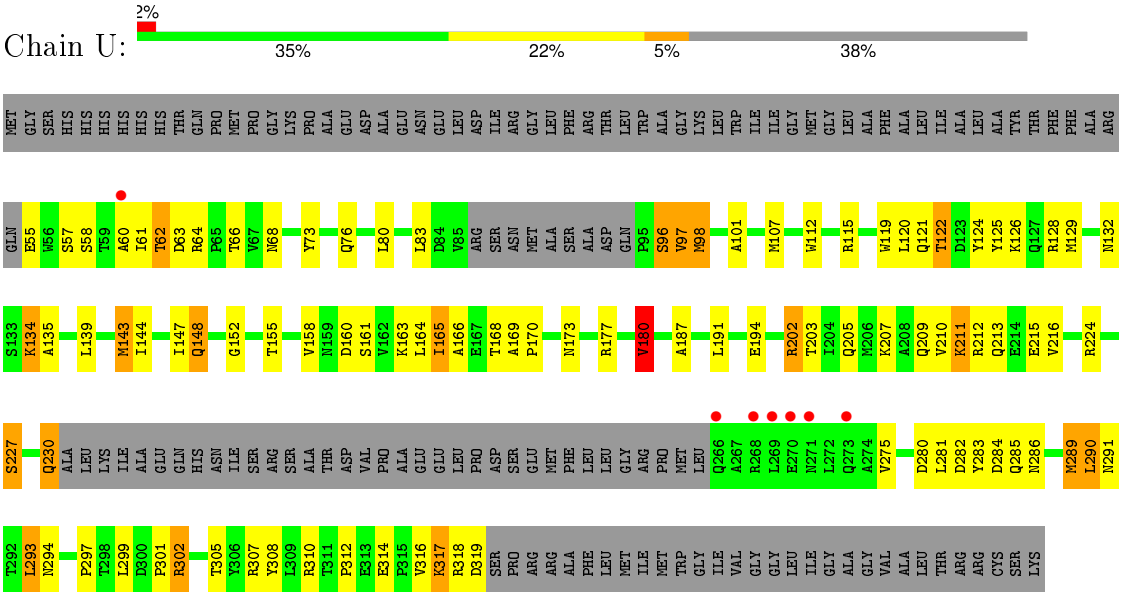
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain T:



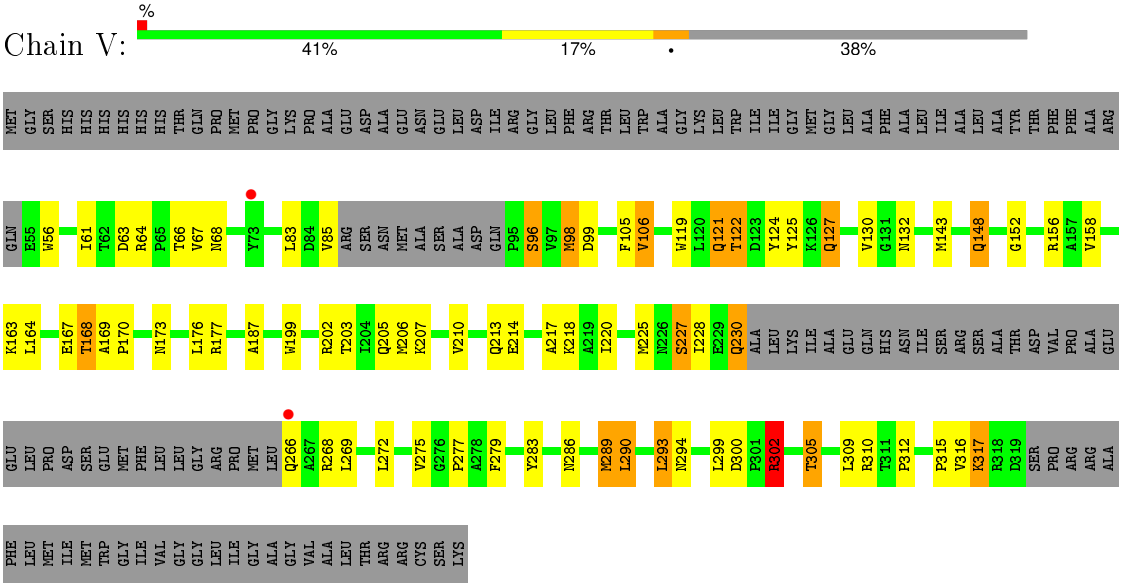
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain U:



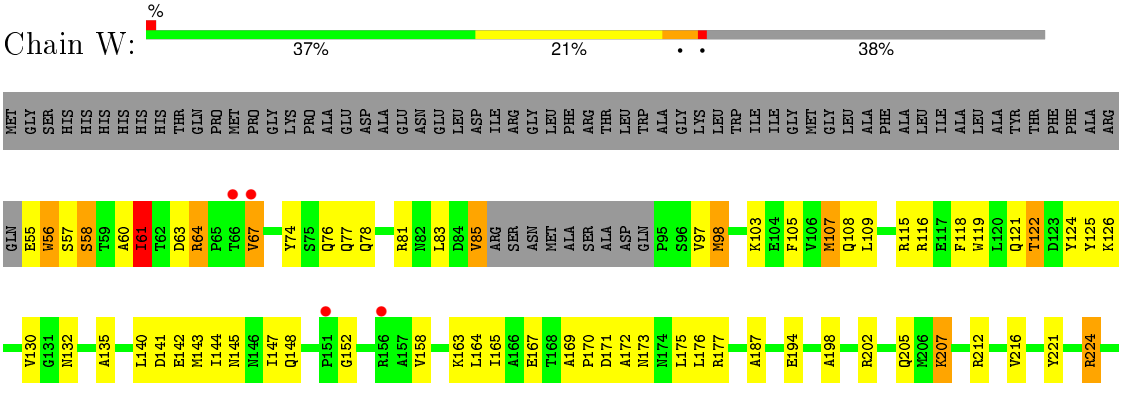
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

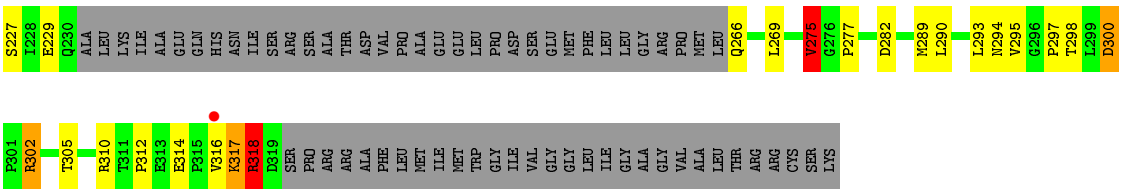
Chain V:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

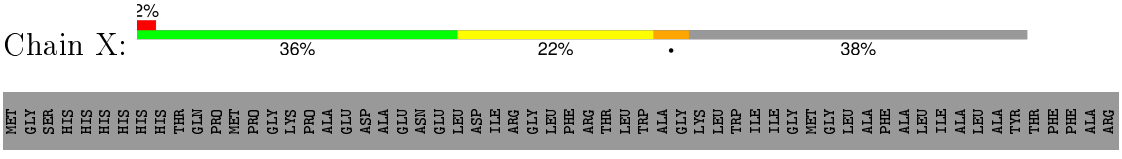
Chain W:





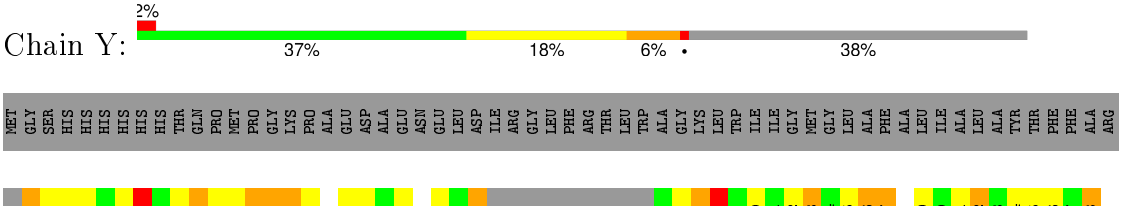
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain X:



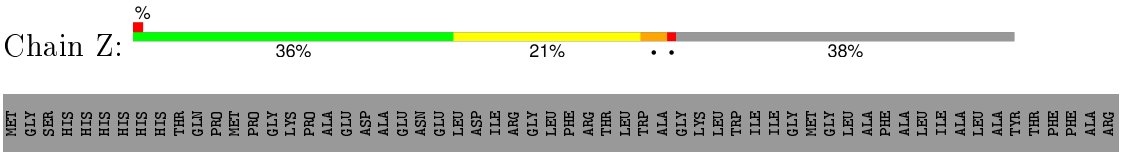
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

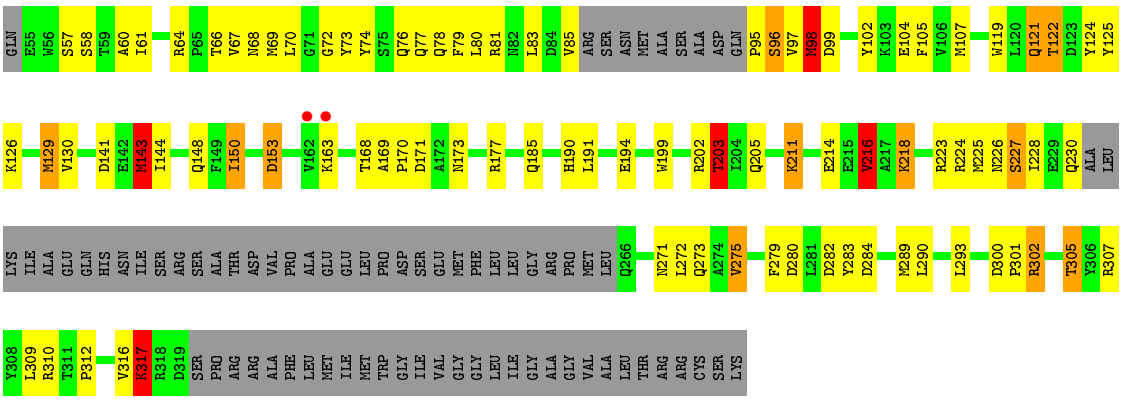
Chain Y:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

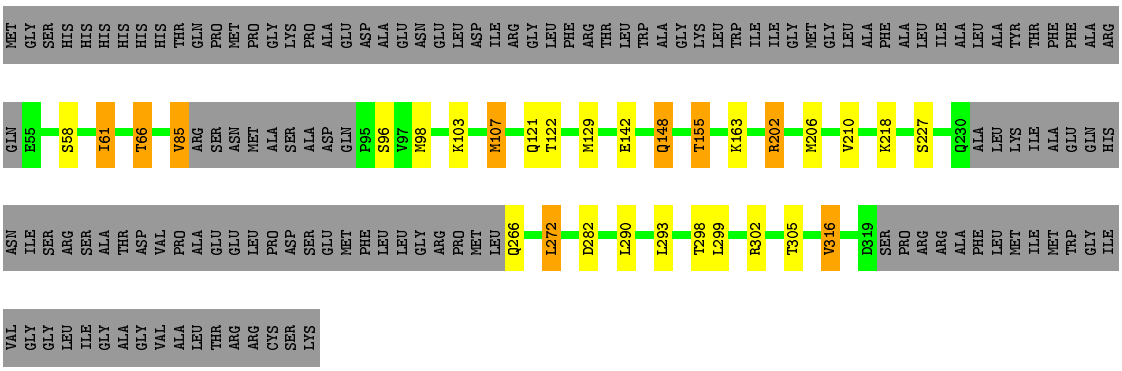
Chain Z:





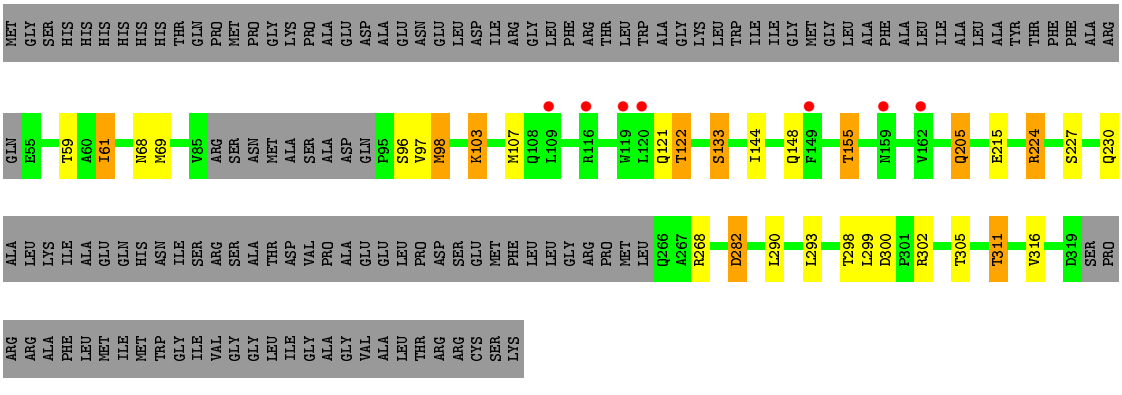
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain a:



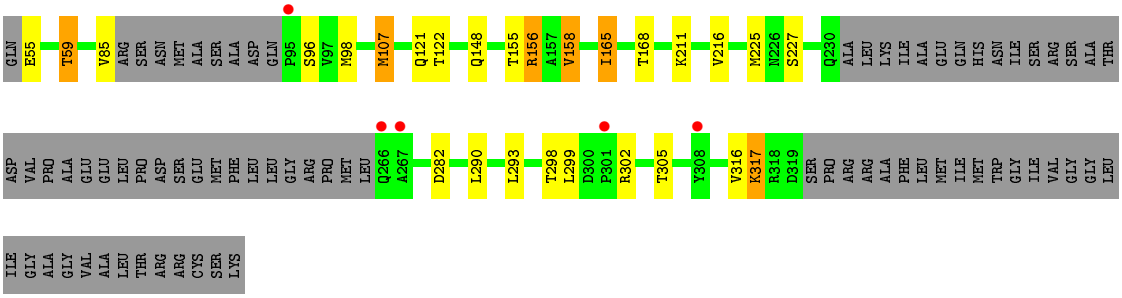
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain b:



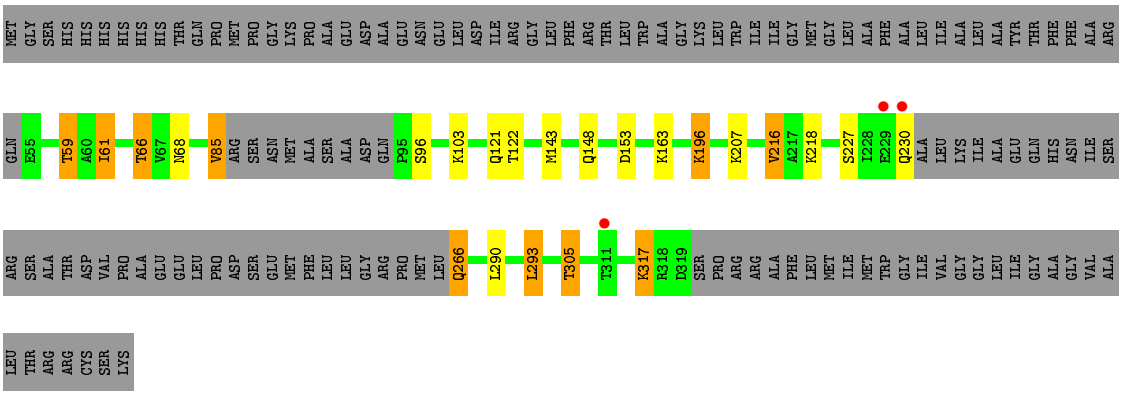
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain c:



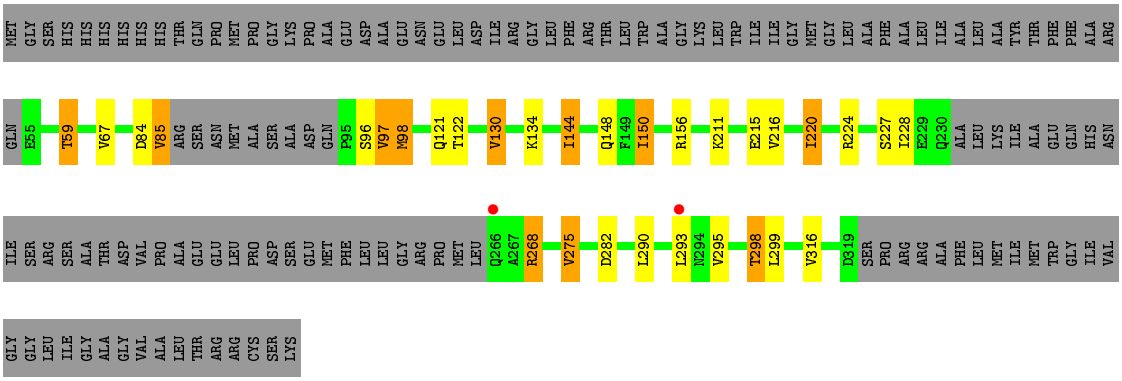
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain d:



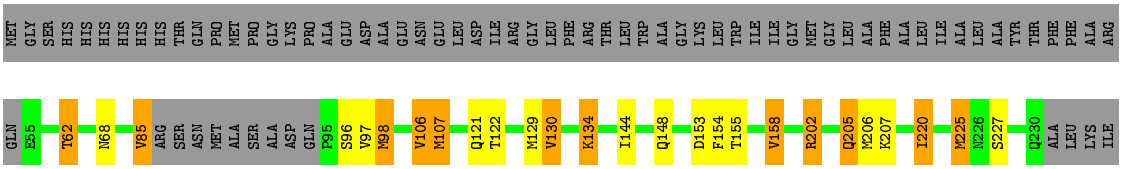
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

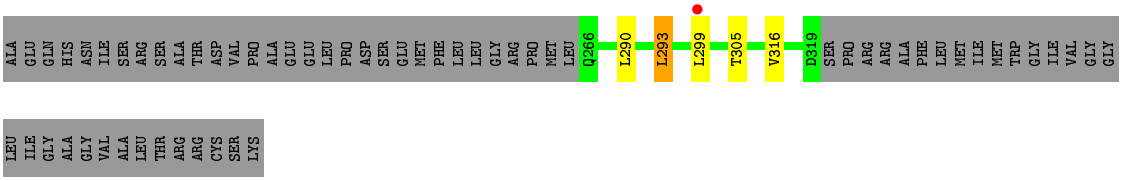
Chain e:



• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain f:




ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 L290 L293 L299 T305 V316 D319 SER PRO ARG ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY GLY
LEU ILE GLY ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	234.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 97.8	EDS
Estimated twinning fraction	0.340 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.52	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
1	T	1797	0	1747	78	0
1	U	1797	0	1748	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1873) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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	Interatomic distance (Å)	Clash overlap (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:P:203:THR:O	1:P:207:LYS:HG3	1.74	0.86
1:H:207:LYS:HG3	1:H:290:LEU:HD21	1.55	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:P:83:LEU:HB3	1:P:202:ARG:NH1	1.96	0.80
1:I:105:PHE:HB2	1:I:305:THR:HG23	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:PHE:HB2	1:L:305:THR:HG23	1.64	0.80
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:X:81:ARG:NH1	1:X:95:PRO:O	2.15	0.79
1:F:61:ILE:HG12	1:F:161:SER:HB3	1.64	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:Z:228:ILE:HD12	1:Z:272:LEU:HD22	1.68	0.76
1:C:132:ASN:HD22	1:C:135:ALA:H	1.32	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:H	1:S:68:ASN:ND2	1.81	0.75
1:Y:61:ILE:HG13	1:Y:310:ARG:HB3	1.69	0.75
1:L:119:TRP:CE2	1:L:143:MET:HB3	2.22	0.74
1:A:292:THR:HG21	1:H:212:ARG:HD3	1.70	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:T:196:LYS:CG	1:T:299:LEU:HD21	2.17	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:B:80:LEU:HD12	1:B:195:LEU:HD12	2.50	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:VAL:HG23	1:A:317:LYS:HD3	1.70	0.73
1:H:105:PHE:HB2	1:H:305:THR:HG23	1.71	0.73
1:A:202:ARG:NH2	1:A:205:GLN:OE1	2.47	0.73
1:G:125:TYR:HD1	1:G:143:MET:HE3	1.53	0.73
1:A:70:LEU:HD11	1:A:98:MET:HB3	1.69	0.73
1:A:60:ALA:HB2	1:A:312:PRO:HG3	1.71	0.72
1:Q:187:ALA:HB3	1:Q:305:THR:HG21	1.70	0.72
1:E:64:ARG:NE	1:E:99:ASP:OD1	2.20	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:Z:81:ARG:NH1	1:Z:95:PRO:O	2.22	0.71
1:I:152:GLY:N	1:I:160:ASP:OD2	2.20	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:P:203:THR:HG22	1:P:207:LYS:HE3	1.72	0.70
1:H:210:VAL:HG22	1:H:286:ASN:HB3	1.73	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:202:ARG:NH2	1:W:205:GLN:OE1	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:224:ARG:HA	1:A:227:SER:OG	1.92	0.69
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:F:80:LEU:HD23	1:F:83:LEU:HD12	3.33	0.69
1:T:83:LEU:HB3	1:T:202:ARG:HH11	1.57	0.69
1:P:119:TRP:NE1	1:P:143:MET:O	2.25	0.69
1:B:141:ASP:HA	1:B:144:ILE:HD12	1.73	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:U:80:LEU:HD23	1:U:83:LEU:HD12	1.73	0.69
1:Q:304:GLN:NE2	1:Q:306:TYR:O	2.24	0.69
1:R:194:GLU:OE2	1:S:68:ASN:ND2	2.26	0.69
1:V:316:VAL:HG23	1:V:317:LYS:HD3	1.74	0.69
1:B:300:ASP:HB2	1:T:295:VAL:HG21	174.85	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: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:D:64:ARG:HE	1:D:99:ASP:HA	2.43	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:B:298:THR:HG21	1:T:294:ASN:CB	172.05	0.67
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:K:60:ALA:HB2	1:K:312:PRO:HG3	1.76	0.67
1:D:228:ILE:HD12	1:D:272:LEU:HD22	1.75	0.67
1:J:211:LYS:HE3	1:J:211:LYS:CA	2.21	0.67
1:D:70:LEU:CD1	1:D:98:MET:HG2	6.32	0.67
1:T:207:LYS:HE3	1:T:294:ASN:HD21	1.58	0.67
1:L:96:SER:OG	1:L:98:MET:HG2	1.95	0.67
1:B:60:ALA:HB2	1:B:312:PRO:HG3	1.77	0.67
1:T:156:ARG:HB3	1:T:158:VAL:HG23	1.76	0.67
1:E:185:GLN:HA	1:E:185:GLN:HE21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HB3	1:B:272:LEU:HD21	3.40	0.67
1:V:173:ASN:OD1	1:V:177:ARG:NE	2.26	0.67
1:B:300:ASP:HB2	1:T:295:VAL:CG2	173.97	0.67
1:P:207:LYS:HE2	1:P:294:ASN:HD21	1.60	0.67
1:N:173:ASN:OD1	1:N:177:ARG:NE	2.26	0.67
1:F:128:ARG:HB3	1:F:139:LEU:HD21	1.75	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: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:224:ARG:O	1:F:228:ILE:HG13	2.55	0.67
1:T:63:ASP:OD1	1:T:64:ARG:HG2	1.95	0.67
1:F:216:VAL:O	1:F:220:ILE:HG13	2.59	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:F:83:LEU:HB3	1:F:202:ARG:HH11	3.26	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:D:168:THR:OG1	1:D:171:ASP:OD2	2.11	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: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:M:216:VAL:O	1:M:220:ILE:HG13	1.95	0.65
1:N:126:LYS:O	1:N:129:MET:HG3	1.96	0.65
1:D:126:LYS:O	1:D:129:MET:HG2	1.95	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:N:64:ARG:HE	1:N:99:ASP:HA	1.61	0.65
1:E:70:LEU:HB2	1:E:74:TYR:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:164:LEU:HB2	1:F:176:LEU:HD13	2.11	0.65
1:D:113:ASP:OD2	1:E:311:THR:OG1	3.34	0.65
1:R:64:ARG:HB3	1:R:102:TYR:HB2	1.79	0.65
1:M:114:THR:HG23	1:M:186:ARG:HD3	1.77	0.65
1:R:122:THR:HG22	1:R:125:TYR:H	1.61	0.65
1:A:66:THR:HG21	1:H:190:HIS:HE1	1.62	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: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:C:56:TRP:HB3	1:C:315:PRO:HG2	2.99	0.64
1:H:210:VAL:CG2	1:H:286:ASN:HB3	2.27	0.64
1:F:177:ARG:NH2	1:F:312:PRO:O	2.31	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:R:173:ASN:OD1	1:R:177:ARG:NE	2.27	0.64
1:A:66:THR:HG21	1:Z:190:HIS:CE1	147.53	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:Z:64:ARG:HG2	1:Z:102:TYR:CG	2.32	0.64
1:W:58:SER:HB2	1:W:176:LEU:HD23	1.79	0.64
1:I:124:TYR:OH	1:I:167:GLU:N	2.31	0.64
1:F:206:MET:HE1	1:F:289:MET:HG2	3.47	0.64
1:A:66:THR:HG21	1:H:190:HIS:CE1	2.32	0.64
1:H:141:ASP:HA	1:H:144:ILE:HD12	1.79	0.64
1:D:66:THR:H	1:D:69:MET:HB2	2.92	0.64
1:C:226:ASN:OD1	1:C:230:GLN:NE2	3.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:210:VAL:HA	1:H:213:GLN:HE21	1.63	0.63
1:A:307:ARG:HH22	1:H:104:GLU:CD	2.01	0.63
1:V:230:GLN:N	1:V:230:GLN:OE1	2.30	0.63
1:B:69:MET:HG2	1:B:304:GLN:HB3	3.10	0.63
1:T:223:ARG:NH1	1:U:284:ASP:OD2	2.29	0.63
1:I:58:SER:OG	1:I:313:GLU:O	2.16	0.63
1:E:266:GLN:HG2	1:E:266:GLN:O	1.99	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:290:LEU:HD22	1:F:294:ASN:HD21	1.64	0.62
1:M:111:SER:HB3	1:M:114:THR:OG1	1.99	0.62
1:F:182:PHE:CE2	1:F:186:ARG:HD2	2.34	0.62
1:Q:66:THR:HG21	1:X:190:HIS:CE1	2.34	0.62
1:K:61:ILE:HB	1:K:310:ARG:HB3	1.80	0.62
1:P:205:GLN:HG3	1:P:206:MET:N	2.14	0.62
1:A:66:THR:HG21	1:Z:190:HIS:NE2	147.62	0.62
1:G:196:LYS:NZ	1:O:296:GLY:O	2.32	0.62
1:Q:119:TRP:NE1	1:Q:143:MET:O	2.32	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: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:A:101:ALA:HA	1:A:191:LEU:HD11	2.48	0.62
1:H:116:ARG:HG3	1:H:144:ILE:HD11	1.81	0.62
1:Z:226:ASN:O	1:Z:230:GLN:HG3	1.99	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:D:119:TRP:CD2	1:D:143:MET:HG3	2.35	0.62
1:Y:119:TRP:CE2	1:Y:143:MET:HB3	2.35	0.62
1:U:83:LEU:O	1:U:202:ARG:NH1	2.33	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: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:Z:96:SER:OG	1:Z:98:MET:SD	2.58	0.61
1:Q:83:LEU:HB3	1:Q:202:ARG:HH11	1.65	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:K:228:ILE:HD12	1:K:272:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:ASP:HA	1:I:144:ILE:HD12	1.82	0.61
1:T:72:GLY:O	1:T:76:GLN:HG3	2.00	0.61
1:H:113:ASP:O	1:H:117:GLU:HG3	2.00	0.61
1:A:177:ARG:NH2	1:A:312:PRO:O	2.32	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
1:B:168:THR:OG1	1:B:171:ASP:OD2	2.50	0.61
1:I:141:ASP:O	1:I:145:ASN:ND2	2.33	0.61
1:A:152:GLY:HA2	1:A:158:VAL:HG12	1.81	0.61
1:K:227:SER:HB2	1:L:275:VAL:HG23	1.82	0.61
1:G:128:ARG:HE	1:G:167:GLU:CD	2.04	0.61
1:E:152:GLY:HA2	1:E:158:VAL:HG12	2.60	0.61
1:H:164:LEU:HB2	1:H:176:LEU:HD13	1.82	0.61
1:Y:124:TYR:OH	1:Y:167:GLU:N	2.28	0.61
1:E:177:ARG:NH2	1:E:312:PRO:O	2.25	0.61
1:C:83:LEU:HD21	1:C:289:MET:SD	2.41	0.61
1:T:80:LEU:HD12	1:T:195:LEU:HD12	1.81	0.61
1:F:59:THR:HB	1:F:310:ARG:CZ	3.12	0.61
1:E:98:MET:CE	1:E:98:MET:H	2.14	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: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: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: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:D:108:GLN:HG3	1:D:187:ALA:HB2	1.82	0.60
1:F:202:ARG:NH2	1:F:205:GLN:HE21	4.07	0.60
1:A:132:ASN:ND2	1:A:135:ALA:H	4.16	0.60
1:I:60:ALA:HB2	1:I:312:PRO:HG3	1.84	0.60
1:E:119:TRP:CD2	1:E:143:MET:HB3	2.83	0.60
1:F:184:SER:HB2	1:F:306:TYR:CE1	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:227:SER:HB2	1:S:275:VAL:HG23	1.84	0.60
1:E:168:THR:OG1	1:E:171:ASP:OD2	2.19	0.60
1:P:187:ALA:CB	1:P:305:THR:HG21	2.29	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:Y:152:GLY:HA2	1:Y:158:VAL:HG12	1.83	0.60
1:E:268:ARG:HA	1:E:271:ASN:HB2	1.82	0.59
1:B:302:ARG:NH1	1:T:292:THR:HG22	177.74	0.59
1:J:223:ARG:HH12	1:K:284:ASP:CG	2.06	0.59
1:B:77:GLN:HG2	1:B:97:VAL:HG13	1.84	0.59
1:I:316:VAL:HG23	1:I:317:LYS:HD2	1.84	0.59
1:U:139:LEU:HG	1:U:143:MET:HE3	1.84	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:F:268:ARG:HA	1:F:271:ASN:HB2	1.83	0.59
1:A:227:SER:HB3	1:B:275:VAL:HG22	1.85	0.59
1:T:223:ARG:HH12	1:U:284:ASP:CG	2.04	0.59
1:J:210:VAL:HA	1:J:213:GLN:HE21	1.67	0.59
1:Z:173:ASN:OD1	1:Z:177:ARG:NE	2.35	0.59
1:Y:122:THR:CG2	1:Y:125:TYR:H	2.14	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:K:69:MET:SD	1:K:307:ARG:HB3	2.43	0.59
1:E:123:ASP:HB3	1:E:127:GLN:HE21	1.68	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:U:122:THR:HG22	1:U:125:TYR:H	1.67	0.59
1:A:207:LYS:HE3	1:A:294:ASN:ND2	3.76	0.59
1:E:120:LEU:HD21	1:E:140:LEU:HD22	2.18	0.59
1:O:119:TRP:CE3	1:O:122:THR:HG21	2.37	0.59
1:E:125:TYR:HD1	1:E:143:MET:HE3	3.41	0.59
1:N:122:THR:HG22	1:N:125:TYR:H	1.68	0.59
1:M:275:VAL:HG13	1:M:276:GLY:H	1.67	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:A:169:ALA:HB3	1:A:170:PRO:HD3	1.85	0.59
1:L:223:ARG:O	1:L:227:SER:OG	2.20	0.59
1:B:119:TRP:NE1	1:B:143:MET:O	2.35	0.59
1:F:61:ILE:HG22	1:F:309:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:56:TRP:HB3	1:R:315:PRO:HG2	1.85	0.59
1:G:227:SER:HB2	1:H:275:VAL:HG23	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:O:217:ALA:HA	1:O:220:ILE:HD12	1.84	0.58
1:I:164:LEU:HB2	1:I:176:LEU:HD13	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
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:G:125:TYR:CD1	1:G:143:MET:CE	2.83	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:C:202:ARG:NH2	1:C:205:GLN:OE1	2.67	0.58
1:K:212:ARG:HH11	1:L:292:THR:HG21	1.69	0.58
1:W:58:SER:HB2	1:W:176:LEU:CD2	2.33	0.58
1:I:223:ARG:NH2	1:J:284:ASP:OD1	2.26	0.58
1:Z:316:VAL:HG23	1:Z:317:LYS:HG2	1.85	0.58
1:J:64:ARG:HG2	1:J:102:TYR:CB	2.33	0.58
1:F:73:TYR:CZ	1:F:191:LEU:HB3	2.38	0.58
1:M:212:ARG:O	1:M:216:VAL:HG23	2.04	0.58
1:E:122:THR:HG22	1:E:125:TYR:H	2.30	0.58
1:Z:122:THR:HG22	1:Z:125:TYR:H	1.68	0.58
1:Q:177:ARG:NH2	1:Q:312:PRO:O	2.36	0.58
1:J:66:THR:H	1:J:69:MET:HB2	1.68	0.58
1:D:58:SER:OG	1:D:313:GLU:O	2.22	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:X:136:ASP:O	1:X:140:LEU:HB2	2.03	0.57
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:B:298:THR:HG21	1:T:294:ASN:HB2	172.71	0.57
1:B:130:VAL:HG23	1:B:132:ASN:H	2.29	0.57
1:R:162:VAL:HG13	1:R:176:LEU:HD11	1.86	0.57
1:I:122:THR:HG22	1:I:125:TYR:H	1.70	0.57
1:D:205:GLN:HG3	1:D:206:MET:N	2.19	0.57
1:Q:122:THR:CG2	1:Q:124:TYR:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:ARG:HH11	1:E:268:ARG:CG	2.61	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:U:169:ALA:HB1	1:U:314:GLU:HG2	1.85	0.57
1:N:283:TYR:CZ	1:N:287:ARG:HD3	2.38	0.57
1:M:187:ALA:HB3	1:M:305:THR:HG21	1.86	0.57
1:D:124:TYR:OH	1:D:167:GLU:HG3	2.48	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
1:E:187:ALA:HB3	1:E:305:THR:HG21	1.85	0.57
1:A:98:MET:CE	1:A:98:MET:H	2.17	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:X:56:TRP:CZ2	1:X:318:ARG:HD2	2.40	0.57
1:V:168:THR:OG1	1:V:170:PRO:HD2	2.04	0.57
1:U:122:THR:CG2	1:U:125:TYR:H	2.17	0.57
1:F:216:VAL:HG12	1:F:220:ILE:HD11	3.21	0.57
1:O:124:TYR:CG	1:O:175:LEU:HD11	2.39	0.57
1:M:168:THR:OG1	1:M:171:ASP:OD2	2.19	0.57
1:P:202:ARG:HE	1:P:205:GLN:HG2	1.70	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:A:226:ASN:O	1:A:230:GLN:HG3	2.05	0.57
1:W:115:ARG:HD3	1:W:147:ILE:HB	1.87	0.57
1:I:148:GLN:N	1:I:148:GLN:HE21	2.03	0.57
1:Q:105:PHE:HB2	1:Q:305:THR:CG2	2.23	0.56
1:P:199:TRP:NE1	1:P:293:LEU:O	2.29	0.56
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:R:56:TRP:CE3	1:R:169:ALA:HB2	2.40	0.56
1:P:63:ASP:O	1:P:307:ARG:N	2.28	0.56
1:R:61:ILE:HB	1:R:310:ARG:HB3	1.87	0.56
1:D:190:HIS:CE1	1:E:66:THR:HG21	2.71	0.56
1:Y:152:GLY:N	1:Y:160:ASP:OD2	2.28	0.56
1:X:164:LEU:HB2	1:X:176:LEU:HD13	1.87	0.56
1:D:199:TRP:CD2	1:D:297:PRO:HD3	2.40	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:L:196:LYS:HG3	1:L:299:LEU:HD21	1.87	0.56
1:B:199:TRP:NE1	1:B:296:GLY:HA2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:ASN:O	1:E:275:VAL:HG12	2.21	0.56
1:G:125:TYR:HD1	1:G:143:MET:HE2	1.67	0.56
1:F:120:LEU:O	1:F:126:LYS:HE2	2.05	0.56
1:K:132:ASN:ND2	1:K:135:ALA:H	2.01	0.56
1:F:188:ALA:HA	1:F:303:PHE:CZ	2.40	0.56
1:P:69:MET:O	1:P:303:PHE:HB2	2.06	0.56
1:L:113:ASP:OD2	1:M:311:THR:OG1	2.23	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:F:64:ARG:O	1:F:307:ARG:HG2	2.05	0.56
1:D:56:TRP:CE3	1:D:169:ALA:HB2	2.40	0.56
1:X:283:TYR:CZ	1:X:287:ARG:HD3	2.41	0.56
1:C:152:GLY:N	1:C:160:ASP:OD2	2.20	0.56
1:Y:177:ARG:NH2	1:Y:312:PRO:O	2.38	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: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:M:139:LEU:O	1:M:143:MET:HG3	2.06	0.56
1:C:96:SER:OG	1:C:98:MET:SD	3.11	0.56
1:A:194:GLU:OE2	1:B:67:VAL:HG23	3.45	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:A:307:ARG:NH2	1:Z:104:GLU:OE1	146.47	0.56
1:S:77:GLN:HB3	1:S:97:VAL:HG11	1.88	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:X:122:THR:HG22	1:X:125:TYR:H	1.71	0.56
1:A:141:ASP:HA	1:A:144:ILE:HD12	1.88	0.56
1:M:124:TYR:CD1	1:M:143:MET:HE1	2.41	0.56
1:Z:64:ARG:HG2	1:Z:102:TYR:CD2	2.40	0.56
1:Q:65:PRO:HD2	1:Q:102:TYR:HB2	1.88	0.56
1:J:223:ARG:NH2	1:K:284:ASP:OD1	2.33	0.56
1:C:122:THR:HG22	1:C:125:TYR:H	1.71	0.56
1:M:225:MET:HE1	1:M:273:GLN:HG3	1.88	0.56
1:Z:79:PHE:O	1:Z:83:LEU:HG	2.06	0.56
1:A:119:TRP:CZ2	1:A:143:MET:HG2	2.41	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:A:76:GLN:NE2	1:A:298:THR:H	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:HA	1:A:211:LYS:HE3	1.88	0.56
1:H:124:TYR:OH	1:H:167:GLU:N	2.37	0.55
1:E:122:THR:CG2	1:E:124:TYR:HB3	2.72	0.55
1:U:173:ASN:OD1	1:U:177:ARG:NE	2.38	0.55
1:D:57:SER:HB3	1:D:165:ILE:HG12	2.17	0.55
1:L:190:HIS:NE2	1:M:66:THR:HG21	2.21	0.55
1:U:120:LEU:HD23	1:U:125:TYR:HE2	1.69	0.55
1:B:182:PHE:CE2	1:B:186:ARG:HD2	2.41	0.55
1:D:76:GLN:OE1	1:D:298:THR:N	2.38	0.55
1:V:96:SER:HB3	1:V:99:ASP:OD2	2.06	0.55
1:V:56:TRP:HE3	1:V:315:PRO:HG2	1.71	0.55
1:L:152:GLY:HA2	1:L:158:VAL:HG12	1.87	0.55
1:C:101:ALA:HA	1:C:191:LEU:HD11	2.13	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:U:132:ASN:HD22	1:U:135:ALA:N	2.01	0.55
1:D:300:ASP:O	1:D:303:PHE:HD2	1.89	0.55
1:B:69:MET:O	1:B:303:PHE:HB2	2.07	0.55
1:D:79:PHE:CE2	1:D:83:LEU:HD11	2.42	0.55
1:J:223:ARG:NH1	1:K:284:ASP:OD2	2.29	0.55
1:V:206:MET:HE2	1:V:289:MET:HG2	1.88	0.55
1:E:202:ARG:NH2	1:E:205:GLN:OE1	2.95	0.55
1:W:229:GLU:HG3	1:W:269:LEU:HD11	1.89	0.55
1:R:96:SER:OG	1:R:98:MET:HG3	2.05	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:B:210:VAL:HA	1:B:213:GLN:HE21	1.71	0.55
1:U:180:VAL:HG11	1:U:308:TYR:OH	2.06	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:G:204:ILE:HD12	1:O:302:ARG:NE	2.21	0.55
1:E:77:GLN:CG	1:E:97:VAL:HG11	3.93	0.55
1:R:110:ALA:HB2	1:R:149:PHE:CD2	2.41	0.55
1:A:152:GLY:HA2	1:A:158:VAL:CG1	2.37	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:C:212:ARG:O	1:C:216:VAL:HG23	2.32	0.55
1:X:124:TYR:OH	1:X:167:GLU:HG3	2.07	0.55
1:A:105:PHE:HB2	1:A:305:THR:CG2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:79:PHE:O	1:T:83:LEU:HG	2.06	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:Y:70:LEU:HD11	1:Y:98:MET:HB3	1.88	0.55
1:R:224:ARG:HG2	1:R:228:ILE:HD11	1.89	0.54
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: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: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:P:141:ASP:HA	1:P:144:ILE:HD12	1.89	0.54
1:P:207:LYS:CE	1:P:294:ASN:HD21	2.20	0.54
1:F:73:TYR:CE1	1:F:191:LEU:HB3	2.42	0.54
1:C:126:LYS:HA	1:C:129:MET:HG3	2.60	0.54
1:E:227:SER:HB2	1:F:275:VAL:HG23	2.54	0.54
1:C:216:VAL:HG13	1:D:284:ASP:HB3	2.11	0.54
1:I:61:ILE:HB	1:I:310:ARG:HB3	1.90	0.54
1:S:122:THR:HG22	1:S:125:TYR:H	1.70	0.54
1:S:122:THR:CG2	1:S:125:TYR:H	2.20	0.54
1:R:141:ASP:HA	1:R:144:ILE:HD12	1.88	0.54
1:X:125:TYR:O	1:X:129:MET:N	2.40	0.54
1:J:64:ARG:HD3	1:J:99:ASP:CA	2.30	0.54
1:O:300:ASP:OD1	1:O:302:ARG:NH1	2.30	0.54
1:Z:78:GLN:HG2	1:Z:97:VAL:HG21	1.89	0.54
1:R:56:TRP:HE3	1:R:315:PRO:HG2	1.72	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:M:83:LEU:HD21	1:M:289:MET:CE	2.38	0.54
1:F:104:GLU:HG2	1:F:191:LEU:HG	1.90	0.54
1:A:153:ASP:H	1:A:158:VAL:HG12	1.73	0.54
1:Q:213:GLN:HE22	1:Q:283:TYR:HA	1.71	0.54
1:X:122:THR:CG2	1:X:125:TYR:H	2.20	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:C:98:MET:N	1:C:98:MET:SD	3.61	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:D:225:MET:HE3	1:D:273:GLN:HG3	1.89	0.54
1:G:200:ALA:HB1	1:O:302:ARG:NH1	2.22	0.54
1:H:213:GLN:NE2	1:H:286:ASN:HD22	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:TRP:CE3	1:F:122:THR:HG21	2.43	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:G:187:ALA:CB	1:G:305:THR:HG21	2.38	0.54
1:T:200:ALA:O	1:T:204:ILE:HG12	2.07	0.54
1:E:57:SER:CB	1:E:163:LYS:HE2	2.58	0.54
1:K:226:ASN:O	1:K:230:GLN:HG3	2.08	0.54
1:X:67:VAL:HG22	1:X:98:MET:HE1	1.89	0.54
1:B:68:ASN:HD22	1:B:68:ASN:H	1.56	0.54
1:N:122:THR:CG2	1:N:125:TYR:H	2.21	0.54
1:I:310:ARG:HB2	1:P:112:TRP:HB3	1.89	0.54
1:T:300:ASP:OD1	1:T:302:ARG:HB2	2.07	0.54
1:F:108:GLN:HG3	1:F:187:ALA:HB2	1.90	0.54
1:T:199:TRP:NE1	1:T:296:GLY:HA2	2.23	0.54
1:E:169:ALA:HB3	1:E:170:PRO:HD3	1.90	0.54
1:A:104:GLU:CD	1:B:307:ARG:HH22	3.53	0.54
1:H:56:TRP:CE3	1:H:169:ALA:HB2	2.43	0.54
1:T:76:GLN:NE2	1:T:298:THR:O	2.41	0.53
1:K:169:ALA:HB3	1:K:170:PRO:HD3	1.90	0.53
1:C:122:THR:CG2	1:C:125:TYR:H	2.19	0.53
1:V:61:ILE:HB	1:V:310:ARG:HB3	1.89	0.53
1:H:119:TRP:CD2	1:H:143:MET:HB3	2.43	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:E:112:TRP:HB3	1:F:310:ARG:HB2	2.73	0.53
1:T:202:ARG:HH21	1:T:205:GLN:NE2	2.06	0.53
1:I:83:LEU:HB3	1:I:202:ARG:HH11	1.74	0.53
1:E:283:TYR:OH	1:E:287:ARG:NH1	3.93	0.53
1:U:227:SER:HB2	1:V:275:VAL:HG23	1.90	0.53
1:K:80:LEU:HD23	1:K:83:LEU:HD12	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:P:206:MET:SD	1:P:289:MET:HG3	2.48	0.53
1:G:119:TRP:O	1:G:125:TYR:HB3	2.08	0.53
1:B:72:GLY:C	1:B:76:GLN:HE21	2.11	0.53
1:K:210:VAL:HG13	1:K:283:TYR:CE1	2.42	0.53
1:Z:80:LEU:HD23	1:Z:83:LEU:HD12	1.90	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:F:184:SER:HA	1:F:305:THR:HG22	1.89	0.53
1:W:57:SER:CB	1:W:163:LYS:HE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:SER:HB3	1:L:99:ASP:OD2	2.09	0.53
1:E:122:THR:O	1:E:126:LYS:HG3	2.24	0.53
1:A:226:ASN:OD1	1:A:230:GLN:NE2	2.40	0.53
1:E:57:SER:HB2	1:E:163:LYS:HE2	2.27	0.53
1:U:76:GLN:HE22	1:U:297:PRO:HA	1.72	0.53
1:A:124:TYR:OH	1:A:167:GLU:HG3	2.08	0.53
1:X:288:ALA:O	1:X:292:THR:OG1	2.26	0.53
1:F:96:SER:O	1:F:100:GLU:HG2	2.08	0.53
1:W:119:TRP:CE2	1:W:143:MET:HB3	2.43	0.53
1:D:64:ARG:O	1:D:307:ARG:HG2	2.19	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:300:ASP:OD1	1:W:302:ARG:HD3	2.09	0.53
1:P:163:LYS:HE3	1:P:165:ILE:HD12	1.91	0.53
1:G:143:MET:HA	1:G:146:ASN:HB2	1.91	0.53
1:W:122:THR:HG22	1:W:125:TYR:H	1.72	0.53
1:U:61:ILE:HB	1:U:310:ARG:HB3	1.91	0.53
1:Q:152:GLY:HA2	1:Q:158:VAL:HG12	1.90	0.53
1:X:124:TYR:OH	1:X:167:GLU:N	2.39	0.53
1:U:120:LEU:HD23	1:U:125:TYR:CE2	2.43	0.53
1:F:266:GLN:HE21	1:F:269:LEU:HD23	1.72	0.53
1:W:108:GLN:HG3	1:W:187:ALA:HB2	1.90	0.53
1:F:105:PHE:CZ	1:F:109:LEU:HD13	2.44	0.53
1:B:57:SER:CB	1:B:163:LYS:HE2	2.39	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:C:199:TRP:CD1	1:C:297:PRO:HD3	2.43	0.53
1:I:275:VAL:HG23	1:P:227:SER:HB2	1.91	0.53
1:A:283:TYR:CZ	1:A:287:ARG:HD3	2.78	0.53
1:U:122:THR:CG2	1:U:124:TYR:HB3	2.39	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: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:P:202:ARG:HH21	1:P:205:GLN:NE2	2.07	0.52
1:U:202:ARG:NH2	1:U:205:GLN:OE1	2.42	0.52
1:D:119:TRP:NE1	1:D:143:MET:O	3.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:119:TRP:CE2	1:U:143:MET:HB3	2.43	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:X:152:GLY:HA2	1:X:158:VAL:HG12	1.91	0.52
1:C:194:GLU:OE2	1:D:67:VAL:HG23	2.36	0.52
1:T:207:LYS:CE	1:T:294:ASN:HD21	2.20	0.52
1:R:125:TYR:HD1	1:R:143:MET:SD	2.32	0.52
1:A:55:GLU:O	1:A:319:ASP:N	2.70	0.52
1:K:155:THR:HB	1:K:156:ARG:HD2	1.90	0.52
1:J:187:ALA:HB3	1:J:305:THR:HG21	1.91	0.52
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:A:221:TYR:CE1	1:A:272:LEU:HG	2.45	0.52
1:W:115:ARG:HD2	1:W:144:ILE:O	2.10	0.52
1:C:73:TYR:CZ	1:C:191:LEU:HB3	2.44	0.52
1:Z:199:TRP:O	1:Z:203:THR:OG1	2.27	0.52
1:L:76:GLN:OE1	1:L:298:THR:N	2.24	0.52
1:D:266:GLN:HG2	1:D:269:LEU:HB3	1.92	0.52
1:A:307:ARG:NH2	1:H:104:GLU:OE1	2.43	0.52
1:L:280:ASP:OD2	1:L:282:ASP:HB3	2.09	0.52
1:A:168:THR:OG1	1:A:171:ASP:OD2	3.94	0.52
1:B:108:GLN:HG3	1:B:187:ALA:HB2	1.90	0.52
1:U:63:ASP:OD1	1:U:64:ARG:N	2.35	0.52
1:A:224:ARG:HA	1:A:227:SER:HG	1.75	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: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:I:203:THR:HA	1:I:293:LEU:HD23	1.92	0.52
1:J:119:TRP:NE1	1:J:147:ILE:HD11	2.25	0.52
1:I:122:THR:CG2	1:I:124:TYR:HB3	2.40	0.52
1:M:275:VAL:HG13	1:M:276:GLY:N	2.24	0.52
1:V:164:LEU:HD13	1:V:176:LEU:HA	1.91	0.52
1:Q:199:TRP:CE2	1:Q:293:LEU:HD12	2.45	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:B:207:LYS:HE3	1:B:290:LEU:HD21	3.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:MET:HA	1:A:206:MET:HE2	4.61	0.52
1:F:122:THR:CG2	1:F:124:TYR:HB3	2.40	0.52
1:E:77:GLN:HG2	1:E:97:VAL:CG1	3.40	0.52
1:D:122:THR:HG22	1:D:125:TYR:H	1.75	0.52
1:C:83:LEU:O	1:C:202:ARG:NH1	3.44	0.52
1:X:57:SER:HA	1:X:164:LEU:O	2.10	0.52
1:U:209:GLN:HA	1:U:212:ARG:NH2	2.25	0.52
1:S:182:PHE:CE2	1:S:186:ARG:HD2	2.45	0.52
1:Z:214:GLU:HA	1:Z:279:PHE:HE2	1.75	0.52
1:J:121:GLN:O	1:J:121:GLN:HG2	2.10	0.52
1:C:55:GLU:O	1:C:318:ARG:HG2	4.63	0.52
1:F:64:ARG:HD3	1:F:99:ASP:OD1	2.10	0.52
1:F:147:ILE:HG12	1:F:164:LEU:HD12	1.92	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
1:F:194:GLU:OE2	1:Y:66:THR:HB	176.08	0.52
1:G:272:LEU:HA	1:G:275:VAL:HG12	1.91	0.52
1:P:184:SER:HB2	1:P:306:TYR:CE1	2.45	0.52
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: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:U:96:SER:HG	1:U:98:MET:HG2	1.75	0.51
1:Q:66:THR:HB	1:X:194:GLU:CD	2.31	0.51
1:V:169:ALA:HB3	1:V:170:PRO:HD3	1.91	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:S:187:ALA:CB	1:S:305:THR:HG21	2.39	0.51
1:G:116:ARG:HG3	1:G:140:LEU:HD21	1.92	0.51
1:E:187:ALA:HB1	1:E:305:THR:HG21	2.50	0.51
1:H:119:TRP:NE1	1:H:143:MET:O	2.43	0.51
1:Q:196:LYS:HD2	1:Q:299:LEU:HD21	1.91	0.51
1:G:295:VAL:HA	1:N:204:ILE:HD11	1.92	0.51
1:H:196:LYS:HD2	1:H:299:LEU:CD1	2.40	0.51
1:F:105:PHE:CG	1:F:306:TYR:HB3	2.46	0.51
1:R:122:THR:HG23	1:R:124:TYR:HB3	1.92	0.51
1:F:269:LEU:O	1:F:273:GLN:HB2	3.26	0.51
1:X:70:LEU:HD11	1:X:98:MET:HB3	1.90	0.51
1:K:119:TRP:HA	1:K:122:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:301:PRO:HD2	1:Y:302:ARG:HH11	1.75	0.51
1:B:187:ALA:CB	1:B:305:THR:HG21	2.40	0.51
1:A:129:MET:HG2	1:A:136:ASP:CG	3.50	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: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: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:L:119:TRP:CD2	1:L:143:MET:HB3	2.45	0.51
1:F:119:TRP:HA	1:F:122:THR:HB	1.92	0.51
1:B:72:GLY:O	1:B:76:GLN:NE2	2.29	0.51
1:S:168:THR:OG1	1:S:171:ASP:OD2	2.23	0.51
1:F:288:ALA:O	1:F:291:ASN:HB2	2.29	0.51
1:Y:63:ASP:OD2	1:Y:64:ARG:HG2	2.11	0.51
1:R:81:ARG:NH2	1:R:95:PRO:O	2.40	0.51
1:F:207:LYS:HG3	1:F:290:LEU:HD21	1.92	0.51
1:Z:70:LEU:HD11	1:Z:98:MET:CB	2.41	0.51
1:E:151:PRO:HG3	1:F:157:ALA:HB3	1.93	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:N:182:PHE:CE2	1:N:186:ARG:HD2	2.46	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:U:125:TYR:CE2	1:U:129:MET:SD	3.04	0.51
1:L:73:TYR:CD1	1:L:195:LEU:HD22	2.46	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: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:D:120:LEU:HD21	1:D:140:LEU:HD22	2.56	0.51
1:A:199:TRP:NE1	1:A:296:GLY:HA2	2.54	0.51
1:D:134:LYS:HZ3	1:E:316:VAL:HB	2.44	0.51
1:W:207:LYS:HZ2	1:W:294:ASN:HD21	1.57	0.50
1:E:115:ARG:HB2	1:E:144:ILE:HG23	3.09	0.50
1:W:58:SER:OG	1:W:172:ALA:C	2.50	0.50
1:B:169:ALA:HB3	1:B:170:PRO:HD3	2.07	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:R:283:TYR:CZ	1:R:287:ARG:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:120:LEU:HG	1:R:140:LEU:HD11	1.93	0.50
1:C:169:ALA:HB3	1:C:170:PRO:HD3	1.93	0.50
1:W:169:ALA:C	1:W:314:GLU:HG2	2.31	0.50
1:G:58:SER:OG	1:G:313:GLU:O	2.29	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: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:E:105:PHE:HB2	1:E:305:THR:CG2	2.38	0.50
1:Y:122:THR:O	1:Y:126:LYS:HG3	2.11	0.50
1:S:198:ALA:HB2	1:T:67:VAL:HG21	1.93	0.50
1:R:139:LEU:O	1:R:143:MET:HG3	2.11	0.50
1:L:177:ARG:NH2	1:L:312:PRO:O	2.44	0.50
1:E:143:MET:O	1:E:146:ASN:HB2	2.12	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:H:196:LYS:HD2	1:H:299:LEU:HD11	1.94	0.50
1:H:299:LEU:HD12	1:O:121:GLN:HE21	1.77	0.50
1:G:229:GLU:HG2	1:G:269:LEU:HD11	1.92	0.50
1:X:77:GLN:HG3	1:X:97:VAL:HG22	1.94	0.50
1:E:134:LYS:NZ	1:F:316:VAL:O	3.11	0.50
1:W:119:TRP:O	1:W:125:TYR:HB3	2.12	0.50
1:B:138:ALA:HB2	1:C:316:VAL:HG11	1.93	0.50
1:M:124:TYR:CE1	1:M:143:MET:HE2	2.47	0.50
1:E:123:ASP:HB3	1:E:127:GLN:NE2	2.27	0.50
1:C:122:THR:HG23	1:C:124:TYR:H	1.77	0.50
1:B:230:GLN:HE21	1:C:274:ALA:HB1	4.28	0.50
1:E:76:GLN:NE2	1:E:298:THR:H	2.10	0.50
1:Z:122:THR:CG2	1:Z:125:TYR:H	2.25	0.50
1:Q:122:THR:HG22	1:Q:125:TYR:H	1.76	0.50
1:L:196:LYS:HA	1:L:297:PRO:HG3	1.94	0.50
1:S:124:TYR:O	1:S:128:ARG:NH1	2.40	0.50
1:M:83:LEU:HD21	1:M:289:MET:HE3	1.94	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:Q:64:ARG:HA	1:Q:102:TYR:CD1	2.47	0.50
1:C:76:GLN:HE22	1:C:297:PRO:HA	2.11	0.50
1:C:225:MET:O	1:C:229:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:MET:HB3	1:F:304:GLN:HB3	1.94	0.50
1:C:104:GLU:O	1:C:108:GLN:HG2	2.47	0.50
1:U:112:TRP:CE2	1:U:144:ILE:HG21	2.47	0.50
1:A:57:SER:HA	1:A:164:LEU:O	2.12	0.50
1:Q:116:ARG:HG3	1:Q:140:LEU:HD21	1.94	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:56:TRP:CD1	1:R:168:THR:HA	2.47	0.50
1:R:138:ALA:N	1:S:316:VAL:HG11	2.27	0.50
1:P:199:TRP:NE1	1:P:296:GLY:HA2	2.26	0.49
1:M:122:THR:CG2	1:M:124:TYR:HB3	2.42	0.49
1:K:119:TRP:CE3	1:K:122:THR:HG21	2.47	0.49
1:Z:141:ASP:HA	1:Z:144:ILE:HD12	1.92	0.49
1:S:56:TRP:CE3	1:S:169:ALA:HB2	2.47	0.49
1:N:56:TRP:CE3	1:N:169:ALA:HB2	2.47	0.49
1:B:118:PHE:CG	1:B:179:TYR:HD1	2.28	0.49
1:F:61:ILE:HB	1:F:310:ARG:HB3	2.15	0.49
1:R:122:THR:CG2	1:R:125:TYR:H	2.24	0.49
1:I:122:THR:CG2	1:I:125:TYR:H	2.26	0.49
1:A:69:MET:HE1	1:A:307:ARG:HB3	1.93	0.49
1:T:271:ASN:O	1:T:275:VAL:HB	2.12	0.49
1:Q:141:ASP:HA	1:Q:144:ILE:HD12	1.94	0.49
1:M:148:GLN:HE21	1:M:148:GLN:N	2.09	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: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:A:83:LEU:HB3	1:A:202:ARG:NH1	2.68	0.49
1:W:119:TRP:CZ3	1:W:175:LEU:HD22	2.47	0.49
1:B:141:ASP:O	1:B:145:ASN:ND2	2.46	0.49
1:B:302:ARG:NH2	1:T:292:THR:HG22	176.48	0.49
1:S:61:ILE:HB	1:S:310:ARG:HB3	1.93	0.49
1:Q:125:TYR:OH	1:Q:136:ASP:O	2.22	0.49
1:S:74:TYR:CD1	1:S:97:VAL:HG21	2.47	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:T:169:ALA:HB3	1:T:170:PRO:HD3	1.93	0.49
1:A:285:GLN:HA	1:Z:216:VAL:CG2	148.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:122:THR:HG23	1:U:124:TYR:HB3	1.94	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:K:267:ALA:O	1:K:271:ASN:ND2	2.45	0.49
1:J:152:GLY:HA2	1:J:158:VAL:HG12	1.94	0.49
1:I:168:THR:OG1	1:I:171:ASP:OD2	2.19	0.49
1:P:203:THR:HA	1:P:293:LEU:HD23	1.95	0.49
1:H:207:LYS:CE	1:H:294:ASN:HD21	2.23	0.49
1:D:70:LEU:HA	1:D:303:PHE:CD1	2.48	0.49
1:P:119:TRP:CD2	1:P:143:MET:HB2	2.47	0.49
1:F:64:ARG:HA	1:F:102:TYR:CD1	2.67	0.49
1:A:69:MET:CE	1:A:307:ARG:HB3	2.42	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:T:114:THR:HG22	1:T:179:TYR:CE1	2.47	0.49
1:T:83:LEU:HB3	1:T:202:ARG:NH1	2.26	0.49
1:D:70:LEU:O	1:D:73:TYR:HB3	2.13	0.49
1:Z:74:TYR:CE1	1:Z:98:MET:SD	3.06	0.49
1:C:76:GLN:HE22	1:C:298:THR:H	1.60	0.49
1:U:76:GLN:NE2	1:U:297:PRO:HA	2.27	0.49
1:Q:57:SER:HA	1:Q:164:LEU:O	2.13	0.49
1:O:169:ALA:HB3	1:O:170:PRO:HD3	1.94	0.49
1:Y:218:LYS:HE2	1:Y:222:ASP:OD2	2.12	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:Q:56:TRP:CD1	1:Q:168:THR:HA	2.48	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:C:230:GLN:OE1	1:D:274:ALA:HB1	2.13	0.49
1:U:55:GLU:N	1:U:166:ALA:O	2.45	0.49
1:A:199:TRP:CD1	1:A:297:PRO:HD3	2.84	0.49
1:N:57:SER:CB	1:N:163:LYS:HE2	2.41	0.49
1:J:169:ALA:HB3	1:J:170:PRO:HD3	1.94	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:A:104:GLU:OE2	1:B:307:ARG:NH1	4.15	0.49
1:U:61:ILE:HG12	1:U:161:SER:HB3	1.95	0.49
1:C:304:GLN:HG2	1:C:306:TYR:CE1	2.91	0.49
1:J:119:TRP:O	1:J:122:THR:HG22	2.13	0.49
1:S:164:LEU:HD13	1:S:176:LEU:HA	1.95	0.49
1:B:190:HIS:CE1	1:C:66:THR:HG21	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:THR:CG2	1:B:125:TYR:H	2.26	0.49
1:J:212:ARG:O	1:J:216:VAL:HG23	2.13	0.49
1:E:216:VAL:CG2	1:F:285:GLN:HA	2.43	0.49
1:D:184:SER:HB2	1:D:306:TYR:CE1	2.47	0.49
1:V:228:ILE:HD12	1:V:272:LEU:HD22	1.95	0.49
1:L:104:GLU:CD	1:M:307:ARG:HH22	2.16	0.49
1:K:301:PRO:HD2	1:K:302:ARG:HH11	1.78	0.49
1:A:207:LYS:HG3	1:A:290:LEU:HD21	3.15	0.48
1:Z:77:GLN:HG2	1:Z:97:VAL:HG13	1.94	0.48
1:C:227:SER:HB2	1:D:275:VAL:HG23	2.69	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:B:55:GLU:O	1:B:318:ARG:HG2	2.13	0.48
1:H:84:ASP:OD1	1:H:85:VAL:HG12	2.13	0.48
1:Z:119:TRP:CE2	1:Z:143:MET:HB3	2.48	0.48
1:I:57:SER:CB	1:I:163:LYS:HE2	2.43	0.48
1:E:211:LYS:CE	1:E:211:LYS:HA	2.29	0.48
1:B:61:ILE:HB	1:B:310:ARG:CB	2.44	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:S:225:MET:CE	1:S:273:GLN:HG3	2.43	0.48
1:M:209:GLN:HA	1:M:212:ARG:NH2	2.28	0.48
1:H:120:LEU:HD21	1:H:140:LEU:HD22	1.95	0.48
1:Q:80:LEU:HD23	1:Q:83:LEU:HD12	1.95	0.48
1:K:168:THR:OG1	1:K:171:ASP:OD2	2.27	0.48
1:P:101:ALA:HA	1:P:191:LEU:HD11	1.95	0.48
1:F:81:ARG:NH1	1:F:95:PRO:O	2.63	0.48
1:K:288:ALA:O	1:K:291:ASN:HB2	2.13	0.48
1:G:169:ALA:HB3	1:G:170:PRO:HD3	1.95	0.48
1:S:300:ASP:OD1	1:S:302:ARG:HD3	2.13	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: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:I:224:ARG:O	1:I:228:ILE:HG13	2.14	0.48
1:U:122:THR:O	1:U:126:LYS:HG3	2.13	0.48
1:P:285:GLN:O	1:P:289:MET:HB2	2.13	0.48
1:G:124:TYR:CG	1:G:175:LEU:HD11	2.48	0.48
1:A:275:VAL:HG13	1:A:276:GLY:O	2.14	0.48
1:L:57:SER:CB	1:L:163:LYS:HE3	2.40	0.48
1:D:126:LYS:HA	1:D:129:MET:HG3	3.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:TYR:OH	1:I:167:GLU:HG3	2.13	0.48
1:A:153:ASP:N	1:A:158:VAL:HG12	2.29	0.48
1:V:214:GLU:HG3	1:V:283:TYR:CE1	2.48	0.48
1:P:122:THR:CG2	1:P:125:TYR:H	2.26	0.48
1:F:226:ASN:OD1	1:F:230:GLN:NE2	4.16	0.48
1:G:125:TYR:HA	1:G:143:MET:HE3	1.94	0.48
1:B:81:ARG:HH12	1:B:96:SER:HA	1.77	0.48
1:N:58:SER:OG	1:N:313:GLU:O	2.28	0.48
1:S:81:ARG:HA	1:S:84:ASP:OD2	2.14	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:U:152:GLY:N	1:U:160:ASP:OD2	2.37	0.48
1:R:108:GLN:OE1	1:R:114:THR:OG1	2.30	0.48
1:K:126:LYS:HA	1:K:129:MET:HG3	1.95	0.48
1:I:169:ALA:HB3	1:I:170:PRO:HD3	1.95	0.48
1:P:199:TRP:CD1	1:P:297:PRO:HD3	2.49	0.48
1:G:200:ALA:C	1:O:302:ARG:NH2	2.63	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:N:272:LEU:HA	1:N:275:VAL:HG12	1.95	0.48
1:D:153:ASP:H	1:D:158:VAL:HB	1.79	0.48
1:B:61:ILE:HG21	1:B:61:ILE:HD13	1.65	0.48
1:E:70:LEU:HD11	1:E:98:MET:HB3	2.04	0.48
1:Q:69:MET:HE1	1:Q:307:ARG:HB3	1.95	0.48
1:B:56:TRP:CD1	1:B:168:THR:HA	2.51	0.48
1:S:300:ASP:OD1	1:S:302:ARG:HB2	2.13	0.48
1:C:57:SER:CB	1:C:163:LYS:HE2	5.44	0.48
1:B:185:GLN:HE22	1:B:301:PRO:HB2	2.67	0.48
1:F:197:GLY:HA3	1:Y:68:ASN:OD1	176.14	0.48
1:N:105:PHE:HB2	1:N:305:THR:HG23	1.95	0.48
1:Z:121:GLN:HG2	1:Z:121:GLN:O	2.14	0.48
1:F:119:TRP:O	1:F:125:TYR:HB3	2.14	0.48
1:R:109:LEU:HD23	1:R:149:PHE:CE1	2.48	0.48
1:A:285:GLN:HG2	1:Z:216:VAL:HG21	148.94	0.48
1:T:134:LYS:NZ	1:U:316:VAL:HB	2.29	0.48
1:Y:316:VAL:HG23	1:Y:317:LYS:HD3	1.96	0.48
1:P:180:VAL:HG11	1:P:308:TYR:CE1	2.49	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:T:73:TYR:CZ	1:T:191:LEU:HB3	2.48	0.48
1:F:300:ASP:OD2	1:F:302:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:63:ASP:HB2	1:F:309:LEU:HD11	1.95	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:G:187:ALA:HB1	1:G:305:THR:HG21	1.96	0.48
1:A:194:GLU:OE2	1:A:194:GLU:HA	2.32	0.48
1:H:205:GLN:HG3	1:H:206:MET:N	2.29	0.48
1:A:292:THR:CG2	1:H:212:ARG:HD3	2.43	0.48
1:A:130:VAL:HG23	1:A:132:ASN:H	1.81	0.48
1:C:213:GLN:NE2	1:C:286:ASN:HD22	2.11	0.48
1:S:223:ARG:O	1:S:227:SER:OG	2.31	0.48
1:M:119:TRP:CE3	1:M:122:THR:HG21	2.48	0.48
1:B:74:TYR:CZ	1:B:78:GLN:HG3	2.49	0.48
1:B:190:HIS:O	1:B:193:ASP:HB2	2.14	0.48
1:L:169:ALA:HB3	1:L:170:PRO:HD3	1.96	0.48
1:B:103:LYS:O	1:B:107:MET:HB2	2.13	0.48
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:H:199:TRP:CG	1:H:297:PRO:HD3	2.48	0.47
1:B:275:VAL:HG13	1:B:276:GLY:O	4.22	0.47
1:N:120:LEU:O	1:N:126:LYS:HE3	2.14	0.47
1:H:55:GLU:HG3	1:H:167:GLU:HA	1.95	0.47
1:A:119:TRP:CE2	1:A:143:MET:HG2	2.49	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:D:141:ASP:O	1:D:145:ASN:ND2	2.73	0.47
1:O:168:THR:OG1	1:O:171:ASP:OD2	2.25	0.47
1:K:74:TYR:HD1	1:K:97:VAL:HG21	1.79	0.47
1:P:168:THR:OG1	1:P:171:ASP:OD2	2.29	0.47
1:F:105:PHE:CE2	1:F:109:LEU:HD22	2.49	0.47
1:A:227:SER:CB	1:B:275:VAL:HG22	2.42	0.47
1:U:119:TRP:CD2	1:U:143:MET:HB3	2.49	0.47
1:C:101:ALA:HA	1:C:191:LEU:HD21	1.96	0.47
1:A:287:ARG:NH2	1:U:302:ARG:HH22	153.56	0.47
1:C:210:VAL:HG13	1:C:283:TYR:HE1	1.79	0.47
1:R:210:VAL:HA	1:R:213:GLN:HE21	1.79	0.47
1:E:116:ARG:HA	1:E:144:ILE:HG12	2.70	0.47
1:R:122:THR:CG2	1:R:124:TYR:HB3	2.44	0.47
1:O:122:THR:O	1:O:126:LYS:CG	2.63	0.47
1:M:228:ILE:HD11	1:M:272:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:77:GLN:HG2	1:W:97:VAL:HG13	1.96	0.47
1:H:61:ILE:O	1:H:309:LEU:N	2.33	0.47
1:V:130:VAL:HG23	1:V:132:ASN:H	1.79	0.47
1:Y:119:TRP:CD2	1:Y:143:MET:HB3	2.49	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:T:293:LEU:HD12	1:T:293:LEU:HA	1.70	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:O:118:PHE:CG	1:O:179:TYR:HD1	2.32	0.47
1:Q:63:ASP:OD2	1:Q:64:ARG:HG2	2.15	0.47
1:V:63:ASP:HB2	1:V:309:LEU:HD11	1.95	0.47
1:P:122:THR:HG22	1:P:125:TYR:H	1.78	0.47
1:A:215:GLU:OE2	1:A:215:GLU:HA	2.14	0.47
1:M:266:GLN:HG2	1:M:266:GLN:O	2.14	0.47
1:F:206:MET:CE	1:F:289:MET:HG2	2.84	0.47
1:C:194:GLU:OE2	1:C:194:GLU:HA	2.87	0.47
1:O:76:GLN:HE21	1:O:298:THR:HG23	1.79	0.47
1:H:128:ARG:HE	1:H:167:GLU:CD	2.18	0.47
1:Y:66:THR:OG1	1:Y:69:MET:HG3	2.14	0.47
1:P:126:LYS:HA	1:P:129:MET:HG3	1.96	0.47
1:F:156:ARG:HG3	1:F:158:VAL:HG23	1.95	0.47
1:S:202:ARG:NH2	1:S:205:GLN:OE1	2.44	0.47
1:R:57:SER:HB3	1:R:319:ASP:OD2	2.14	0.47
1:K:187:ALA:HB3	1:K:305:THR:HG21	1.96	0.47
1:W:124:TYR:OH	1:W:167:GLU:HG3	2.14	0.47
1:R:109:LEU:HD23	1:R:149:PHE:CD1	2.50	0.47
1:C:286:ASN:O	1:C:290:LEU:HB2	2.14	0.47
1:B:224:ARG:HD2	1:B:224:ARG:HA	4.20	0.47
1:E:98:MET:HG2	1:E:98:MET:H	3.55	0.47
1:A:198:ALA:HB2	1:B:67:VAL:HG21	3.25	0.47
1:V:61:ILE:HG22	1:V:309:LEU:HB2	1.97	0.47
1:W:216:VAL:HG13	1:X:284:ASP:HB2	1.97	0.47
1:A:147:ILE:HG12	1:A:164:LEU:HD12	2.37	0.47
1:Q:120:LEU:HD21	1:Q:140:LEU:HD22	1.95	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:L:229:GLU:HG3	1:L:269:LEU:HD11	1.97	0.47
1:X:122:THR:CG2	1:X:124:TYR:HB3	2.44	0.47
1:A:112:TRP:CD1	1:B:310:ARG:HG3	2.49	0.47
1:P:199:TRP:CG	1:P:297:PRO:HD3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASP:OD2	1:T:295:VAL:HG11	173.67	0.47
1:L:96:SER:HG	1:L:98:MET:HG2	1.79	0.47
1:F:216:VAL:HG21	1:Y:285:GLN:HG2	157.80	0.47
1:F:56:TRP:HE3	1:F:315:PRO:HG2	1.79	0.47
1:O:124:TYR:OH	1:O:167:GLU:HG3	2.15	0.47
1:Q:64:ARG:HE	1:Q:99:ASP:HA	1.80	0.47
1:S:60:ALA:HB2	1:S:312:PRO:HG3	1.96	0.47
1:F:272:LEU:HA	1:F:275:VAL:HG12	1.96	0.47
1:G:292:THR:O	1:G:295:VAL:HG22	2.15	0.47
1:S:118:PHE:CG	1:S:179:TYR:HD1	2.33	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:V:61:ILE:O	1:V:309:LEU:N	2.33	0.47
1:L:66:THR:O	1:L:69:MET:HB2	2.14	0.47
1:T:56:TRP:CE3	1:T:169:ALA:HB2	2.50	0.47
1:Q:57:SER:CB	1:Q:163:LYS:HE2	2.45	0.47
1:Q:108:GLN:OE1	1:Q:186:ARG:NE	2.39	0.47
1:X:122:THR:HG23	1:X:124:TYR:HB3	1.96	0.47
1:R:119:TRP:NE1	1:R:143:MET:O	2.48	0.47
1:D:69:MET:O	1:D:304:GLN:N	2.48	0.47
1:C:76:GLN:NE2	1:C:298:THR:H	2.13	0.47
1:O:130:VAL:HG23	1:O:132:ASN:H	1.80	0.47
1:M:60:ALA:HB2	1:M:312:PRO:HG3	1.97	0.47
1:F:206:MET:HG3	1:F:290:LEU:HG	2.39	0.46
1:G:124:TYR:HE1	1:G:143:MET:SD	2.38	0.46
1:K:130:VAL:HG23	1:K:132:ASN:H	1.80	0.46
1:B:120:LEU:HD11	1:B:140:LEU:HD21	1.97	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:A:56:TRP:CE3	1:A:169:ALA:HB2	2.87	0.46
1:T:100:GLU:OE1	1:T:103:LYS:HD3	2.14	0.46
1:I:211:LYS:HA	1:I:211:LYS:HE3	1.97	0.46
1:A:96:SER:HB3	1:A:99:ASP:OD2	2.22	0.46
1:D:66:THR:OG1	1:D:69:MET:HG3	2.14	0.46
1:D:124:TYR:HE1	1:D:143:MET:SD	2.86	0.46
1:G:81:ARG:NH1	1:G:95:PRO:O	2.42	0.46
1:F:58:SER:OG	1:F:173:ASN:HA	2.68	0.46
1:B:61:ILE:CG2	1:B:309:LEU:HB2	2.45	0.46
1:X:79:PHE:O	1:X:83:LEU:HG	2.16	0.46
1:B:76:GLN:O	1:B:79:PHE:HB3	2.50	0.46
1:M:114:THR:HG23	1:M:186:ARG:CD	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:63:ASP:HB2	1:P:309:LEU:HD11	1.97	0.46
1:V:122:THR:CG2	1:V:124:TYR:HB3	2.46	0.46
1:S:120:LEU:HD21	1:S:140:LEU:HD22	1.97	0.46
1:J:206:MET:CE	1:J:289:MET:HG2	2.46	0.46
1:E:121:GLN:HG2	1:E:121:GLN:O	2.39	0.46
1:X:121:GLN:O	1:X:121:GLN:HG2	2.15	0.46
1:F:184:SER:HA	1:F:305:THR:CG2	2.46	0.46
1:U:132:ASN:HD21	1:U:134:LYS:HB3	1.80	0.46
1:B:164:LEU:HB2	1:B:176:LEU:HD13	1.98	0.46
1:A:96:SER:OG	1:A:98:MET:HG2	4.33	0.46
1:C:199:TRP:CE2	1:C:293:LEU:HD12	2.90	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:D:210:VAL:HA	1:D:213:GLN:HE21	2.35	0.46
1:F:77:GLN:HA	1:F:77:GLN:OE1	2.64	0.46
1:T:194:GLU:OE2	1:U:66:THR:HB	2.15	0.46
1:E:61:ILE:HG21	1:E:61:ILE:HD13	1.67	0.46
1:A:74:TYR:CE1	1:A:98:MET:CE	3.15	0.46
1:P:119:TRP:CE2	1:P:143:MET:HB2	2.50	0.46
1:C:126:LYS:O	1:C:129:MET:HG3	3.56	0.46
1:B:122:THR:HG22	1:B:125:TYR:H	1.81	0.46
1:O:64:ARG:HA	1:O:102:TYR:CD1	2.50	0.46
1:E:228:ILE:HD13	1:E:228:ILE:HG21	2.09	0.46
1:D:132:ASN:HB3	1:D:135:ALA:HB3	2.77	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:W:198:ALA:HA	1:X:67:VAL:HG11	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:C:214:GLU:HG3	1:C:283:TYR:CE1	3.06	0.46
1:L:210:VAL:HG13	1:L:283:TYR:CE1	2.51	0.46
1:K:188:ALA:HA	1:K:303:PHE:CZ	2.50	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:B:121:GLN:O	1:B:121:GLN:HG2	4.24	0.46
1:A:112:TRP:CE2	1:A:144:ILE:HG21	3.38	0.46
1:E:275:VAL:HG13	1:E:276:GLY:N	2.21	0.46
1:P:289:MET:O	1:P:293:LEU:HB2	2.16	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:B:96:SER:HB3	1:B:99:ASP:OD2	3.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:MET:HA	1:C:292:THR:HG1	1.79	0.46
1:V:214:GLU:OE2	1:V:283:TYR:OH	2.17	0.46
1:G:199:TRP:CZ2	1:G:293:LEU:HA	2.51	0.46
1:D:268:ARG:HA	1:D:268:ARG:HD2	2.00	0.46
1:N:164:LEU:HB2	1:N:176:LEU:HD13	1.96	0.46
1:U:280:ASP:OD2	1:U:283:TYR:N	2.47	0.46
1:Y:97:VAL:O	1:Y:100:GLU:HB2	2.15	0.46
1:T:201:ALA:O	1:T:205:GLN:HB3	2.16	0.46
1:F:122:THR:HG23	1:F:124:TYR:HB3	1.98	0.46
1:C:122:THR:HG23	1:C:124:TYR:N	2.31	0.46
1:I:202:ARG:NH2	1:I:205:GLN:OE1	2.48	0.46
1:E:101:ALA:HA	1:E:191:LEU:HD11	2.42	0.46
1:Z:57:SER:CB	1:Z:163:LYS:HE2	2.46	0.46
1:W:266:GLN:O	1:W:266:GLN:HG2	2.16	0.46
1:K:185:GLN:HA	1:K:185:GLN:OE1	2.16	0.46
1:A:122:THR:O	1:A:126:LYS:HG3	2.15	0.46
1:L:101:ALA:HA	1:L:191:LEU:HD11	1.98	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:M:216:VAL:CG2	1:N:285:GLN:HA	2.45	0.46
1:V:96:SER:OG	1:V:98:MET:HG2	2.15	0.46
1:Q:64:ARG:HA	1:Q:102:TYR:CG	2.51	0.46
1:I:57:SER:HB2	1:I:163:LYS:HE2	1.98	0.46
1:J:63:ASP:CG	1:J:64:ARG:H	2.20	0.46
1:Z:96:SER:HB3	1:Z:99:ASP:OD2	2.16	0.46
1:F:64:ARG:CZ	1:F:102:TYR:HD2	2.28	0.46
1:J:213:GLN:NE2	1:J:286:ASN:HD22	2.13	0.46
1:P:63:ASP:OD1	1:P:64:ARG:HG2	2.16	0.46
1:U:301:PRO:HD2	1:U:302:ARG:CD	2.46	0.46
1:V:214:GLU:HA	1:V:279:PHE:HE2	1.81	0.46
1:G:96:SER:HB3	1:G:99:ASP:OD2	2.15	0.46
1:G:304:GLN:OE1	1:G:306:TYR:CZ	2.68	0.46
1:H:60:ALA:HA	1:H:310:ARG:O	2.15	0.46
1:L:168:THR:OG1	1:L:171:ASP:OD2	2.27	0.46
1:Z:169:ALA:HB3	1:Z:170:PRO:HD3	1.98	0.46
1:E:128:ARG:HB3	1:E:139:LEU:HD21	2.13	0.46
1:R:209:GLN:HA	1:R:212:ARG:NH2	2.31	0.46
1:U:57:SER:OG	1:U:319:ASP:OD1	2.32	0.46
1:W:141:ASP:O	1:W:145:ASN:ND2	2.49	0.46
1:E:64:ARG:H	1:E:64:ARG:HG2	1.59	0.45
1:W:119:TRP:CH2	1:W:175:LEU:HD13	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ASN:CG	1:C:230:GLN:HE22	3.10	0.45
1:Q:69:MET:CE	1:Q:307:ARG:HB3	2.46	0.45
1:Y:169:ALA:HB3	1:Y:170:PRO:HD3	1.98	0.45
1:D:81:ARG:NH1	1:D:95:PRO:O	2.63	0.45
1:Q:214:GLU:HA	1:Q:279:PHE:HE2	1.81	0.45
1:Y:286:ASN:O	1:Y:290:LEU:HB2	2.16	0.45
1:L:300:ASP:O	1:L:303:PHE:HD2	1.99	0.45
1:U:187:ALA:HB3	1:U:305:THR:HG21	1.97	0.45
1:P:185:GLN:HA	1:P:185:GLN:OE1	2.16	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:N:124:TYR:CG	1:N:175:LEU:HD11	2.50	0.45
1:G:109:LEU:HD23	1:G:149:PHE:CE1	2.51	0.45
1:D:212:ARG:HD3	1:E:292:THR:HG21	2.99	0.45
1:B:66:THR:O	1:B:70:LEU:HG	2.16	0.45
1:N:192:ASN:HB3	1:N:299:LEU:HD22	1.97	0.45
1:X:120:LEU:HD23	1:X:125:TYR:CE2	2.51	0.45
1:O:301:PRO:HD2	1:O:302:ARG:HD2	1.96	0.45
1:D:180:VAL:HG11	1:D:308:TYR:OH	3.51	0.45
1:P:269:LEU:O	1:P:273:GLN:HB2	2.15	0.45
1:D:67:VAL:HG22	1:D:98:MET:CE	2.46	0.45
1:R:109:LEU:HD21	1:R:162:VAL:HB	1.98	0.45
1:T:156:ARG:HD2	1:T:156:ARG:HA	1.33	0.45
1:F:220:ILE:HG13	1:F:220:ILE:H	2.21	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:A:199:TRP:CE2	1:A:293:LEU:HD12	2.51	0.45
1:E:212:ARG:HH11	1:F:292:THR:HG21	1.91	0.45
1:O:152:GLY:HA2	1:O:158:VAL:HG12	1.98	0.45
1:A:288:ALA:O	1:A:291:ASN:HB2	2.16	0.45
1:J:117:GLU:OE1	1:J:186:ARG:NH1	2.38	0.45
1:Y:148:GLN:HE21	1:Y:148:GLN:HB2	1.53	0.45
1:B:64:ARG:HA	1:B:102:TYR:CD1	2.51	0.45
1:J:122:THR:O	1:J:126:LYS:HG3	2.15	0.45
1:P:61:ILE:HG13	1:P:161:SER:HB3	1.97	0.45
1:A:304:GLN:NE2	1:A:306:TYR:O	2.50	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:D:199:TRP:CE2	1:D:297:PRO:HD3	2.52	0.45
1:K:106:VAL:HG13	1:K:149:PHE:CZ	2.51	0.45
1:B:58:SER:HB2	1:B:176:LEU:CD2	3.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:GLU:CD	1:Y:307:ARG:HH22	182.35	0.45
1:W:124:TYR:CE2	1:W:171:ASP:HB3	2.51	0.45
1:Z:74:TYR:HE1	1:Z:98:MET:SD	2.38	0.45
1:M:96:SER:HB3	1:M:99:ASP:OD2	2.17	0.45
1:W:115:ARG:HG2	1:W:147:ILE:HD12	1.98	0.45
1:E:216:VAL:HG21	1:F:285:GLN:HG3	1.98	0.45
1:U:101:ALA:HA	1:U:191:LEU:HD11	1.99	0.45
1:J:106:VAL:HG13	1:J:149:PHE:CZ	2.52	0.45
1:X:270:GLU:O	1:X:273:GLN:HB2	2.17	0.45
1:V:119:TRP:NE1	1:V:143:MET:O	2.50	0.45
1:Z:105:PHE:HB2	1:Z:305:THR:CG2	2.39	0.45
1:T:202:ARG:HE	1:T:205:GLN:CG	2.25	0.45
1:F:120:LEU:HD23	1:F:125:TYR:CE2	2.51	0.45
1:Z:67:VAL:HG13	1:Z:74:TYR:CD2	2.52	0.45
1:U:177:ARG:NH2	1:U:312:PRO:O	2.49	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: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
1:D:228:ILE:HG22	1:D:269:LEU:HD13	1.98	0.45
1:L:64:ARG:HA	1:L:102:TYR:HB2	1.98	0.45
1:F:169:ALA:HB3	1:F:170:PRO:HD3	2.03	0.45
1:A:307:ARG:HH22	1:Z:104:GLU:CD	146.25	0.45
1:H:125:TYR:OH	1:H:140:LEU:HB2	2.15	0.45
1:X:105:PHE:HB2	1:X:305:THR:CG2	2.46	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:F:153:ASP:O	1:F:158:VAL:HG23	3.65	0.45
1:J:109:LEU:HD23	1:J:149:PHE:CD1	2.52	0.45
1:O:60:ALA:HB2	1:O:312:PRO:HG3	1.99	0.45
1:M:202:ARG:HH21	1:M:205:GLN:CD	2.18	0.45
1:W:305:THR:HG22	1:W:305:THR:O	2.16	0.45
1:F:101:ALA:HA	1:F:191:LEU:HD21	1.99	0.45
1:Z:122:THR:O	1:Z:126:LYS:HG3	2.16	0.45
1:L:100:GLU:OE1	1:L:103:LYS:HD3	2.17	0.45
1:W:74:TYR:HE1	1:W:98:MET:HE1	1.80	0.45
1:S:77:GLN:HG2	1:S:97:VAL:HG12	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASP:O	1:B:303:PHE:HD2	1.99	0.45
1:V:64:ARG:HD3	1:V:99:ASP:OD1	2.17	0.45
1:E:216:VAL:HG22	1:F:285:GLN:HA	1.98	0.45
1:C:69:MET:O	1:C:303:PHE:HB2	2.44	0.45
1:T:266:GLN:HE21	1:T:269:LEU:HD22	1.81	0.45
1:A:182:PHE:CE2	1:A:186:ARG:HD2	2.62	0.45
1:F:123:ASP:O	1:F:127:GLN:HB2	2.17	0.45
1:Z:66:THR:H	1:Z:69:MET:HB2	1.81	0.45
1:U:126:LYS:O	1:U:129:MET:HB2	2.17	0.45
1:A:141:ASP:O	1:A:145:ASN:ND2	2.50	0.45
1:I:290:LEU:HD23	1:I:290:LEU:HA	1.81	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:P:122:THR:CG2	1:P:124:TYR:HB3	2.47	0.45
1:J:199:TRP:CD1	1:J:297:PRO:HD3	2.52	0.45
1:H:192:ASN:HA	1:H:192:ASN:HD22	1.64	0.45
1:X:120:LEU:HG	1:X:140:LEU:HD11	1.99	0.44
1:E:300:ASP:HA	1:E:302:ARG:NH1	2.32	0.44
1:A:66:THR:HB	1:H:194:GLU:OE2	2.16	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:Y:301:PRO:HD2	1:Y:302:ARG:HD3	1.99	0.44
1:A:293:LEU:HA	1:A:293:LEU:HD12	2.10	0.44
1:Q:169:ALA:HB3	1:Q:170:PRO:HD3	1.99	0.44
1:A:116:ARG:HG3	1:A:140:LEU:HD21	1.99	0.44
1:B:215:GLU:OE1	1:B:218:LYS:HG2	2.17	0.44
1:O:300:ASP:OD1	1:O:302:ARG:HD3	2.17	0.44
1:X:81:ARG:HH21	1:X:100:GLU:HG3	1.82	0.44
1:K:130:VAL:N	1:K:136:ASP:OD1	2.42	0.44
1:B:298:THR:HA	1:T:291:ASN:HD22	176.63	0.44
1:F:57:SER:N	1:F:315:PRO:HG3	2.92	0.44
1:H:299:LEU:HD12	1:O:121:GLN:NE2	2.33	0.44
1:V:213:GLN:HE22	1:V:283:TYR:HA	1.81	0.44
1:K:117:GLU:OE1	1:K:186:ARG:NH1	2.40	0.44
1:H:156:ARG:HG3	1:H:158:VAL:HG23	1.99	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:N:218:LYS:HG3	1:N:218:LYS:O	2.17	0.44
1:C:268:ARG:HA	1:C:268:ARG:HD2	1.92	0.44
1:P:206:MET:HG2	1:P:290:LEU:HG	2.00	0.44
1:E:119:TRP:CE2	1:E:143:MET:HB3	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:169:ALA:HB3	1:R:170:PRO:HD3	1.99	0.44
1:C:119:TRP:CE2	1:C:143:MET:HB3	3.07	0.44
1:U:289:MET:O	1:U:293:LEU:HB2	2.17	0.44
1:P:164:LEU:HB2	1:P:176:LEU:HD13	1.99	0.44
1:B:156:ARG:HA	1:B:156:ARG:HD2	4.45	0.44
1:R:152:GLY:HA2	1:R:158:VAL:HG12	2.00	0.44
1:F:184:SER:HB2	1:F:306:TYR:CD1	2.52	0.44
1:B:116:ARG:HG3	1:B:144:ILE:HD11	1.99	0.44
1:F:164:LEU:HD13	1:F:176:LEU:N	3.01	0.44
1:B:56:TRP:CE3	1:B:169:ALA:HB2	2.52	0.44
1:V:56:TRP:CE3	1:V:315:PRO:HG2	2.50	0.44
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.83	0.44
1:D:146:ASN:O	1:D:164:LEU:HA	2.18	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:K:105:PHE:HB2	1:K:305:THR:CG2	2.39	0.44
1:Q:68:ASN:ND2	1:X:194:GLU:OE2	2.49	0.44
1:B:139:LEU:O	1:B:143:MET:HG3	2.18	0.44
1:G:66:THR:O	1:G:69:MET:HB3	2.18	0.44
1:M:118:PHE:CG	1:M:179:TYR:HD1	2.35	0.44
1:E:148:GLN:HE21	1:E:148:GLN:HB2	3.02	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:H:207:LYS:HG2	1:H:290:LEU:HD11	1.98	0.44
1:H:105:PHE:CE2	1:H:109:LEU:HD22	2.52	0.44
1:X:119:TRP:CD2	1:X:143:MET:HB3	2.52	0.44
1:Y:128:ARG:HE	1:Y:167:GLU:CD	2.20	0.44
1:E:122:THR:HG23	1:E:124:TYR:HB3	2.19	0.44
1:A:268:ARG:O	1:A:272:LEU:HD23	4.74	0.44
1:X:169:ALA:HB3	1:X:170:PRO:HD3	2.00	0.44
1:W:83:LEU:C	1:W:85:VAL:H	2.21	0.44
1:F:184:SER:HB2	1:F:306:TYR:HE1	1.82	0.44
1:A:206:MET:HG2	1:A:290:LEU:HA	3.67	0.44
1:U:96:SER:OG	1:U:97:VAL:N	2.49	0.44
1:O:212:ARG:O	1:O:216:VAL:HG23	2.18	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:D:193:ASP:O	1:D:196:LYS:HB3	3.19	0.44
1:Q:272:LEU:HA	1:Q:275:VAL:HG12	2.00	0.44
1:D:289:MET:O	1:D:293:LEU:HB2	2.53	0.44
1:O:221:TYR:HB2	1:O:277:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:ASP:C	1:E:84:ASP:OD1	2.56	0.44
1:A:64:ARG:HE	1:A:99:ASP:HA	1.83	0.44
1:U:83:LEU:HB3	1:U:202:ARG:NH1	2.29	0.44
1:D:129:MET:HA	1:D:136:ASP:OD1	2.18	0.44
1:Z:64:ARG:HG2	1:Z:102:TYR:CB	2.48	0.44
1:H:122:THR:HG22	1:H:125:TYR:H	1.82	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:G:105:PHE:HB2	1:G:305:THR:CG2	2.48	0.44
1:A:128:ARG:HE	1:A:167:GLU:CD	2.21	0.44
1:T:56:TRP:CD1	1:T:168:THR:HA	2.52	0.44
1:Y:77:GLN:HB3	1:Y:97:VAL:HG11	1.99	0.44
1:H:76:GLN:O	1:H:79:PHE:HB3	2.18	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:P:229:GLU:HG3	1:P:269:LEU:HD11	2.00	0.44
1:F:212:ARG:HD3	1:Y:292:THR:HG21	159.34	0.44
1:D:80:LEU:HD12	1:D:195:LEU:HD12	2.00	0.44
1:D:76:GLN:NE2	1:D:195:LEU:HD21	3.64	0.44
1:V:124:TYR:OH	1:V:167:GLU:N	2.42	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:D:212:ARG:HH11	1:E:292:THR:HG21	1.82	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:V:266:GLN:HE21	1:V:269:LEU:CD2	2.30	0.44
1:K:98:MET:HG2	1:K:98:MET:H	1.11	0.43
1:B:58:SER:HB2	1:B:176:LEU:HD22	3.55	0.43
1:B:120:LEU:HG	1:B:140:LEU:HD11	2.00	0.43
1:N:96:SER:HB3	1:N:99:ASP:OD2	2.18	0.43
1:R:62:THR:HG1	1:R:102:TYR:HH	1.56	0.43
1:O:122:THR:HG23	1:O:124:TYR:HB3	2.00	0.43
1:J:57:SER:CB	1:J:163:LYS:HE2	2.47	0.43
1:V:122:THR:HG23	1:V:124:TYR:HB3	1.99	0.43
1:F:72:GLY:O	1:F:76:GLN:HG3	2.17	0.43
1:B:202:ARG:HH21	1:B:205:GLN:CD	2.22	0.43
1:B:61:ILE:O	1:B:309:LEU:N	2.36	0.43
1:A:61:ILE:HG23	1:A:160:ASP:O	2.30	0.43
1:K:228:ILE:HD12	1:K:272:LEU:CD2	2.48	0.43
1:H:210:VAL:HG22	1:H:286:ASN:CB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:LEU:HB3	1:L:202:ARG:HD3	2.00	0.43
1:S:67:VAL:HG13	1:S:74:TYR:CD2	2.53	0.43
1:Q:300:ASP:OD1	1:Q:302:ARG:HB2	2.18	0.43
1:D:81:ARG:O	1:D:85:VAL:HG12	2.18	0.43
1:M:304:GLN:HG2	1:M:306:TYR:CE1	2.53	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:X:290:LEU:HD23	1:X:290:LEU:HA	1.79	0.43
1:B:80:LEU:HD23	1:B:83:LEU:HD12	2.88	0.43
1:U:202:ARG:HH21	1:U:205:GLN:CD	2.22	0.43
1:B:221:TYR:CE1	1:B:272:LEU:HG	2.81	0.43
1:S:198:ALA:CA	1:T:67:VAL:HG11	2.49	0.43
1:H:206:MET:HB2	1:H:206:MET:HE2	1.88	0.43
1:U:210:VAL:HG13	1:U:283:TYR:CE1	2.53	0.43
1:S:280:ASP:O	1:S:283:TYR:HB3	2.18	0.43
1:G:103:LYS:O	1:G:107:MET:HB2	2.18	0.43
1:Z:218:LYS:HE3	1:Z:218:LYS:HB2	1.72	0.43
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.81	0.43
1:B:298:THR:HA	1:T:291:ASN:ND2	177.05	0.43
1:D:64:ARG:HD3	1:D:99:ASP:OD1	2.87	0.43
1:L:64:ARG:H	1:L:64:ARG:HG2	1.58	0.43
1:T:64:ARG:NE	1:T:99:ASP:OD1	2.50	0.43
1:F:266:GLN:O	1:F:269:LEU:HB3	2.18	0.43
1:Z:214:GLU:HG3	1:Z:283:TYR:CE1	2.53	0.43
1:B:216:VAL:O	1:B:220:ILE:HG13	2.19	0.43
1:I:300:ASP:OD1	1:I:302:ARG:HB2	2.19	0.43
1:H:63:ASP:CG	1:H:64:ARG:H	2.22	0.43
1:X:177:ARG:NH2	1:X:312:PRO:O	2.52	0.43
1:W:152:GLY:HA2	1:W:158:VAL:HG12	2.00	0.43
1:Y:293:LEU:HD12	1:Y:293:LEU:HA	1.84	0.43
1:F:105:PHE:HA	1:F:187:ALA:HB2	2.28	0.43
1:A:223:ARG:O	1:A:227:SER:HB3	3.25	0.43
1:R:227:SER:HB2	1:S:275:VAL:CG2	2.48	0.43
1:W:169:ALA:HB3	1:W:170:PRO:HD3	1.99	0.43
1:G:266:GLN:O	1:G:269:LEU:N	2.45	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:Q:114:THR:HG22	1:Q:179:TYR:CE1	2.53	0.43
1:D:150:ILE:HA	1:D:151:PRO:HD2	1.91	0.43
1:B:98:MET:HG2	1:B:98:MET:H	2.36	0.43
1:W:130:VAL:HG23	1:W:132:ASN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:ALA:C	1:F:314:GLU:HG2	3.97	0.43
1:B:67:VAL:HG13	1:B:74:TYR:CG	2.53	0.43
1:U:212:ARG:O	1:U:216:VAL:HG23	2.18	0.43
1:X:174:ASN:HB3	1:X:178:GLN:NE2	2.33	0.43
1:G:141:ASP:HB2	1:H:316:VAL:HG11	1.99	0.43
1:R:118:PHE:CG	1:R:179:TYR:HD1	2.36	0.43
1:J:132:ASN:HB3	1:J:135:ALA:HB3	2.00	0.43
1:B:203:THR:OG1	1:B:293:LEU:HD11	2.19	0.43
1:L:293:LEU:HD12	1:L:293:LEU:HA	1.80	0.43
1:W:61:ILE:HG21	1:W:61:ILE:HD13	1.59	0.43
1:G:204:ILE:HB	1:O:302:ARG:HH21	1.84	0.43
1:B:58:SER:HB3	1:B:312:PRO:HB3	2.00	0.43
1:D:194:GLU:CD	1:E:66:THR:HB	2.58	0.43
1:C:169:ALA:HB1	1:C:314:GLU:HG2	3.68	0.43
1:D:122:THR:HG23	1:D:124:TYR:N	2.34	0.43
1:C:80:LEU:HD11	1:C:199:TRP:HB2	2.27	0.43
1:O:107:MET:CE	1:P:63:ASP:OD2	2.66	0.43
1:P:116:ARG:HA	1:P:144:ILE:HG12	2.00	0.43
1:O:169:ALA:HA	1:O:315:PRO:HG2	2.00	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: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:B:162:VAL:HG13	1:B:176:LEU:HD11	2.01	0.43
1:W:119:TRP:CD2	1:W:143:MET:HB3	2.53	0.43
1:B:302:ARG:HH12	1:T:292:THR:CG2	177.81	0.43
1:M:61:ILE:HB	1:M:310:ARG:HB3	2.00	0.43
1:W:81:ARG:NE	1:W:97:VAL:HG22	2.33	0.43
1:I:170:PRO:O	1:I:174:ASN:ND2	2.52	0.43
1:I:104:GLU:CD	1:J:307:ARG:HH22	2.21	0.43
1:L:141:ASP:OD2	1:L:145:ASN:ND2	2.49	0.43
1:M:280:ASP:OD2	1:M:283:TYR:N	2.48	0.43
1:H:269:LEU:O	1:H:273:GLN:HG3	2.18	0.43
1:L:61:ILE:HB	1:L:310:ARG:HB3	2.01	0.43
1:X:115:ARG:HD3	1:X:147:ILE:HB	2.01	0.43
1:F:61:ILE:N	1:F:310:ARG:HB3	2.34	0.43
1:F:122:THR:HG23	1:F:124:TYR:H	1.84	0.43
1:G:196:LYS:CE	1:O:298:THR:HG22	2.46	0.43
1:A:285:GLN:HA	1:Z:216:VAL:HG22	148.10	0.43
1:S:228:ILE:HD13	1:S:268:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:102:TYR:O	1:N:106:VAL:HG23	2.18	0.43
1:Y:211:LYS:HE3	1:Y:211:LYS:HA	2.01	0.43
1:S:98:MET:N	1:S:98:MET:SD	2.79	0.43
1:G:204:ILE:HB	1:O:302:ARG:NH2	2.34	0.43
1:W:122:THR:CG2	1:W:124:TYR:HB3	2.48	0.43
1:T:207:LYS:NZ	1:T:294:ASN:HD21	2.17	0.43
1:M:98:MET:HG2	1:M:98:MET:H	1.50	0.43
1:D:125:TYR:HA	1:D:143:MET:HE1	3.69	0.43
1:Z:122:THR:CG2	1:Z:124:TYR:HB3	2.48	0.43
1:V:56:TRP:CD1	1:V:168:THR:HA	2.53	0.43
1:E:57:SER:HA	1:E:164:LEU:O	2.18	0.43
1:P:122:THR:O	1:P:126:LYS:HG3	2.19	0.43
1:U:73:TYR:CZ	1:U:191:LEU:HB3	2.54	0.43
1:L:141:ASP:HA	1:L:144:ILE:HD12	2.00	0.43
1:B:153:ASP:H	1:B:158:VAL:HB	1.84	0.43
1:E:268:ARG:NH1	1:E:268:ARG:CG	3.11	0.42
1:A:64:ARG:HA	1:A:102:TYR:CG	2.54	0.42
1:D:275:VAL:HG13	1:D:276:GLY:O	2.53	0.42
1:C:124:TYR:O	1:C:128:ARG:HD2	2.19	0.42
1:M:126:LYS:O	1:M:129:MET:HE2	2.19	0.42
1:A:214:GLU:OE2	1:A:283:TYR:OH	2.62	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:C:211:LYS:HE3	1:C:211:LYS:HA	3.37	0.42
1:F:120:LEU:HD21	1:F:140:LEU:HD22	2.10	0.42
1:B:300:ASP:HB2	1:T:295:VAL:HG22	173.98	0.42
1:R:105:PHE:CE2	1:R:109:LEU:HD22	2.53	0.42
1:D:64:ARG:HA	1:D:102:TYR:HB2	2.01	0.42
1:Y:125:TYR:HD1	1:Y:143:MET:CE	2.32	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:F:58:SER:CB	1:F:173:ASN:HA	3.31	0.42
1:H:153:ASP:H	1:H:158:VAL:HB	1.84	0.42
1:G:153:ASP:H	1:G:158:VAL:HB	1.84	0.42
1:V:105:PHE:HB2	1:V:305:THR:HG23	2.00	0.42
1:H:58:SER:O	1:H:163:LYS:HG3	2.18	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:K:294:ASN:HA	1:K:294:ASN:HD22	1.63	0.42
1:R:293:LEU:HD12	1:R:293:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:TRP:CZ2	1:A:144:ILE:HG21	3.55	0.42
1:F:280:ASP:OD1	1:F:283:TYR:N	2.35	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:H:56:TRP:O	1:H:165:ILE:HA	2.20	0.42
1:B:203:THR:HA	1:B:293:LEU:HG	2.01	0.42
1:V:187:ALA:HB3	1:V:305:THR:HG21	2.01	0.42
1:P:104:GLU:O	1:P:108:GLN:HG2	2.19	0.42
1:F:61:ILE:HG23	1:F:160:ASP:O	2.19	0.42
1:R:107:MET:HE3	1:S:309:LEU:HD22	2.00	0.42
1:T:63:ASP:OD1	1:T:64:ARG:N	2.44	0.42
1:I:223:ARG:HH12	1:J:284:ASP:CG	2.20	0.42
1:Z:79:PHE:CE2	1:Z:83:LEU:HD11	2.54	0.42
1:F:150:ILE:HA	1:F:151:PRO:HD2	1.87	0.42
1:I:118:PHE:CG	1:I:179:TYR:HD1	2.37	0.42
1:H:96:SER:O	1:H:99:ASP:HB2	2.19	0.42
1:S:57:SER:CB	1:S:163:LYS:HE2	2.49	0.42
1:A:301:PRO:HD2	1:A:302:ARG:HH11	1.84	0.42
1:T:148:GLN:HE21	1:T:148:GLN:HB2	1.61	0.42
1:M:268:ARG:HD3	1:M:268:ARG:HA	1.91	0.42
1:B:268:ARG:HA	1:B:268:ARG:HD2	1.76	0.42
1:Y:177:ARG:HG3	1:Y:312:PRO:HB2	2.01	0.42
1:R:62:THR:OG1	1:R:102:TYR:OH	2.27	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:D:290:LEU:HD23	1:D:290:LEU:HA	1.92	0.42
1:N:210:VAL:HG13	1:N:283:TYR:HE1	1.83	0.42
1:N:169:ALA:HB3	1:N:170:PRO:HD3	2.01	0.42
1:G:203:THR:HA	1:G:293:LEU:HD23	2.01	0.42
1:L:266:GLN:HE21	1:L:269:LEU:HD22	1.83	0.42
1:E:294:ASN:HA	1:E:294:ASN:HD22	1.81	0.42
1:G:267:ALA:O	1:G:271:ASN:HB2	2.19	0.42
1:Y:194:GLU:HA	1:Y:194:GLU:OE2	2.20	0.42
1:D:73:TYR:OH	1:D:191:LEU:HD22	2.20	0.42
1:F:126:LYS:HG2	1:F:129:MET:HE2	3.29	0.42
1:B:64:ARG:H	1:B:64:ARG:HG2	3.29	0.42
1:R:177:ARG:HG3	1:R:312:PRO:HB2	2.02	0.42
1:E:152:GLY:N	1:E:160:ASP:OD2	2.36	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:F:185:GLN:HE22	1:F:301:PRO:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:GLU:HG3	1:J:269:LEU:HD11	2.01	0.42
1:I:194:GLU:HA	1:I:194:GLU:OE2	2.20	0.42
1:W:194:GLU:HA	1:W:194:GLU:OE2	2.20	0.42
1:W:60:ALA:HB2	1:W:312:PRO:HG3	2.01	0.42
1:F:164:LEU:HD13	1:F:175:LEU:C	3.26	0.42
1:C:272:LEU:HA	1:C:275:VAL:HG12	2.16	0.42
1:I:216:VAL:HG13	1:J:284:ASP:HB3	2.01	0.42
1:Q:60:ALA:HB2	1:Q:312:PRO:HG3	2.02	0.42
1:N:280:ASP:OD1	1:N:283:TYR:N	2.50	0.42
1:W:115:ARG:HB3	1:W:144:ILE:HA	2.01	0.42
1:P:64:ARG:HG2	1:P:64:ARG:H	1.51	0.42
1:A:119:TRP:CH2	1:A:143:MET:HG2	2.55	0.42
1:R:137:ALA:C	1:S:316:VAL:HG11	2.40	0.42
1:O:141:ASP:O	1:O:145:ASN:ND2	2.53	0.42
1:B:180:VAL:HG11	1:B:308:TYR:OH	2.49	0.42
1:P:268:ARG:HD2	1:P:268:ARG:HA	1.60	0.42
1:P:202:ARG:CZ	1:P:205:GLN:HE21	2.33	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:E:228:ILE:HG22	1:E:269:LEU:HD13	2.01	0.42
1:D:130:VAL:HG23	1:D:132:ASN:H	2.41	0.42
1:U:57:SER:CB	1:U:163:LYS:HE2	2.49	0.42
1:L:300:ASP:O	1:L:303:PHE:CD2	2.73	0.42
1:U:291:ASN:O	1:U:294:ASN:HB2	2.20	0.42
1:C:102:TYR:HA	1:C:105:PHE:HB3	2.29	0.42
1:G:210:VAL:HA	1:G:213:GLN:NE2	2.31	0.42
1:D:96:SER:HB3	1:D:99:ASP:OD2	2.98	0.42
1:D:275:VAL:HG13	1:D:276:GLY:N	2.34	0.42
1:C:216:VAL:HG13	1:D:284:ASP:CB	2.74	0.42
1:O:63:ASP:HB2	1:O:309:LEU:HD11	2.01	0.42
1:A:58:SER:O	1:A:163:LYS:HA	2.19	0.42
1:G:217:ALA:HB1	1:G:277:PRO:HB3	2.02	0.42
1:Y:65:PRO:HD2	1:Y:102:TYR:HB2	2.02	0.42
1:H:266:GLN:HG2	1:H:266:GLN:O	2.19	0.42
1:O:58:SER:HB2	1:O:172:ALA:C	2.40	0.42
1:D:224:ARG:HA	1:D:227:SER:OG	2.20	0.42
1:C:132:ASN:HB3	1:C:135:ALA:HB3	2.02	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:C:73:TYR:CE1	1:C:191:LEU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:57:SER:HA	1:U:164:LEU:O	2.20	0.42
1:S:66:THR:OG1	1:S:69:MET:SD	2.73	0.42
1:S:153:ASP:OD2	1:S:156:ARG:HD2	2.19	0.42
1:Q:109:LEU:HD23	1:Q:149:PHE:CE1	2.54	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:N:268:ARG:HD2	1:N:268:ARG:HA	1.59	0.42
1:D:148:GLN:HE21	1:D:148:GLN:HB2	3.20	0.42
1:P:207:LYS:O	1:P:211:LYS:HB2	2.20	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:A:74:TYR:HA	1:A:97:VAL:HG11	2.66	0.41
1:E:77:GLN:OE1	1:E:77:GLN:HA	2.96	0.41
1:H:56:TRP:CD1	1:H:168:THR:HA	2.55	0.41
1:Q:293:LEU:HA	1:Q:293:LEU:HD12	1.91	0.41
1:P:184:SER:HB2	1:P:306:TYR:CD1	2.55	0.41
1:S:198:ALA:HA	1:T:67:VAL:HG11	2.01	0.41
1:H:74:TYR:CZ	1:H:78:GLN:HG3	2.55	0.41
1:D:280:ASP:O	1:D:283:TYR:HB3	2.43	0.41
1:N:226:ASN:OD1	1:N:230:GLN:NE2	2.48	0.41
1:M:102:TYR:OH	1:M:160:ASP:OD1	2.35	0.41
1:S:188:ALA:HA	1:S:303:PHE:CZ	2.55	0.41
1:X:112:TRP:CD2	1:X:144:ILE:HG21	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:X:119:TRP:NE1	1:X:143:MET:O	2.53	0.41
1:B:224:ARG:HB3	1:B:272:LEU:CD2	4.11	0.41
1:D:223:ARG:NH1	1:E:284:ASP:OD2	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:K:182:PHE:CE2	1:K:186:ARG:HD2	2.55	0.41
1:S:268:ARG:HD2	1:S:268:ARG:HA	1.76	0.41
1:J:130:VAL:HG23	1:J:132:ASN:H	1.86	0.41
1:D:55:GLU:O	1:D:319:ASP:N	2.39	0.41
1:Q:101:ALA:HA	1:Q:191:LEU:HD11	2.02	0.41
1:S:63:ASP:OD1	1:S:64:ARG:N	2.48	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:N:98:MET:HG2	1:N:98:MET:H	1.00	0.41
1:D:68:ASN:ND2	1:D:68:ASN:H	2.18	0.41
1:V:121:GLN:HG2	1:V:121:GLN:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:211:LYS:HA	1:M:211:LYS:HE3	2.01	0.41
1:N:173:ASN:HB2	1:N:314:GLU:HA	2.01	0.41
1:W:57:SER:OG	1:W:163:LYS:HE2	2.20	0.41
1:L:63:ASP:OD1	1:L:64:ARG:HG2	2.20	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:R:124:TYR:HH	1:R:167:GLU:H	1.60	0.41
1:I:293:LEU:HA	1:I:293:LEU:HD12	1.88	0.41
1:D:293:LEU:HA	1:D:293:LEU:HD12	1.78	0.41
1:X:101:ALA:HA	1:X:191:LEU:HD11	2.01	0.41
1:D:60:ALA:HB2	1:D:312:PRO:HG3	2.02	0.41
1:U:281:LEU:O	1:U:285:GLN:HG3	2.20	0.41
1:F:223:ARG:O	1:F:227:SER:HB3	2.78	0.41
1:A:77:GLN:HA	1:A:77:GLN:OE1	2.20	0.41
1:Q:194:GLU:OE2	1:Q:194:GLU:HA	2.21	0.41
1:E:304:GLN:HG2	1:E:306:TYR:O	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:M:56:TRP:CD1	1:M:168:THR:HA	2.56	0.41
1:B:199:TRP:CG	1:B:297:PRO:HD3	2.58	0.41
1:O:194:GLU:OE2	1:P:66:THR:HB	2.20	0.41
1:U:73:TYR:OH	1:U:191:LEU:HB3	2.20	0.41
1:Z:61:ILE:HG22	1:Z:309:LEU:HB2	2.03	0.41
1:M:156:ARG:O	1:M:157:ALA:HB3	2.20	0.41
1:P:179:TYR:O	1:P:182:PHE:HB3	2.20	0.41
1:N:203:THR:O	1:N:207:LYS:HB2	2.20	0.41
1:X:74:TYR:OH	1:X:78:GLN:NE2	2.46	0.41
1:A:125:TYR:OH	1:A:136:ASP:HB3	2.20	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:C:187:ALA:CB	1:C:305:THR:HG21	2.48	0.41
1:B:302:ARG:CZ	1:T:292:THR:HG22	176.60	0.41
1:K:177:ARG:NH2	1:K:312:PRO:O	2.54	0.41
1:C:291:ASN:O	1:C:295:VAL:HG23	2.21	0.41
1:C:56:TRP:CE3	1:C:169:ALA:HB2	2.55	0.41
1:U:301:PRO:HD2	1:U:302:ARG:HD3	2.02	0.41
1:K:115:ARG:HG3	1:K:179:TYR:OH	2.20	0.41
1:M:57:SER:HA	1:M:164:LEU:O	2.20	0.41
1:W:63:ASP:OD1	1:W:64:ARG:HG2	2.20	0.41
1:J:188:ALA:HB1	1:J:303:PHE:CE2	2.55	0.41
1:A:180:VAL:HG11	1:A:308:TYR:OH	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:MET:CE	1:J:273:GLN:HG2	2.50	0.41
1:A:122:THR:HG22	1:A:125:TYR:H	1.85	0.41
1:K:225:MET:CB	1:K:272:LEU:HD11	2.44	0.41
1:D:180:VAL:HG23	1:D:181:ALA:N	2.36	0.41
1:F:73:TYR:OH	1:F:191:LEU:HD22	2.21	0.41
1:B:300:ASP:OD1	1:B:302:ARG:HB2	3.72	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:N:64:ARG:NE	1:N:99:ASP:OD1	2.53	0.41
1:R:124:TYR:OH	1:R:167:GLU:HG3	2.20	0.41
1:O:119:TRP:HE3	1:O:122:THR:HG21	1.80	0.41
1:H:122:THR:O	1:H:126:LYS:HE3	2.21	0.41
1:Y:56:TRP:O	1:Y:165:ILE:HA	2.20	0.41
1:A:198:ALA:HA	1:B:67:VAL:HG11	3.16	0.41
1:B:55:GLU:HG2	1:B:167:GLU:HA	2.02	0.41
1:G:65:PRO:HB2	1:G:69:MET:HG2	2.02	0.41
1:C:74:TYR:CE2	1:C:78:GLN:HG3	2.55	0.41
1:B:223:ARG:NH2	1:C:284:ASP:OD1	2.90	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:P:202:ARG:HH21	1:P:205:GLN:HE21	1.68	0.41
1:F:96:SER:OG	1:F:98:MET:SD	2.68	0.41
1:E:74:TYR:HE1	1:E:98:MET:CE	2.33	0.41
1:D:225:MET:HE1	1:D:273:GLN:HA	2.03	0.41
1:W:198:ALA:CA	1:X:67:VAL:HG11	2.51	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:J:206:MET:HG3	1:J:206:MET:O	2.21	0.41
1:J:182:PHE:CE2	1:J:186:ARG:HD2	2.55	0.41
1:X:177:ARG:HG3	1:X:312:PRO:HB2	2.03	0.41
1:B:214:GLU:OE2	1:B:283:TYR:OH	2.31	0.41
1:Z:168:THR:OG1	1:Z:171:ASP:OD2	2.31	0.41
1:W:221:TYR:HB2	1:W:277:PRO:HB3	2.03	0.41
1:O:176:LEU:HA	1:O:176:LEU:HD12	1.85	0.41
1:R:127:GLN:HB2	1:R:127:GLN:HE21	1.77	0.41
1:D:182:PHE:CE2	1:D:186:ARG:HD2	2.56	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:G:125:TYR:CD1	1:G:143:MET:HE2	2.52	0.41
1:E:64:ARG:HA	1:E:102:TYR:CG	2.68	0.41
1:D:266:GLN:NE2	1:D:269:LEU:HD23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:OE1	1:B:307:ARG:NH2	3.78	0.41
1:Z:280:ASP:O	1:Z:283:TYR:HB3	2.20	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:Y:290:LEU:HD23	1:Y:290:LEU:HA	1.92	0.41
1:E:291:ASN:O	1:E:294:ASN:HB2	2.21	0.41
1:P:288:ALA:O	1:P:291:ASN:HB2	2.21	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:I:63:ASP:OD2	1:I:159:ASN:ND2	2.54	0.41
1:Y:216:VAL:HG13	1:Z:284:ASP:HB3	2.03	0.41
1:U:290:LEU:HA	1:U:290:LEU:HD23	1.84	0.41
1:E:293:LEU:HD12	1:E:293:LEU:HA	1.73	0.41
1:E:275:VAL:CG1	1:E:276:GLY:H	2.24	0.41
1:B:57:SER:HA	1:B:164:LEU:O	2.21	0.41
1:D:300:ASP:OD1	1:D:302:ARG:NH1	2.54	0.41
1:O:209:GLN:HA	1:O:212:ARG:NH2	2.36	0.41
1:L:97:VAL:HB	1:L:98:MET:HE2	2.03	0.41
1:S:61:ILE:HG22	1:S:309:LEU:HD12	2.01	0.41
1:O:128:ARG:HE	1:O:167:GLU:CD	2.24	0.41
1:Q:146:ASN:HA	1:Q:146:ASN:HD22	1.68	0.41
1:D:122:THR:HG23	1:D:124:TYR:H	1.84	0.41
1:Y:122:THR:CG2	1:Y:124:TYR:HB3	2.51	0.41
1:Y:305:THR:HG23	1:Y:305:THR:O	2.21	0.41
1:J:69:MET:HG2	1:J:304:GLN:HB3	2.03	0.41
1:S:74:TYR:CD1	1:S:97:VAL:HG22	2.56	0.41
1:C:283:TYR:OH	1:C:287:ARG:HD3	2.20	0.41
1:K:120:LEU:O	1:K:126:LYS:HE3	2.21	0.41
1:R:213:GLN:NE2	1:R:286:ASN:HD22	2.18	0.41
1:A:137:ALA:O	1:A:140:LEU:HB3	2.21	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:K:206:MET:HG2	1:K:290:LEU:HG	2.03	0.41
1:J:294:ASN:HA	1:J:294:ASN:HD22	1.66	0.41
1:G:268:ARG:HA	1:G:268:ARG:HD2	1.72	0.41
1:T:122:THR:CG2	1:T:125:TYR:H	2.34	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:C:300:ASP:OD1	1:C:302:ARG:HD3	4.32	0.41
1:J:61:ILE:HB	1:J:310:ARG:HB3	2.03	0.41
1:O:272:LEU:HA	1:O:275:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:77:GLN:OE1	1:N:77:GLN:HA	2.21	0.41
1:F:207:LYS:NZ	1:F:294:ASN:HD21	4.23	0.41
1:D:305:THR:O	1:D:305:THR:HG23	2.33	0.41
1:B:69:MET:HG3	1:B:304:GLN:HB3	4.29	0.41
1:E:119:TRP:CG	1:E:143:MET:HB3	3.41	0.41
1:B:67:VAL:HG13	1:B:74:TYR:CD1	2.56	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:I:300:ASP:OD1	1:I:302:ARG:HD3	2.21	0.41
1:P:280:ASP:O	1:P:283:TYR:HB3	2.21	0.41
1:K:280:ASP:OD1	1:K:282:ASP:HB2	2.21	0.41
1:Q:61:ILE:O	1:Q:309:LEU:N	2.33	0.41
1:C:147:ILE:HG12	1:C:164:LEU:HD12	2.45	0.41
1:H:118:PHE:HE1	1:H:178:GLN:HB3	1.86	0.41
1:F:59:THR:O	1:F:312:PRO:HA	2.93	0.40
1:P:228:ILE:HG22	1:P:269:LEU:HD12	2.03	0.40
1:Z:74:TYR:CD1	1:Z:97:VAL:HB	2.56	0.40
1:G:76:GLN:HE21	1:G:298:THR:H	1.68	0.40
1:F:268:ARG:HA	1:F:268:ARG:HD2	2.14	0.40
1:B:74:TYR:OH	1:B:78:GLN:NE2	2.53	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:S:198:ALA:N	1:T:67:VAL:HG11	2.36	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: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:G:80:LEU:HD23	1:G:80:LEU:HA	1.80	0.40
1:Q:105:PHE:HA	1:Q:187:ALA:HB2	2.03	0.40
1:A:122:THR:CG2	1:A:125:TYR:H	2.34	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:W:119:TRP:NE1	1:W:143:MET:O	2.54	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:F:221:TYR:HE1	1:F:272:LEU:O	2.08	0.40
1:U:209:GLN:O	1:U:213:GLN:HG3	2.21	0.40
1:U:203:THR:HA	1:U:293:LEU:HG	2.04	0.40
1:E:188:ALA:HB1	1:E:303:PHE:CE2	2.66	0.40
1:Y:162:VAL:HG13	1:Y:176:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:76:GLN:NE2	1:W:297:PRO:HA	2.36	0.40
1:X:137:ALA:O	1:X:140:LEU:HB3	2.21	0.40
1:G:125:TYR:OH	1:G:140:LEU:HB2	2.22	0.40
1:W:294:ASN:HA	1:W:294:ASN:HD22	1.60	0.40
1:S:212:ARG:HG2	1:T:288:ALA:CB	2.48	0.40
1:G:128:ARG:HB3	1:G:139:LEU:HD21	2.04	0.40
1:D:199:TRP:CG	1:D:297:PRO:HD3	2.56	0.40
1:F:188:ALA:HB1	1:F:303:PHE:CE2	2.77	0.40
1:D:147:ILE:HG12	1:D:164:LEU:HD12	2.14	0.40
1:V:286:ASN:O	1:V:290:LEU:HB2	2.21	0.40
1:R:210:VAL:O	1:R:213:GLN:HB2	2.21	0.40
1:C:150:ILE:HA	1:C:151:PRO:HD2	1.91	0.40
1:L:216:VAL:O	1:L:220:ILE:HG13	2.22	0.40
1:X:146:ASN:HB3	1:X:165:ILE:HB	2.04	0.40
1:E:80:LEU:HA	1:E:80:LEU:HD23	1.90	0.40
1:U:132:ASN:ND2	1:U:134:LYS:HB3	2.37	0.40
1:D:191:LEU:O	1:D:194:GLU:HB2	2.88	0.40
1:A:98:MET:H	1:A:98:MET:HG2	3.58	0.40
1:W:124:TYR:OH	1:W:167:GLU:N	2.42	0.40
1:P:143:MET:HB3	1:P:143:MET:HE2	1.97	0.40
1:C:169:ALA:CB	1:C:314:GLU:HG2	4.30	0.40
1:F:56:TRP:CE3	1:F:169:ALA:HB2	2.56	0.40
1:C:199:TRP:NE1	1:C:293:LEU:O	2.68	0.40
1:I:61:ILE:HG22	1:I:309:LEU:HB2	2.02	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:N:57:SER:O	1:N:315:PRO:HB3	2.22	0.40
1:P:122:THR:HG23	1:P:124:TYR:HB3	2.02	0.40
1:B:126:LYS:HA	1:B:129:MET:SD	3.79	0.40
1:G:123:ASP:O	1:G:127:GLN:HG3	2.22	0.40
1:O:180:VAL:HG11	1:O:308:TYR:CE1	2.57	0.40
1:A:59:THR:HA	1:A:162:VAL:O	2.30	0.40
1:R:148:GLN:HE21	1:R:148:GLN:HB2	1.55	0.40
1:O:77:GLN:HA	1:O:77:GLN:OE1	2.21	0.40
1:P:79:PHE:O	1:P:83:LEU:HG	2.21	0.40
1:D:61:ILE:HG13	1:D:161:SER:HB3	3.56	0.40
1:F:70:LEU:HD11	1:F:98:MET:HA	2.04	0.40
1:E:77:GLN:OE1	1:E:195:LEU:HD13	2.21	0.40
1:M:119:TRP:HE3	1:M:122:THR:HG21	1.85	0.40
1:Z:64:ARG:O	1:Z:307:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLU:CD	1:C:66:THR:HB	2.42	0.40
1:H:206:MET:HE1	1:H:289:MET:HG2	2.03	0.40
1:S:308:TYR:CE2	1:S:311:THR:HG23	2.57	0.40
1:A:148:GLN:HB2	1:A:148:GLN:HE21	1.57	0.40
1:W:109:LEU:HA	1:W:109:LEU:HD12	1.96	0.40
1:A:81:ARG:O	1:A:85:VAL:HG22	2.76	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	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LYS:NZ	1:L:296:GLY:O[2_546]	1.93	0.27

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	34	77
1	F	215/356 (60%)	210 (98%)	4 (2%)	1 (0%)	34	77
1	G	215/356 (60%)	211 (98%)	3 (1%)	1 (0%)	34	77
1	H	215/356 (60%)	211 (98%)	3 (1%)	1 (0%)	34	77
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	56	90

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	190/296 (64%)	165 (87%)	25 (13%)	5 28
1	B	190/296 (64%)	174 (92%)	16 (8%)	14 49
1	C	190/296 (64%)	169 (89%)	21 (11%)	8 34
1	D	190/296 (64%)	173 (91%)	17 (9%)	12 44
1	E	190/296 (64%)	166 (87%)	24 (13%)	5 30
1	F	190/296 (64%)	175 (92%)	15 (8%)	15 51
1	G	190/296 (64%)	175 (92%)	15 (8%)	15 51
1	H	190/296 (64%)	167 (88%)	23 (12%)	6 31
1	I	190/296 (64%)	165 (87%)	25 (13%)	5 28
1	J	190/296 (64%)	169 (89%)	21 (11%)	8 34
1	K	190/296 (64%)	167 (88%)	23 (12%)	6 31
1	L	190/296 (64%)	164 (86%)	26 (14%)	4 27
1	M	190/296 (64%)	162 (85%)	28 (15%)	4 24
1	N	190/296 (64%)	174 (92%)	16 (8%)	14 49
1	O	190/296 (64%)	172 (90%)	18 (10%)	11 41
1	P	190/296 (64%)	166 (87%)	24 (13%)	5 30
1	Q	190/296 (64%)	172 (90%)	18 (10%)	11 41
1	R	190/296 (64%)	170 (90%)	20 (10%)	8 36
1	S	190/296 (64%)	167 (88%)	23 (12%)	6 31
1	T	190/296 (64%)	171 (90%)	19 (10%)	9 38
1	U	190/296 (64%)	165 (87%)	25 (13%)	5 28
1	V	190/296 (64%)	172 (90%)	18 (10%)	11 41
1	W	190/296 (64%)	173 (91%)	17 (9%)	12 44
1	X	190/296 (64%)	171 (90%)	19 (10%)	9 38
1	Y	190/296 (64%)	161 (85%)	29 (15%)	3 22
1	Z	190/296 (64%)	166 (87%)	24 (13%)	5 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	190/296 (64%)	168 (88%)	22 (12%)	7 32
1	b	190/296 (64%)	167 (88%)	23 (12%)	6 31
1	c	190/296 (64%)	169 (89%)	21 (11%)	8 34
1	d	190/296 (64%)	171 (90%)	19 (10%)	9 38
1	e	190/296 (64%)	168 (88%)	22 (12%)	7 32
1	f	190/296 (64%)	169 (89%)	21 (11%)	8 34
All	All	6080/9472 (64%)	5403 (89%)	677 (11%)	8 34

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	221/356 (62%)	-0.19	0 100 100	232, 286, 334, 403	0
1	B	221/356 (62%)	-0.27	0 100 100	200, 271, 345, 382	0
1	C	221/356 (62%)	0.04	11 (4%) 32 32	248, 300, 381, 438	0
1	D	221/356 (62%)	-0.26	1 (0%) 91 88	223, 281, 331, 361	0
1	E	221/356 (62%)	0.27	17 (7%) 16 19	255, 337, 447, 534	0
1	F	221/356 (62%)	-0.10	8 (3%) 46 43	208, 275, 322, 362	0
1	G	221/356 (62%)	-0.05	3 (1%) 78 71	229, 279, 337, 357	0
1	H	221/356 (62%)	-0.20	1 (0%) 91 88	228, 263, 309, 327	0
1	I	221/356 (62%)	-0.09	8 (3%) 46 43	245, 316, 404, 442	0
1	J	221/356 (62%)	-0.19	6 (2%) 58 54	244, 286, 351, 372	0
1	K	221/356 (62%)	-0.27	3 (1%) 78 71	249, 287, 346, 389	0
1	L	221/356 (62%)	-0.14	2 (0%) 85 81	223, 284, 405, 432	0
1	M	221/356 (62%)	-0.23	2 (0%) 85 81	205, 265, 333, 351	0
1	N	221/356 (62%)	-0.02	5 (2%) 64 59	206, 290, 339, 361	0
1	O	221/356 (62%)	-0.10	3 (1%) 78 71	214, 267, 337, 376	0
1	P	221/356 (62%)	-0.16	2 (0%) 85 81	245, 283, 320, 341	0
1	Q	221/356 (62%)	-0.27	2 (0%) 85 81	204, 276, 333, 350	0
1	R	221/356 (62%)	0.05	10 (4%) 37 36	229, 322, 389, 429	0
1	S	221/356 (62%)	-0.32	0 100 100	236, 300, 344, 456	0
1	T	221/356 (62%)	0.13	9 (4%) 41 39	205, 313, 404, 456	0
1	U	221/356 (62%)	-0.18	7 (3%) 51 46	199, 286, 401, 509	0
1	V	221/356 (62%)	-0.12	2 (0%) 85 81	237, 309, 351, 378	0
1	W	221/356 (62%)	-0.21	5 (2%) 64 59	211, 301, 375, 398	0
1	X	221/356 (62%)	-0.13	6 (2%) 58 54	240, 303, 398, 414	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	221/356 (62%)	0.01	8 (3%) 46 43	236, 326, 449, 465	0
1	Z	221/356 (62%)	-0.25	2 (0%) 85 81	228, 310, 395, 408	0
1	a	221/356 (62%)	-0.23	0 100 100	231, 299, 363, 391	0
1	b	221/356 (62%)	0.05	7 (3%) 51 46	256, 348, 475, 550	0
1	c	221/356 (62%)	-0.12	5 (2%) 64 59	256, 314, 369, 399	0
1	d	221/356 (62%)	-0.37	3 (1%) 78 71	235, 284, 331, 372	0
1	e	221/356 (62%)	-0.26	2 (0%) 85 81	237, 321, 358, 384	0
1	f	221/356 (62%)	-0.28	1 (0%) 91 88	214, 289, 334, 393	0
All	All	7072/11392 (62%)	-0.14	141 (1%) 68 63	199, 295, 383, 550	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	266	GLN	6.4
1	X	305	THR	6.2
1	Y	277	PRO	6.1
1	M	319	ASP	5.5
1	G	156	ARG	5.2
1	d	229	GLU	4.6
1	R	266	GLN	4.5
1	E	60	ALA	4.4
1	Y	228	ILE	4.4
1	E	314	GLU	4.3
1	b	116	ARG	4.3
1	d	230	GLN	4.2
1	J	230	GLN	4.1
1	X	304	GLN	3.9
1	G	155	THR	3.9
1	N	270	GLU	3.7
1	C	298	THR	3.7
1	F	230	GLN	3.7
1	X	306	TYR	3.7
1	c	95	PRO	3.6
1	C	276	GLY	3.6
1	Q	62	THR	3.5
1	T	279	PHE	3.5
1	Y	278	ALA	3.5
1	N	266	GLN	3.5
1	E	162	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	313	GLU	3.4
1	U	270	GLU	3.4
1	T	266	GLN	3.3
1	J	227	SER	3.3
1	b	119	TRP	3.3
1	L	277	PRO	3.3
1	I	266	GLN	3.2
1	F	229	GLU	3.2
1	E	266	GLN	3.2
1	E	316	VAL	3.1
1	U	271	ASN	3.1
1	Y	132	ASN	3.1
1	P	299	LEU	3.1
1	I	224	ARG	3.1
1	O	297	PRO	3.0
1	E	163	LYS	3.0
1	T	267	ALA	3.0
1	W	151	PRO	3.0
1	F	228	ILE	3.0
1	C	156	ARG	3.0
1	C	299	LEU	2.9
1	C	277	PRO	2.9
1	O	294	ASN	2.9
1	R	74	TYR	2.9
1	T	268	ARG	2.9
1	E	61	ILE	2.8
1	F	227	SER	2.8
1	U	273	GLN	2.8
1	R	206	MET	2.8
1	R	267	ALA	2.8
1	I	298	THR	2.7
1	E	270	GLU	2.7
1	Y	135	ALA	2.7
1	K	275	VAL	2.7
1	F	297	PRO	2.7
1	c	267	ALA	2.6
1	E	156	ARG	2.6
1	W	66	THR	2.6
1	b	120	LEU	2.6
1	H	134	LYS	2.5
1	F	84	ASP	2.5
1	E	315	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	279	PHE	2.5
1	T	120	LEU	2.5
1	C	275	VAL	2.5
1	b	109	LEU	2.5
1	R	270	GLU	2.5
1	T	316	VAL	2.5
1	U	266	GLN	2.5
1	T	317	LYS	2.5
1	d	311	THR	2.5
1	Z	162	VAL	2.5
1	c	308	TYR	2.5
1	O	295	VAL	2.5
1	W	316	VAL	2.5
1	R	73	TYR	2.5
1	N	267	ALA	2.4
1	N	73	TYR	2.4
1	L	276	GLY	2.4
1	G	299	LEU	2.4
1	c	301	PRO	2.4
1	V	73	TYR	2.4
1	N	207	LYS	2.4
1	Y	276	GLY	2.4
1	J	317	LYS	2.4
1	I	195	LEU	2.3
1	X	307	ARG	2.3
1	J	228	ILE	2.3
1	U	269	LEU	2.3
1	X	188	ALA	2.3
1	E	112	TRP	2.3
1	J	297	PRO	2.3
1	T	315	PRO	2.3
1	e	266	GLN	2.3
1	U	268	ARG	2.3
1	Y	134	LYS	2.3
1	J	226	ASN	2.3
1	I	73	TYR	2.2
1	E	59	THR	2.2
1	I	162	VAL	2.2
1	R	129	MET	2.2
1	K	274	ALA	2.2
1	R	98	MET	2.2
1	C	279	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	228	ILE	2.2
1	R	275	VAL	2.2
1	D	175	LEU	2.2
1	C	155	THR	2.1
1	C	297	PRO	2.1
1	Y	279	PHE	2.1
1	E	267	ALA	2.1
1	E	309	LEU	2.1
1	e	293	LEU	2.1
1	I	225	MET	2.1
1	M	317	LYS	2.1
1	F	85	VAL	2.1
1	C	228	ILE	2.1
1	E	148	GLN	2.1
1	E	145	ASN	2.1
1	b	149	PHE	2.1
1	V	266	GLN	2.1
1	T	163	LYS	2.1
1	R	207	LYS	2.1
1	b	159	ASN	2.1
1	f	299	LEU	2.1
1	W	156	ARG	2.1
1	X	156	ARG	2.1
1	Z	163	LYS	2.1
1	K	271	ASN	2.0
1	Q	266	GLN	2.0
1	b	162	VAL	2.0
1	U	60	ALA	2.0
1	C	278	ALA	2.0
1	F	145	ASN	2.0
1	W	67	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.