



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 3, 2019 – 08:20 PM EST

PDB ID : 6V1G
EMDB ID: : EMD-21011
Title : Genome-containing AAVrh.10
Authors : Mietzsch, M.; Agbandje-McKenna, M.
Deposited on : 2019-11-20
Resolution : 2.98 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

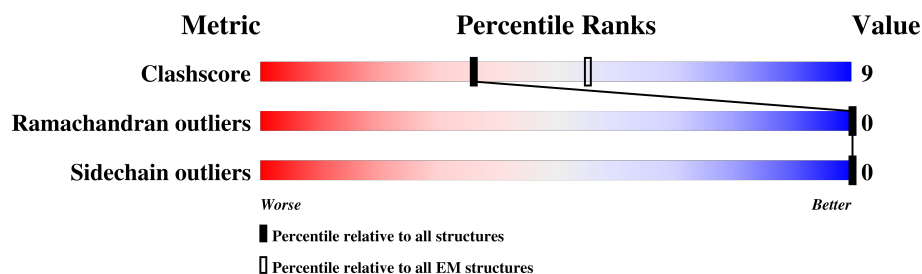
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	520	70% 30%
1	2	520	70% 30%
1	3	520	70% 30%
1	4	520	71% 29%
1	5	520	71% 29%
1	6	520	71% 29%
1	7	520	71% 29%
1	8	520	71% 29%
1	A	520	70% 30%
















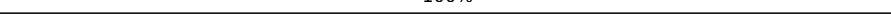
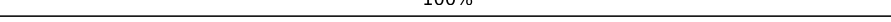
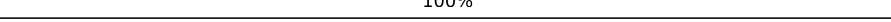

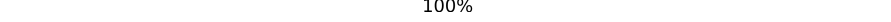
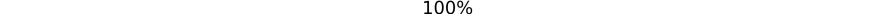
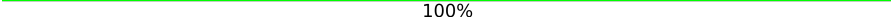
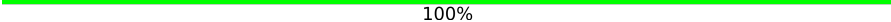


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Mol	Chain	Length	Quality of chain	
1	B	520	<div><div></div></div>	<div><div></div></div>
1	C	520	<div><div></div></div>	<div><div></div></div>
1	D	520	<div><div></div></div>	<div><div></div></div>
1	E	520	<div><div></div></div>	<div><div></div></div>
1	F	520	<div><div></div></div>	<div><div></div></div>
1	G	520	<div><div></div></div>	<div><div></div></div>
1	H	520	<div><div></div></div>	<div><div></div></div>
1	I	520	<div><div></div></div>	<div><div></div></div>
1	J	520	<div><div></div></div>	<div><div></div></div>
1	K	520	<div><div></div></div>	<div><div></div></div>
1	L	520	<div><div></div></div>	<div><div></div></div>
1	M	520	<div><div></div></div>	<div><div></div></div>
1	N	520	<div><div></div></div>	<div><div></div></div>
1	O	520	<div><div></div></div>	<div><div></div></div>
1	P	520	<div><div></div></div>	<div><div></div></div>
1	Q	520	<div><div></div></div>	<div><div></div></div>
1	R	520	<div><div></div></div>	<div><div></div></div>
1	S	520	<div><div></div></div>	<div><div></div></div>
1	T	520	<div><div></div></div>	<div><div></div></div>
1	U	520	<div><div></div></div>	<div><div></div></div>
1	V	520	<div><div></div></div>	<div><div></div></div>
1	W	520	<div><div></div></div>	<div><div></div></div>
1	X	520	<div><div></div></div>	<div><div></div></div>
1	Y	520	<div><div></div></div>	<div><div></div></div>
1	Z	520	<div><div></div></div>	<div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	a	520	 100%
1	b	520	 100%
1	c	520	 100%
1	d	520	 100%
1	e	520	 100%
1	f	520	 100%
1	g	520	 100%
1	h	520	 100%
1	i	520	 100%
1	j	520	 100%
1	k	520	 100%
1	l	520	 100%
1	m	520	 100%
1	n	520	 100%
1	o	520	 100%
1	p	520	 100%
1	q	520	 100%
1	r	520	 100%
1	s	520	 100%
1	t	520	 100%
1	u	520	 100%
1	v	520	 100%
1	w	520	 100%
1	x	520	 100%
1	y	520	 100%

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Mol	Chain	Length	Quality of chain
1	z	520	<div><div></div><div>100%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 249900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	B	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	C	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	D	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	E	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	F	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	G	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	H	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	I	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	J	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	K	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	L	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	M	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	N	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	O	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	P	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	Q	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	S	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	T	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	U	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	V	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	W	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	X	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	Y	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	Z	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	a	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	b	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	c	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	d	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	e	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	f	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	g	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	h	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	i	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	j	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	k	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	l	520	Total 4128	C 2608	N 712	O 794	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	n	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	o	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	p	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	q	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	r	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	s	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	t	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	u	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	v	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	w	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	x	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	y	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	z	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	1	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	2	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	3	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	4	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	5	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	6	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	7	520	Total 4128	C 2608	N 712	O 794	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LEU	PRO	conflict	UNP Q6JC62
A	406	LEU	ARG	conflict	UNP Q6JC62
A	720	ASP	GLU	conflict	UNP Q6JC62
B	365	LEU	PRO	conflict	UNP Q6JC62
B	406	LEU	ARG	conflict	UNP Q6JC62
B	720	ASP	GLU	conflict	UNP Q6JC62
C	365	LEU	PRO	conflict	UNP Q6JC62
C	406	LEU	ARG	conflict	UNP Q6JC62
C	720	ASP	GLU	conflict	UNP Q6JC62
D	365	LEU	PRO	conflict	UNP Q6JC62
D	406	LEU	ARG	conflict	UNP Q6JC62
D	720	ASP	GLU	conflict	UNP Q6JC62
E	365	LEU	PRO	conflict	UNP Q6JC62
E	406	LEU	ARG	conflict	UNP Q6JC62
E	720	ASP	GLU	conflict	UNP Q6JC62
F	365	LEU	PRO	conflict	UNP Q6JC62
F	406	LEU	ARG	conflict	UNP Q6JC62
F	720	ASP	GLU	conflict	UNP Q6JC62
G	365	LEU	PRO	conflict	UNP Q6JC62
G	406	LEU	ARG	conflict	UNP Q6JC62
G	720	ASP	GLU	conflict	UNP Q6JC62
H	365	LEU	PRO	conflict	UNP Q6JC62
H	406	LEU	ARG	conflict	UNP Q6JC62
H	720	ASP	GLU	conflict	UNP Q6JC62
I	365	LEU	PRO	conflict	UNP Q6JC62
I	406	LEU	ARG	conflict	UNP Q6JC62
I	720	ASP	GLU	conflict	UNP Q6JC62
J	365	LEU	PRO	conflict	UNP Q6JC62
J	406	LEU	ARG	conflict	UNP Q6JC62
J	720	ASP	GLU	conflict	UNP Q6JC62
K	365	LEU	PRO	conflict	UNP Q6JC62
K	406	LEU	ARG	conflict	UNP Q6JC62
K	720	ASP	GLU	conflict	UNP Q6JC62
L	365	LEU	PRO	conflict	UNP Q6JC62
L	406	LEU	ARG	conflict	UNP Q6JC62
L	720	ASP	GLU	conflict	UNP Q6JC62

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Chain	Residue	Modelled	Actual	Comment	Reference
M	365	LEU	PRO	conflict	UNP Q6JC62
M	406	LEU	ARG	conflict	UNP Q6JC62
M	720	ASP	GLU	conflict	UNP Q6JC62
N	365	LEU	PRO	conflict	UNP Q6JC62
N	406	LEU	ARG	conflict	UNP Q6JC62
N	720	ASP	GLU	conflict	UNP Q6JC62
O	365	LEU	PRO	conflict	UNP Q6JC62
O	406	LEU	ARG	conflict	UNP Q6JC62
O	720	ASP	GLU	conflict	UNP Q6JC62
P	365	LEU	PRO	conflict	UNP Q6JC62
P	406	LEU	ARG	conflict	UNP Q6JC62
P	720	ASP	GLU	conflict	UNP Q6JC62
Q	365	LEU	PRO	conflict	UNP Q6JC62
Q	406	LEU	ARG	conflict	UNP Q6JC62
Q	720	ASP	GLU	conflict	UNP Q6JC62
R	365	LEU	PRO	conflict	UNP Q6JC62
R	406	LEU	ARG	conflict	UNP Q6JC62
R	720	ASP	GLU	conflict	UNP Q6JC62
S	365	LEU	PRO	conflict	UNP Q6JC62
S	406	LEU	ARG	conflict	UNP Q6JC62
S	720	ASP	GLU	conflict	UNP Q6JC62
T	365	LEU	PRO	conflict	UNP Q6JC62
T	406	LEU	ARG	conflict	UNP Q6JC62
T	720	ASP	GLU	conflict	UNP Q6JC62
U	365	LEU	PRO	conflict	UNP Q6JC62
U	406	LEU	ARG	conflict	UNP Q6JC62
U	720	ASP	GLU	conflict	UNP Q6JC62
V	365	LEU	PRO	conflict	UNP Q6JC62
V	406	LEU	ARG	conflict	UNP Q6JC62
V	720	ASP	GLU	conflict	UNP Q6JC62
W	365	LEU	PRO	conflict	UNP Q6JC62
W	406	LEU	ARG	conflict	UNP Q6JC62
W	720	ASP	GLU	conflict	UNP Q6JC62
X	365	LEU	PRO	conflict	UNP Q6JC62
X	406	LEU	ARG	conflict	UNP Q6JC62
X	720	ASP	GLU	conflict	UNP Q6JC62
Y	365	LEU	PRO	conflict	UNP Q6JC62
Y	406	LEU	ARG	conflict	UNP Q6JC62
Y	720	ASP	GLU	conflict	UNP Q6JC62
Z	365	LEU	PRO	conflict	UNP Q6JC62
Z	406	LEU	ARG	conflict	UNP Q6JC62
Z	720	ASP	GLU	conflict	UNP Q6JC62

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Chain	Residue	Modelled	Actual	Comment	Reference
a	365	LEU	PRO	conflict	UNP Q6JC62
a	406	LEU	ARG	conflict	UNP Q6JC62
a	720	ASP	GLU	conflict	UNP Q6JC62
b	365	LEU	PRO	conflict	UNP Q6JC62
b	406	LEU	ARG	conflict	UNP Q6JC62
b	720	ASP	GLU	conflict	UNP Q6JC62
c	365	LEU	PRO	conflict	UNP Q6JC62
c	406	LEU	ARG	conflict	UNP Q6JC62
c	720	ASP	GLU	conflict	UNP Q6JC62
d	365	LEU	PRO	conflict	UNP Q6JC62
d	406	LEU	ARG	conflict	UNP Q6JC62
d	720	ASP	GLU	conflict	UNP Q6JC62
e	365	LEU	PRO	conflict	UNP Q6JC62
e	406	LEU	ARG	conflict	UNP Q6JC62
e	720	ASP	GLU	conflict	UNP Q6JC62
f	365	LEU	PRO	conflict	UNP Q6JC62
f	406	LEU	ARG	conflict	UNP Q6JC62
f	720	ASP	GLU	conflict	UNP Q6JC62
g	365	LEU	PRO	conflict	UNP Q6JC62
g	406	LEU	ARG	conflict	UNP Q6JC62
g	720	ASP	GLU	conflict	UNP Q6JC62
h	365	LEU	PRO	conflict	UNP Q6JC62
h	406	LEU	ARG	conflict	UNP Q6JC62
h	720	ASP	GLU	conflict	UNP Q6JC62
i	365	LEU	PRO	conflict	UNP Q6JC62
i	406	LEU	ARG	conflict	UNP Q6JC62
i	720	ASP	GLU	conflict	UNP Q6JC62
j	365	LEU	PRO	conflict	UNP Q6JC62
j	406	LEU	ARG	conflict	UNP Q6JC62
j	720	ASP	GLU	conflict	UNP Q6JC62
k	365	LEU	PRO	conflict	UNP Q6JC62
k	406	LEU	ARG	conflict	UNP Q6JC62
k	720	ASP	GLU	conflict	UNP Q6JC62
l	365	LEU	PRO	conflict	UNP Q6JC62
l	406	LEU	ARG	conflict	UNP Q6JC62
l	720	ASP	GLU	conflict	UNP Q6JC62
m	365	LEU	PRO	conflict	UNP Q6JC62
m	406	LEU	ARG	conflict	UNP Q6JC62
m	720	ASP	GLU	conflict	UNP Q6JC62
n	365	LEU	PRO	conflict	UNP Q6JC62
n	406	LEU	ARG	conflict	UNP Q6JC62
n	720	ASP	GLU	conflict	UNP Q6JC62

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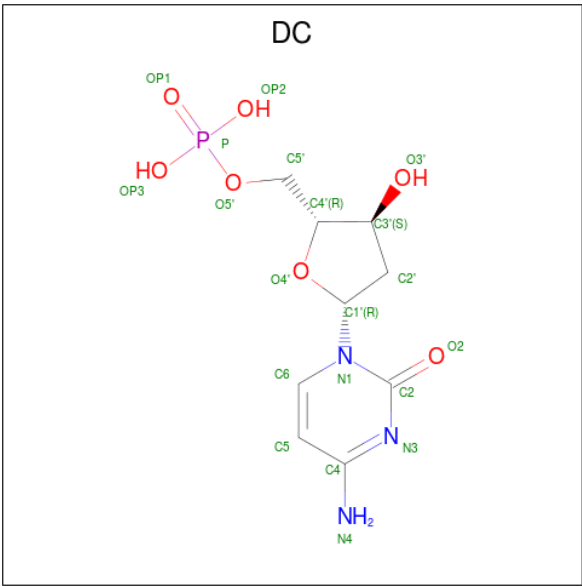
Chain	Residue	Modelled	Actual	Comment	Reference
o	365	LEU	PRO	conflict	UNP Q6JC62
o	406	LEU	ARG	conflict	UNP Q6JC62
o	720	ASP	GLU	conflict	UNP Q6JC62
p	365	LEU	PRO	conflict	UNP Q6JC62
p	406	LEU	ARG	conflict	UNP Q6JC62
p	720	ASP	GLU	conflict	UNP Q6JC62
q	365	LEU	PRO	conflict	UNP Q6JC62
q	406	LEU	ARG	conflict	UNP Q6JC62
q	720	ASP	GLU	conflict	UNP Q6JC62
r	365	LEU	PRO	conflict	UNP Q6JC62
r	406	LEU	ARG	conflict	UNP Q6JC62
r	720	ASP	GLU	conflict	UNP Q6JC62
s	365	LEU	PRO	conflict	UNP Q6JC62
s	406	LEU	ARG	conflict	UNP Q6JC62
s	720	ASP	GLU	conflict	UNP Q6JC62
t	365	LEU	PRO	conflict	UNP Q6JC62
t	406	LEU	ARG	conflict	UNP Q6JC62
t	720	ASP	GLU	conflict	UNP Q6JC62
u	365	LEU	PRO	conflict	UNP Q6JC62
u	406	LEU	ARG	conflict	UNP Q6JC62
u	720	ASP	GLU	conflict	UNP Q6JC62
v	365	LEU	PRO	conflict	UNP Q6JC62
v	406	LEU	ARG	conflict	UNP Q6JC62
v	720	ASP	GLU	conflict	UNP Q6JC62
w	365	LEU	PRO	conflict	UNP Q6JC62
w	406	LEU	ARG	conflict	UNP Q6JC62
w	720	ASP	GLU	conflict	UNP Q6JC62
x	365	LEU	PRO	conflict	UNP Q6JC62
x	406	LEU	ARG	conflict	UNP Q6JC62
x	720	ASP	GLU	conflict	UNP Q6JC62
y	365	LEU	PRO	conflict	UNP Q6JC62
y	406	LEU	ARG	conflict	UNP Q6JC62
y	720	ASP	GLU	conflict	UNP Q6JC62
z	365	LEU	PRO	conflict	UNP Q6JC62
z	406	LEU	ARG	conflict	UNP Q6JC62
z	720	ASP	GLU	conflict	UNP Q6JC62
1	365	LEU	PRO	conflict	UNP Q6JC62
1	406	LEU	ARG	conflict	UNP Q6JC62
1	720	ASP	GLU	conflict	UNP Q6JC62
2	365	LEU	PRO	conflict	UNP Q6JC62
2	406	LEU	ARG	conflict	UNP Q6JC62
2	720	ASP	GLU	conflict	UNP Q6JC62

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Chain	Residue	Modelled	Actual	Comment	Reference
3	365	LEU	PRO	conflict	UNP Q6JC62
3	406	LEU	ARG	conflict	UNP Q6JC62
3	720	ASP	GLU	conflict	UNP Q6JC62
4	365	LEU	PRO	conflict	UNP Q6JC62
4	406	LEU	ARG	conflict	UNP Q6JC62
4	720	ASP	GLU	conflict	UNP Q6JC62
5	365	LEU	PRO	conflict	UNP Q6JC62
5	406	LEU	ARG	conflict	UNP Q6JC62
5	720	ASP	GLU	conflict	UNP Q6JC62
6	365	LEU	PRO	conflict	UNP Q6JC62
6	406	LEU	ARG	conflict	UNP Q6JC62
6	720	ASP	GLU	conflict	UNP Q6JC62
7	365	LEU	PRO	conflict	UNP Q6JC62
7	406	LEU	ARG	conflict	UNP Q6JC62
7	720	ASP	GLU	conflict	UNP Q6JC62
8	365	LEU	PRO	conflict	UNP Q6JC62
8	406	LEU	ARG	conflict	UNP Q6JC62
8	720	ASP	GLU	conflict	UNP Q6JC62

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DC) (formula: C₉H₁₄N₃O₇P).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			16	9	3	4	
2	B	1	Total	C	N	O	0
			16	9	3	4	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			16	9	3	4	
2	D	1	Total	C	N	O	0
			16	9	3	4	
2	E	1	Total	C	N	O	0
			16	9	3	4	
2	F	1	Total	C	N	O	0
			16	9	3	4	
2	G	1	Total	C	N	O	0
			16	9	3	4	
2	H	1	Total	C	N	O	0
			16	9	3	4	
2	I	1	Total	C	N	O	0
			16	9	3	4	
2	J	1	Total	C	N	O	0
			16	9	3	4	
2	K	1	Total	C	N	O	0
			16	9	3	4	
2	L	1	Total	C	N	O	0
			16	9	3	4	
2	M	1	Total	C	N	O	0
			16	9	3	4	
2	N	1	Total	C	N	O	0
			16	9	3	4	
2	O	1	Total	C	N	O	0
			16	9	3	4	
2	P	1	Total	C	N	O	0
			16	9	3	4	
2	Q	1	Total	C	N	O	0
			16	9	3	4	
2	R	1	Total	C	N	O	0
			16	9	3	4	
2	S	1	Total	C	N	O	0
			16	9	3	4	
2	T	1	Total	C	N	O	0
			16	9	3	4	
2	U	1	Total	C	N	O	0
			16	9	3	4	
2	V	1	Total	C	N	O	0
			16	9	3	4	
2	W	1	Total	C	N	O	0
			16	9	3	4	

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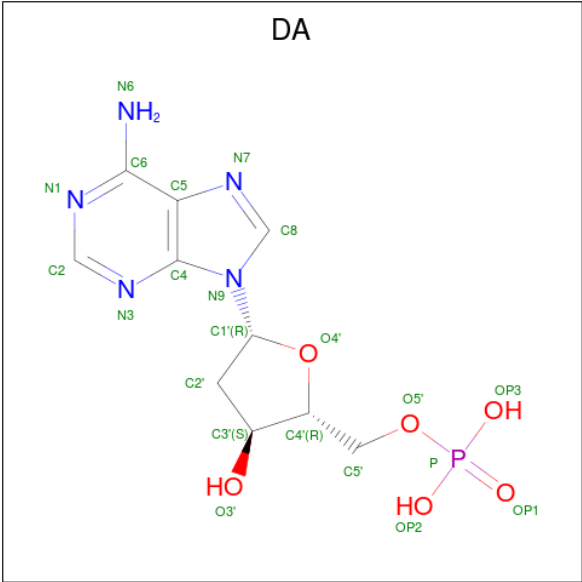
Mol	Chain	Residues	Atoms				AltConf
2	X	1	Total	C	N	O	0
			16	9	3	4	
2	Y	1	Total	C	N	O	0
			16	9	3	4	
2	Z	1	Total	C	N	O	0
			16	9	3	4	
2	a	1	Total	C	N	O	0
			16	9	3	4	
2	b	1	Total	C	N	O	0
			16	9	3	4	
2	c	1	Total	C	N	O	0
			16	9	3	4	
2	d	1	Total	C	N	O	0
			16	9	3	4	
2	e	1	Total	C	N	O	0
			16	9	3	4	
2	f	1	Total	C	N	O	0
			16	9	3	4	
2	g	1	Total	C	N	O	0
			16	9	3	4	
2	h	1	Total	C	N	O	0
			16	9	3	4	
2	i	1	Total	C	N	O	0
			16	9	3	4	
2	j	1	Total	C	N	O	0
			16	9	3	4	
2	k	1	Total	C	N	O	0
			16	9	3	4	
2	l	1	Total	C	N	O	0
			16	9	3	4	
2	m	1	Total	C	N	O	0
			16	9	3	4	
2	n	1	Total	C	N	O	0
			16	9	3	4	
2	o	1	Total	C	N	O	0
			16	9	3	4	
2	p	1	Total	C	N	O	0
			16	9	3	4	
2	q	1	Total	C	N	O	0
			16	9	3	4	
2	r	1	Total	C	N	O	0
			16	9	3	4	

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Mol	Chain	Residues	Atoms				AltConf
2	s	1	Total	C	N	O	0
			16	9	3	4	
2	t	1	Total	C	N	O	0
			16	9	3	4	
2	u	1	Total	C	N	O	0
			16	9	3	4	
2	v	1	Total	C	N	O	0
			16	9	3	4	
2	w	1	Total	C	N	O	0
			16	9	3	4	
2	x	1	Total	C	N	O	0
			16	9	3	4	
2	y	1	Total	C	N	O	0
			16	9	3	4	
2	z	1	Total	C	N	O	0
			16	9	3	4	
2	1	1	Total	C	N	O	0
			16	9	3	4	
2	2	1	Total	C	N	O	0
			16	9	3	4	
2	3	1	Total	C	N	O	0
			16	9	3	4	
2	4	1	Total	C	N	O	0
			16	9	3	4	
2	5	1	Total	C	N	O	0
			16	9	3	4	
2	6	1	Total	C	N	O	0
			16	9	3	4	
2	7	1	Total	C	N	O	0
			16	9	3	4	
2	8	1	Total	C	N	O	0
			16	9	3	4	

- Molecule 3 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: DA) (formula: C₁₀H₁₄N₅O₆P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	B	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	C	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	D	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	E	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	F	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	G	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	H	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	I	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	J	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	K	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	L	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	M	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	N	1	Total	C	N	O	P	0
			21	10	5	5	1	

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Mol	Chain	Residues	Atoms					AltConf
3	O	1	Total 21	C 10	N 5	O 5	P 1	0
3	P	1	Total 21	C 10	N 5	O 5	P 1	0
3	Q	1	Total 21	C 10	N 5	O 5	P 1	0
3	R	1	Total 21	C 10	N 5	O 5	P 1	0
3	S	1	Total 21	C 10	N 5	O 5	P 1	0
3	T	1	Total 21	C 10	N 5	O 5	P 1	0
3	U	1	Total 21	C 10	N 5	O 5	P 1	0
3	V	1	Total 21	C 10	N 5	O 5	P 1	0
3	W	1	Total 21	C 10	N 5	O 5	P 1	0
3	X	1	Total 21	C 10	N 5	O 5	P 1	0
3	Y	1	Total 21	C 10	N 5	O 5	P 1	0
3	Z	1	Total 21	C 10	N 5	O 5	P 1	0
3	a	1	Total 21	C 10	N 5	O 5	P 1	0
3	b	1	Total 21	C 10	N 5	O 5	P 1	0
3	c	1	Total 21	C 10	N 5	O 5	P 1	0
3	d	1	Total 21	C 10	N 5	O 5	P 1	0
3	e	1	Total 21	C 10	N 5	O 5	P 1	0
3	f	1	Total 21	C 10	N 5	O 5	P 1	0
3	g	1	Total 21	C 10	N 5	O 5	P 1	0
3	h	1	Total 21	C 10	N 5	O 5	P 1	0
3	i	1	Total 21	C 10	N 5	O 5	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
3	j	1	Total 21	C 10	N 5	O 5	P 1	0
3	k	1	Total 21	C 10	N 5	O 5	P 1	0
3	l	1	Total 21	C 10	N 5	O 5	P 1	0
3	m	1	Total 21	C 10	N 5	O 5	P 1	0
3	n	1	Total 21	C 10	N 5	O 5	P 1	0
3	o	1	Total 21	C 10	N 5	O 5	P 1	0
3	p	1	Total 21	C 10	N 5	O 5	P 1	0
3	q	1	Total 21	C 10	N 5	O 5	P 1	0
3	r	1	Total 21	C 10	N 5	O 5	P 1	0
3	s	1	Total 21	C 10	N 5	O 5	P 1	0
3	t	1	Total 21	C 10	N 5	O 5	P 1	0
3	u	1	Total 21	C 10	N 5	O 5	P 1	0
3	v	1	Total 21	C 10	N 5	O 5	P 1	0
3	w	1	Total 21	C 10	N 5	O 5	P 1	0
3	x	1	Total 21	C 10	N 5	O 5	P 1	0
3	y	1	Total 21	C 10	N 5	O 5	P 1	0
3	z	1	Total 21	C 10	N 5	O 5	P 1	0
3	1	1	Total 21	C 10	N 5	O 5	P 1	0
3	2	1	Total 21	C 10	N 5	O 5	P 1	0
3	3	1	Total 21	C 10	N 5	O 5	P 1	0
3	4	1	Total 21	C 10	N 5	O 5	P 1	0

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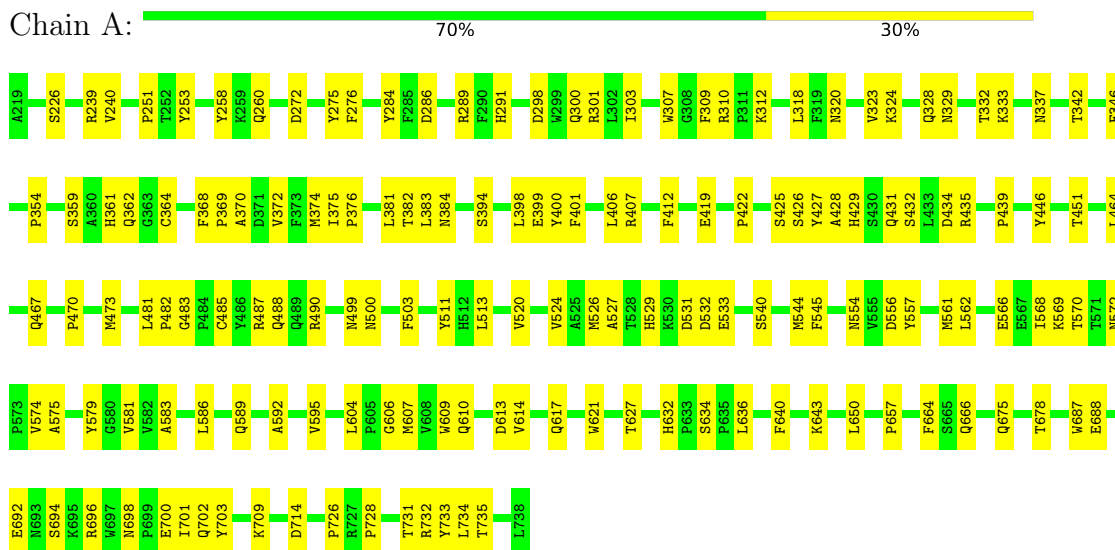
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Mol	Chain	Residues	Atoms					AltConf
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			21	10	5	5	1	
3	6	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	7	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	8	1	Total	C	N	O	P	0
			21	10	5	5	1	

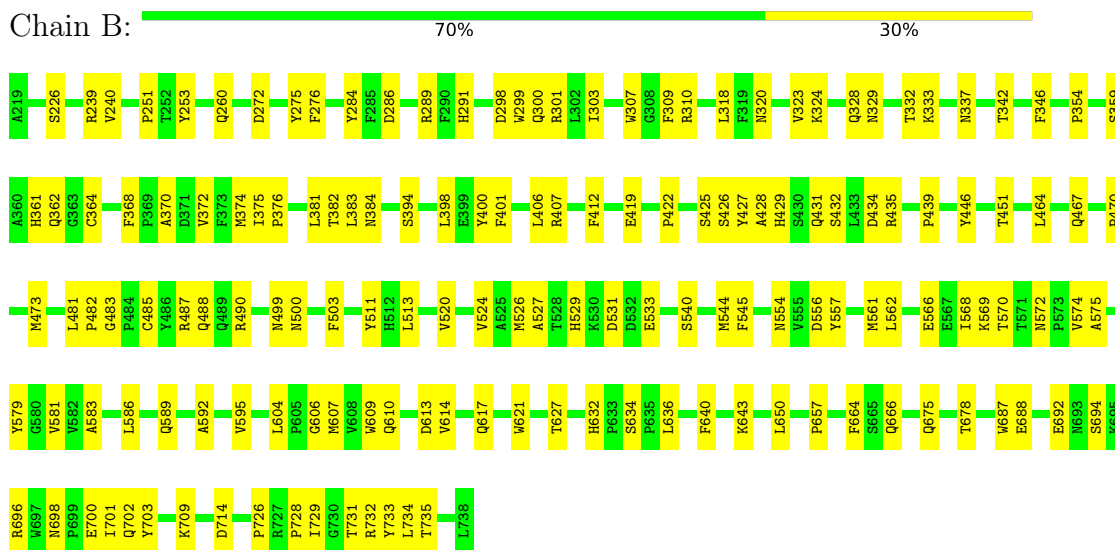
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

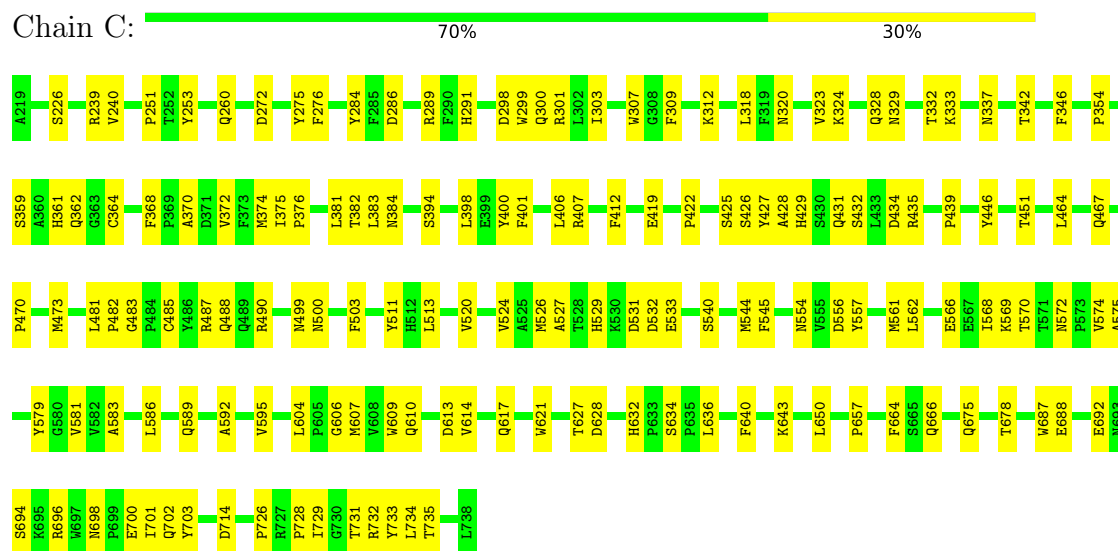
• Molecule 1: Capsid protein VP1



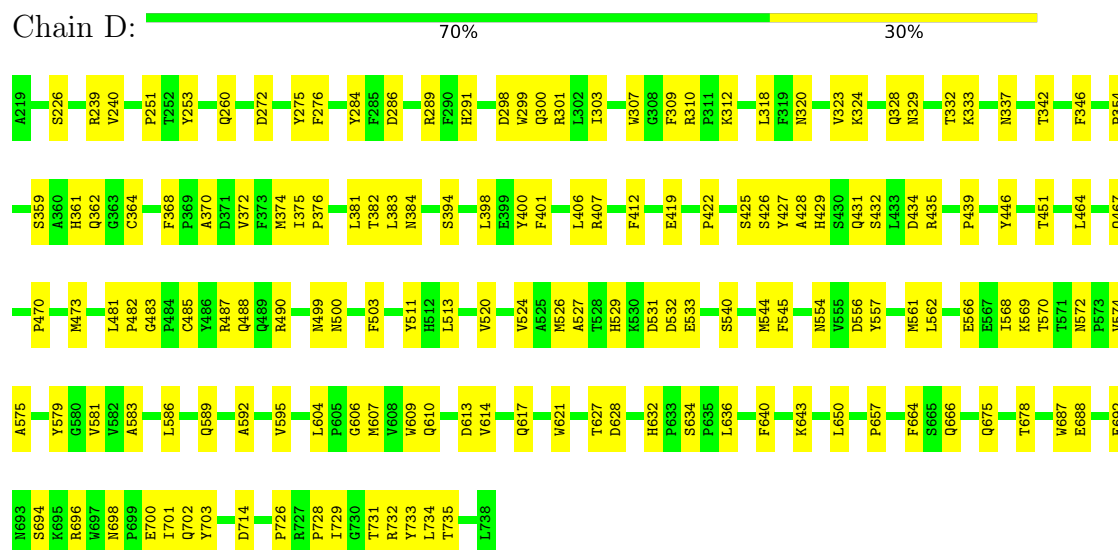
• Molecule 1: Capsid protein VP1



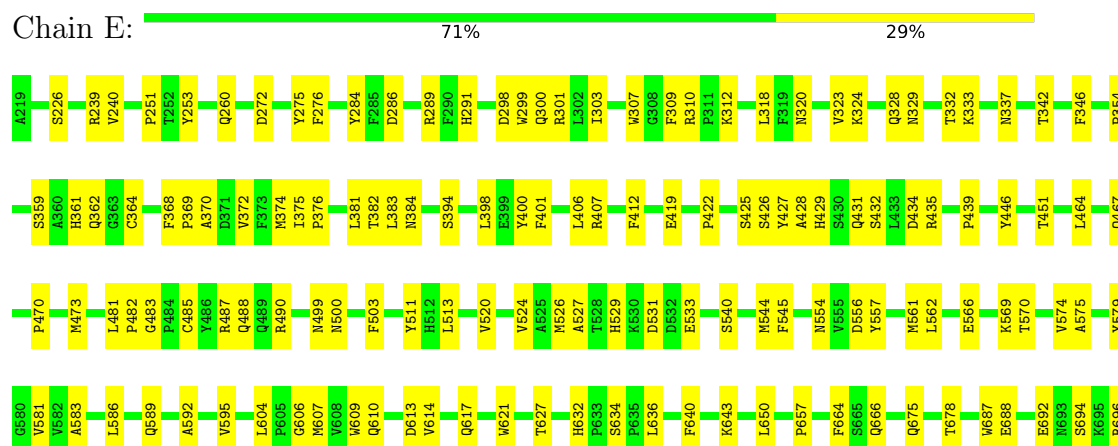
• Molecule 1: Capsid protein VP1

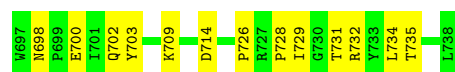


• Molecule 1: Capsid protein VP1



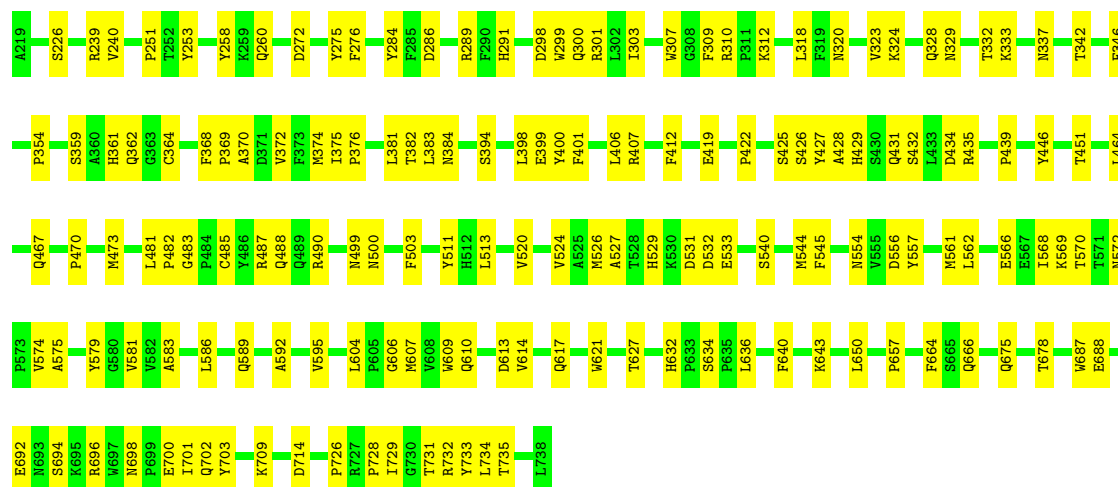
• Molecule 1: Capsid protein VP1





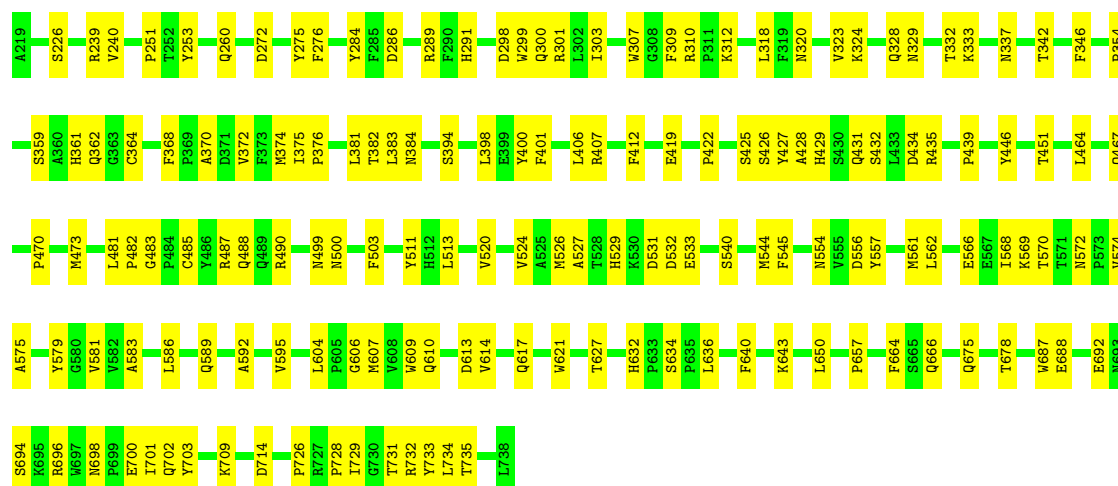
• Molecule 1: Capsid protein VP1

Chain F: 69% 31%



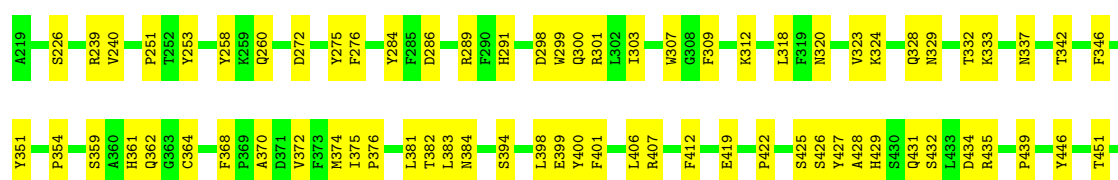
• Molecule 1: Capsid protein VP1

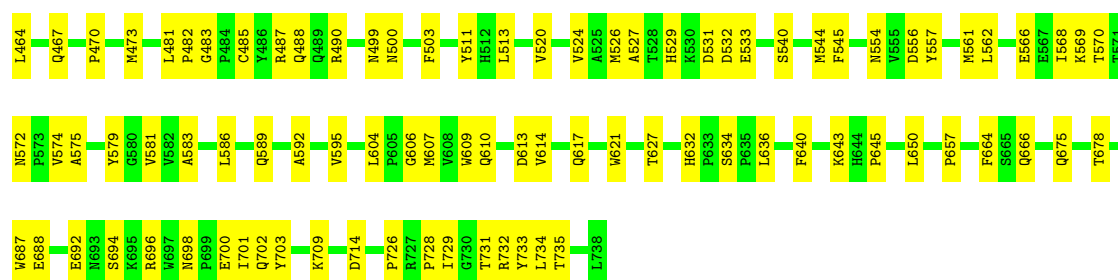
Chain G: 70% 30%



• Molecule 1: Capsid protein VP1

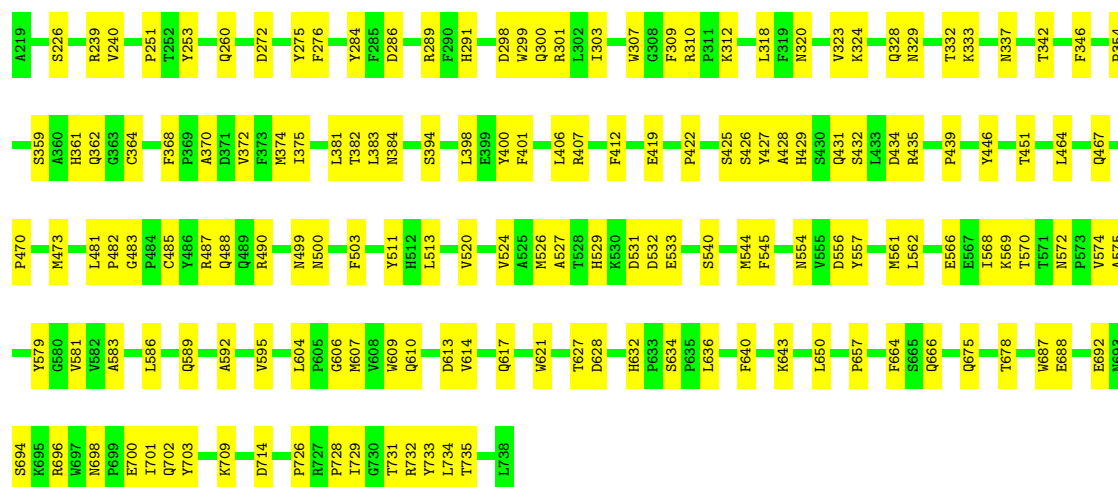
Chain H: 69% 31%





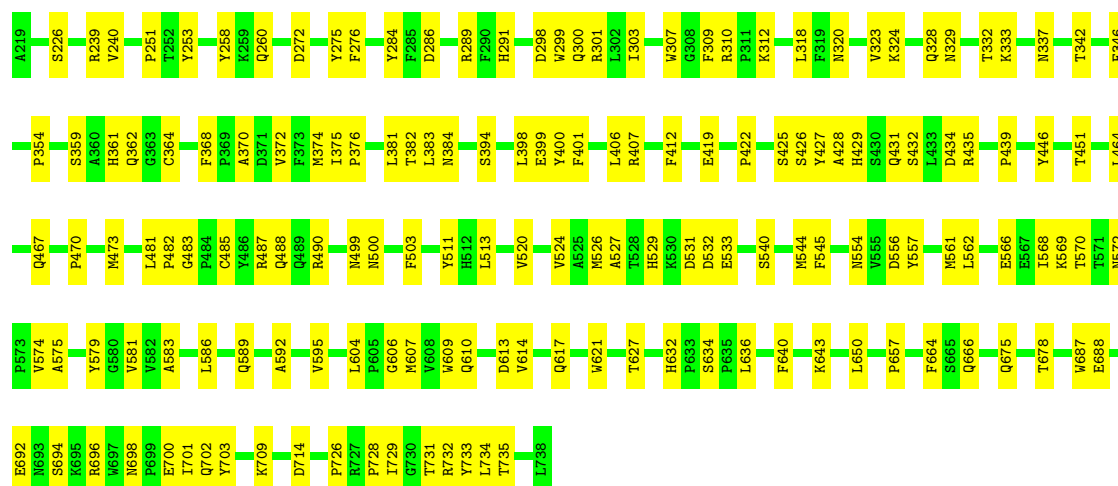
• Molecule 1: Capsid protein VP1

Chain I: 70% 30%



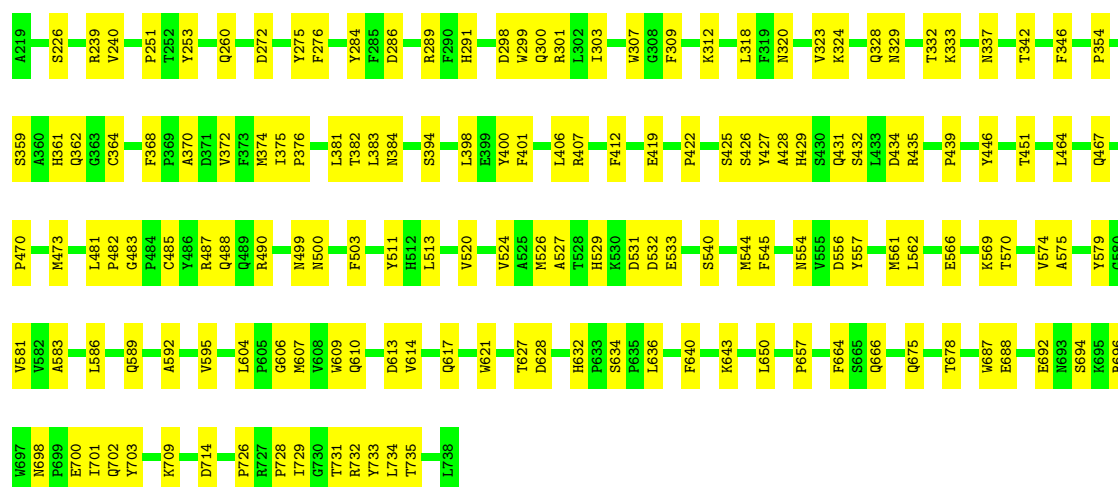
• Molecule 1: Capsid protein VP1

Chain J: 70% 30%



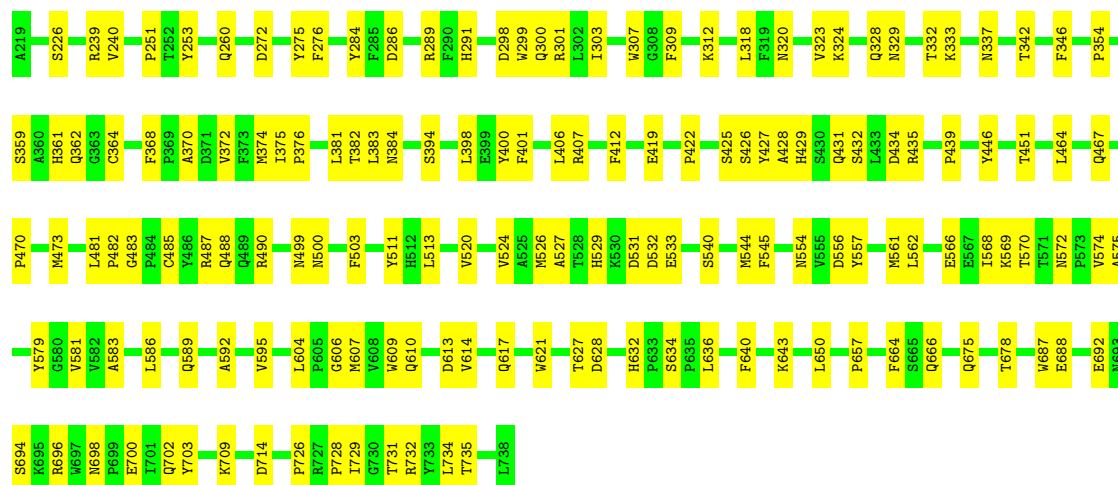
• Molecule 1: Capsid protein VP1

Chain K: 70% 30%



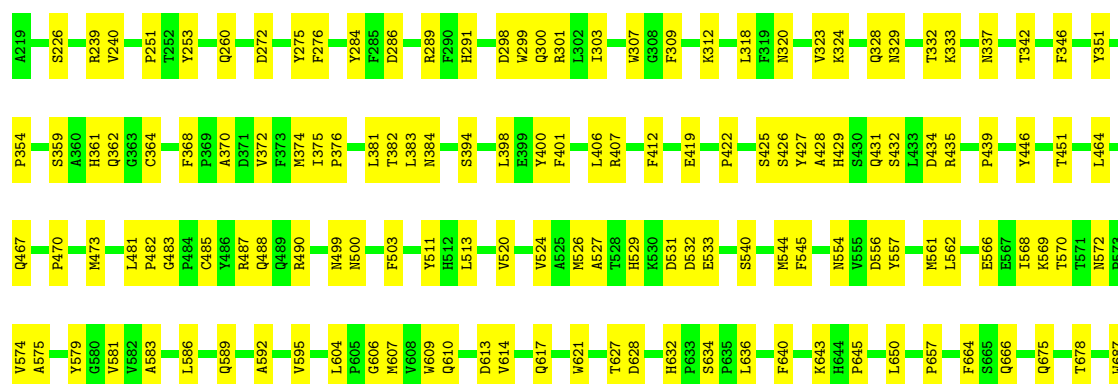
• Molecule 1: Capsid protein VP1

Chain L: 70% 30%



• Molecule 1: Capsid protein VP1

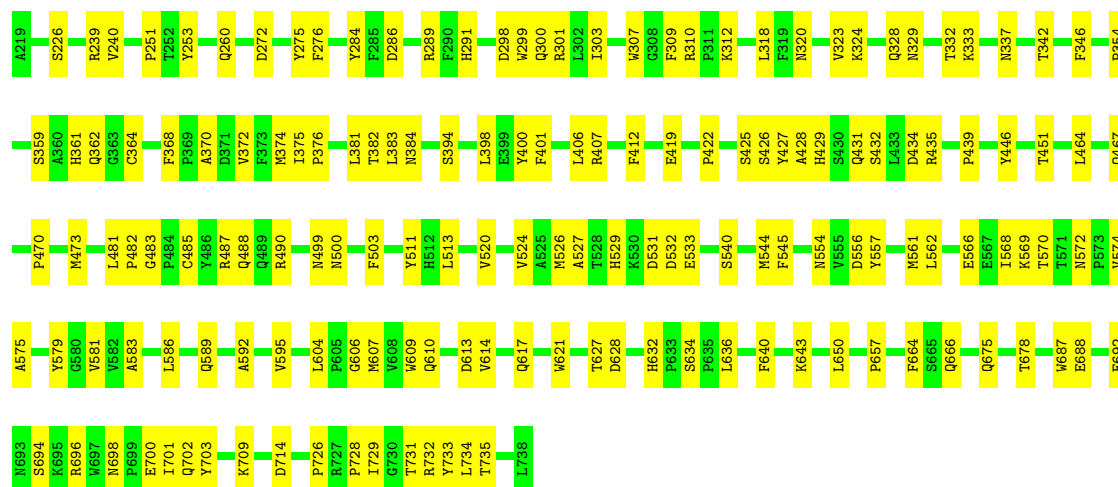
Chain M: 70% 30%





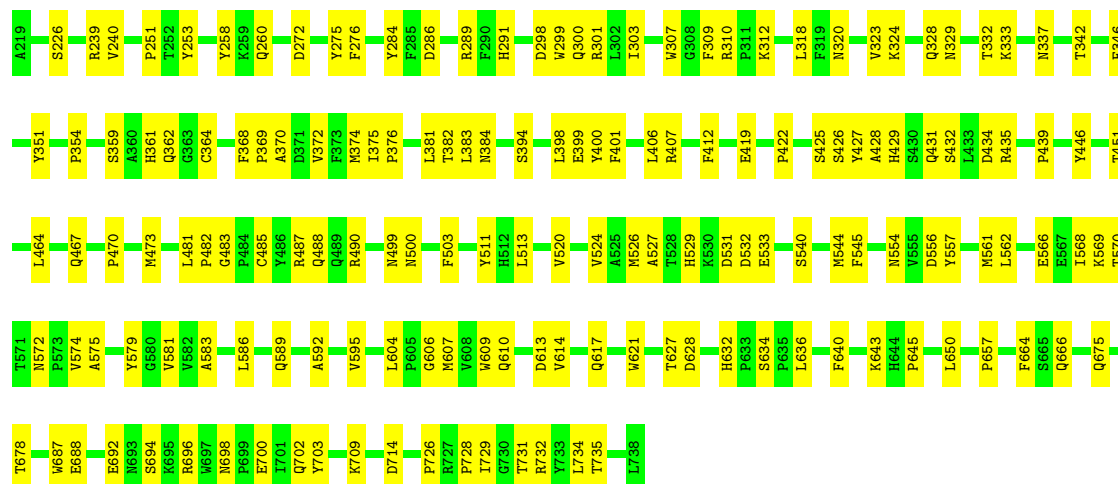
● Molecule 1: Capsid protein VP1

Chain N: 70% 30%



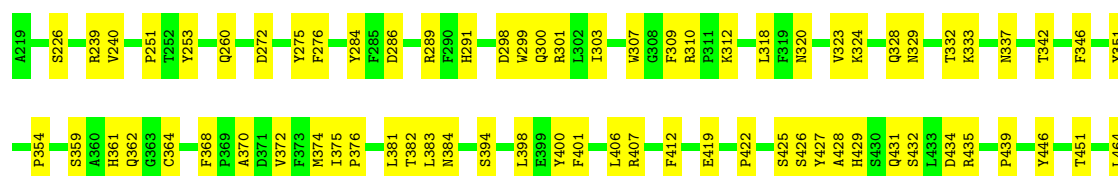
● Molecule 1: Capsid protein VP1

Chain O: 69% 31%



● Molecule 1: Capsid protein VP1

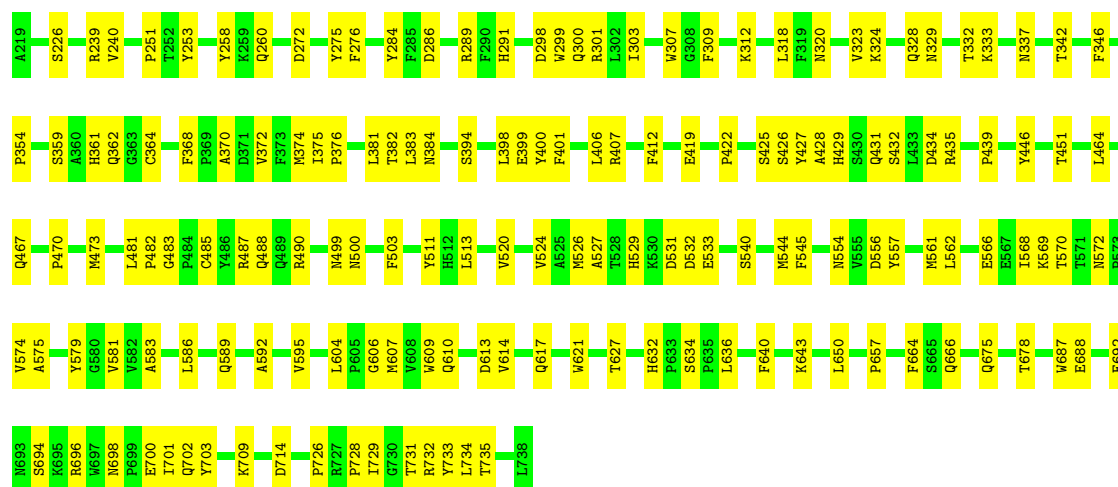
Chain P: 70% 30%





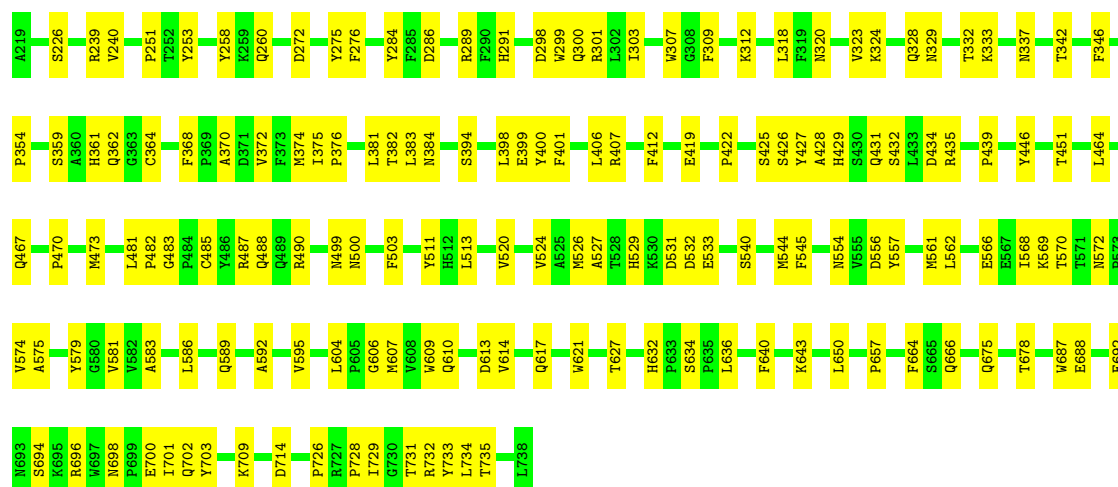
• Molecule 1: Capsid protein VP1

Chain Q: 70% 30%



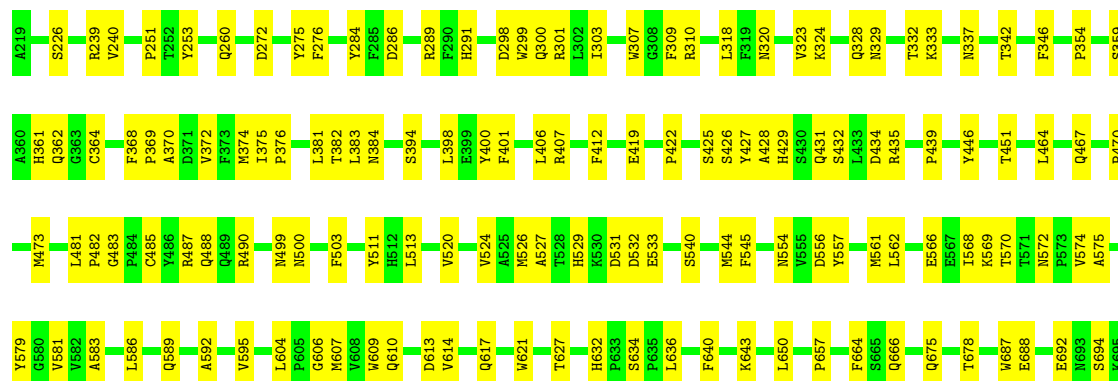
• Molecule 1: Capsid protein VP1

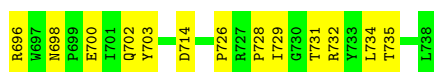
Chain R: 70% 30%



• Molecule 1: Capsid protein VP1

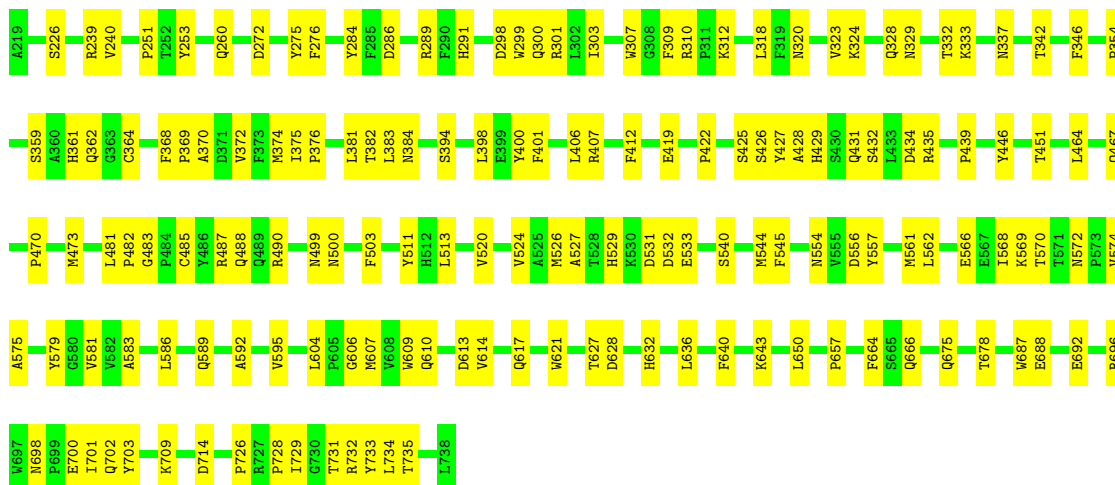
Chain S: 70% 30%





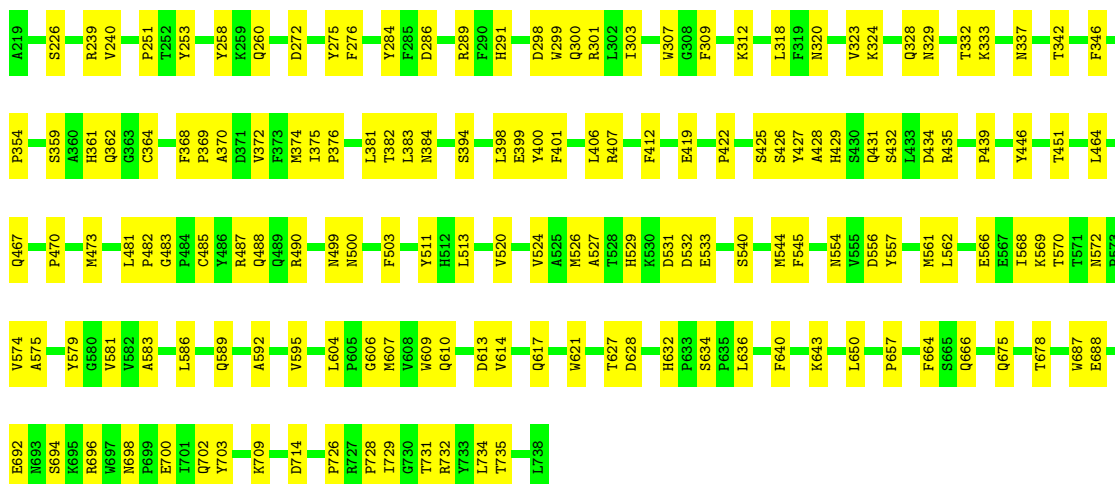
● Molecule 1: Capsid protein VP1

Chain V: 70% 30%



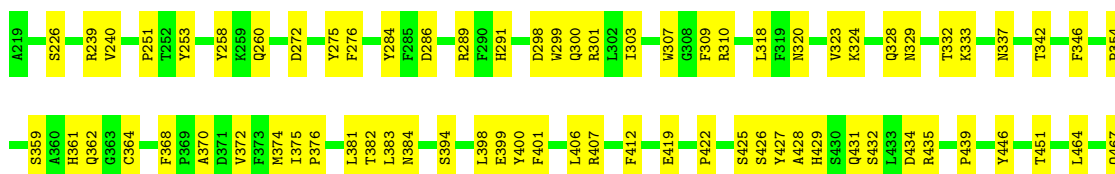
● Molecule 1: Capsid protein VP1

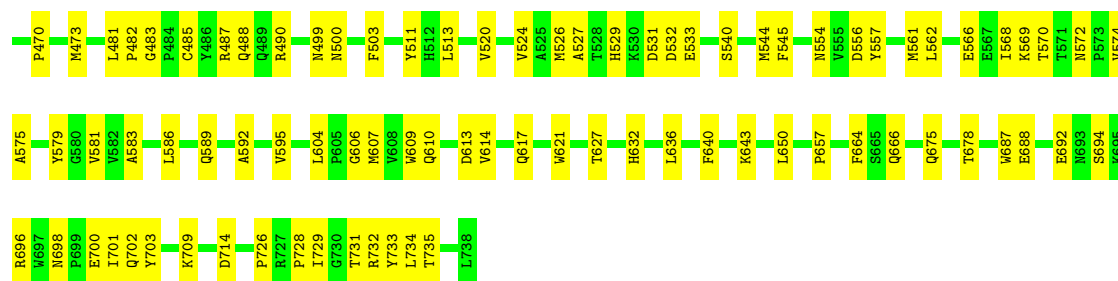
Chain W: 70% 30%



● Molecule 1: Capsid protein VP1

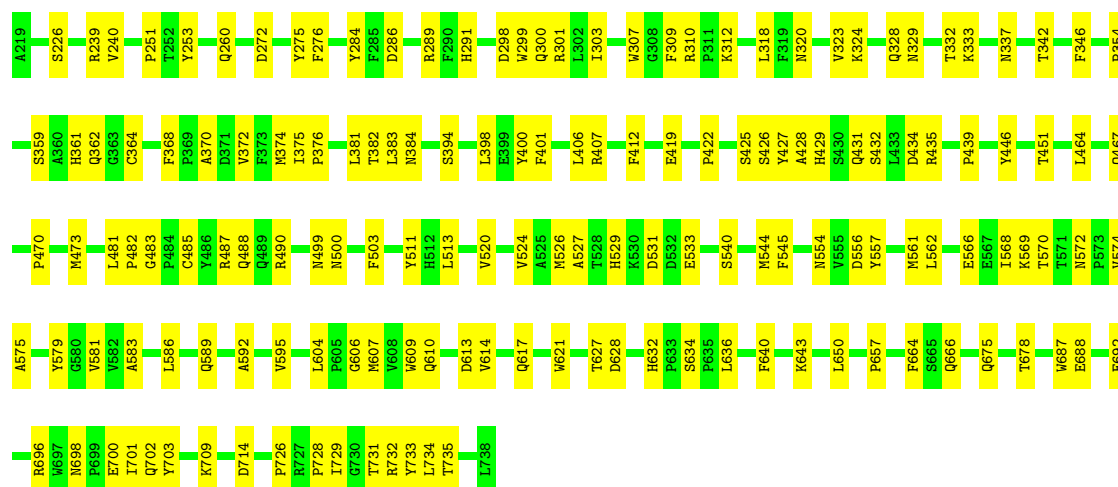
Chain X: 70% 30%





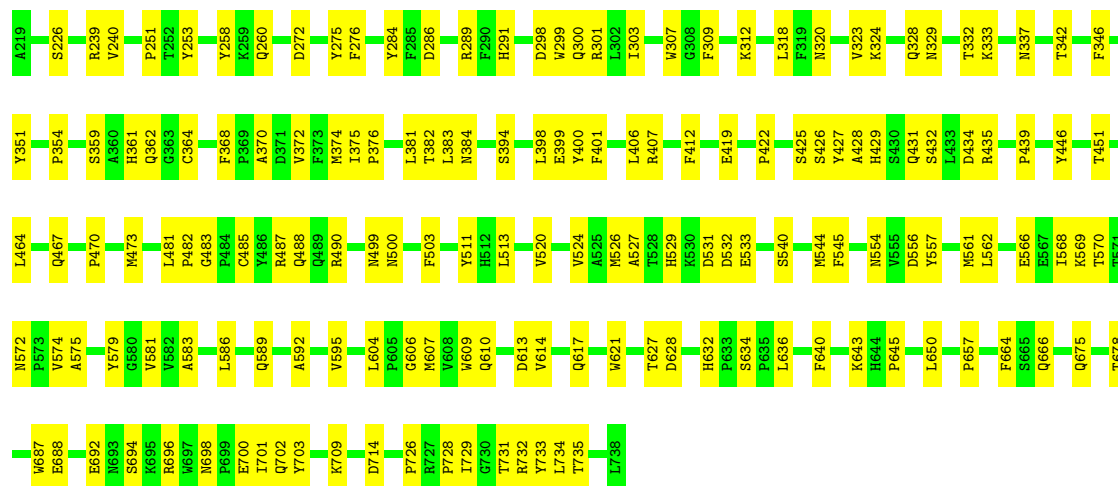
• Molecule 1: Capsid protein VP1

Chain Y: 70% 30%



• Molecule 1: Capsid protein VP1

Chain Z: 69% 31%



• Molecule 1: Capsid protein VP1

Chain a: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain y:  100%

There are no outlier residues recorded for this chain.

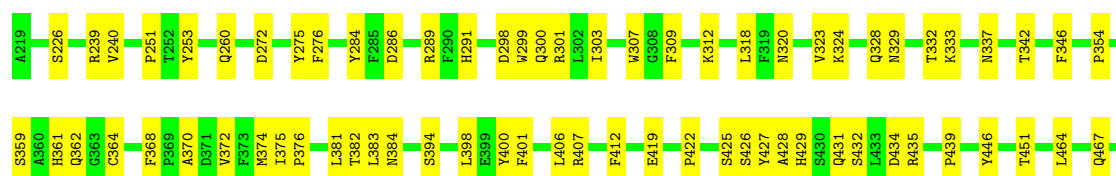
- Molecule 1: Capsid protein VP1

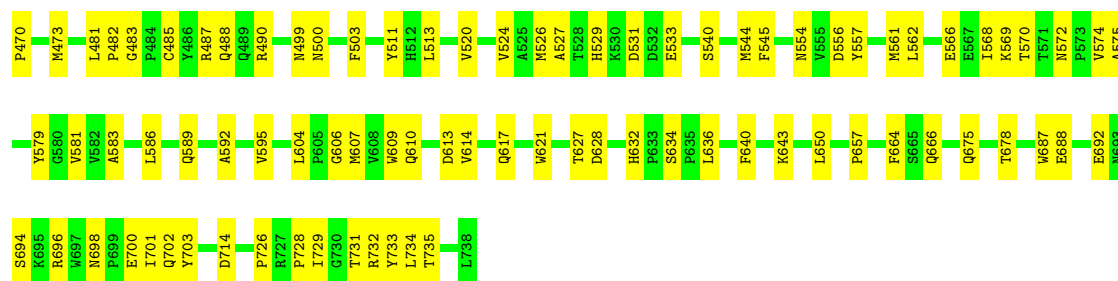
Chain z:  100%

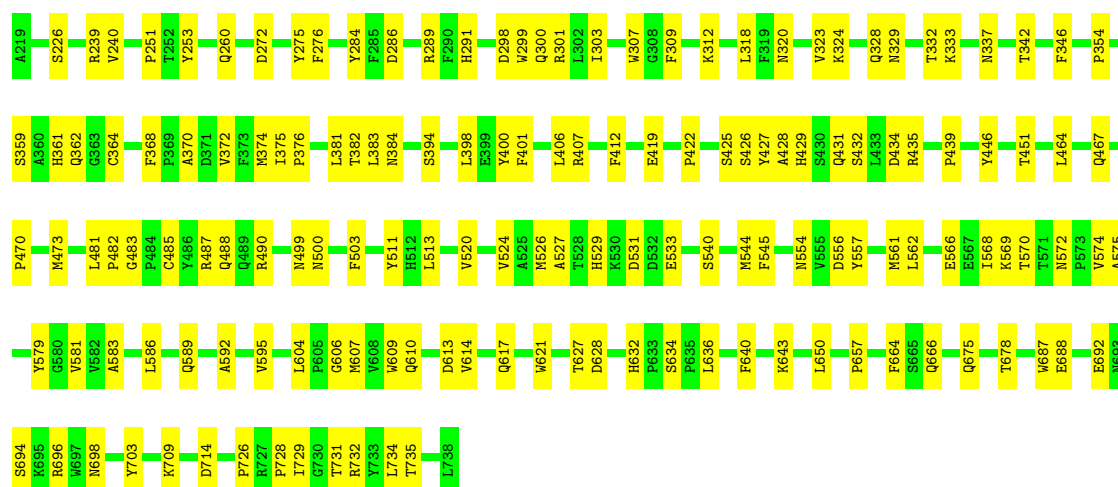
There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

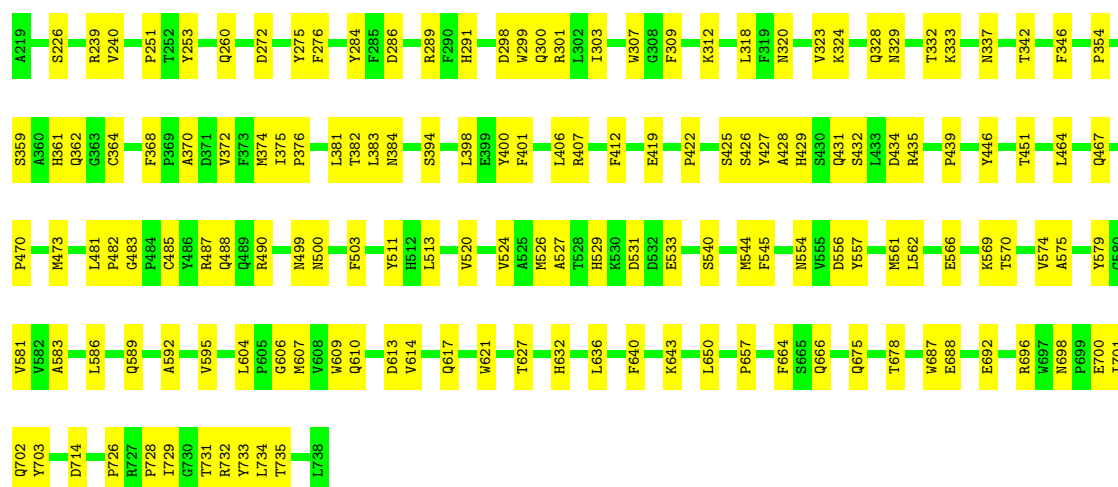
Chain 1:  70% 30%



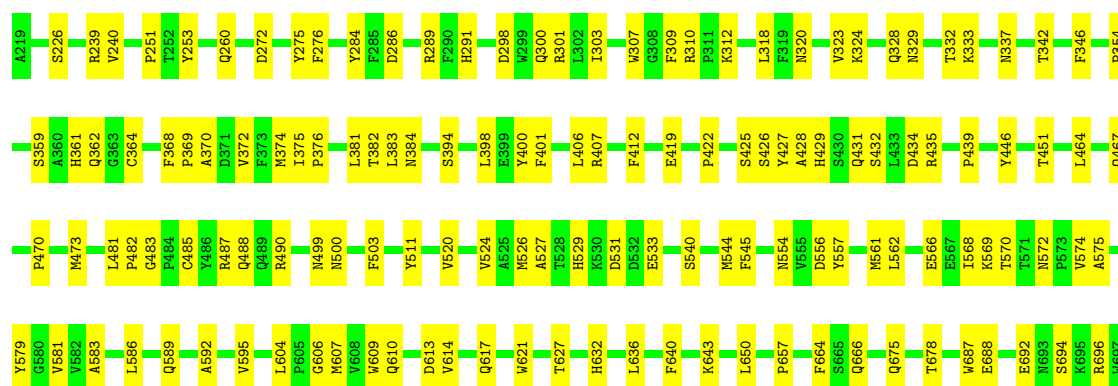


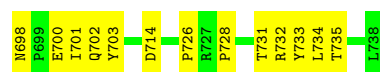


- Molecule 1: Capsid protein VP1



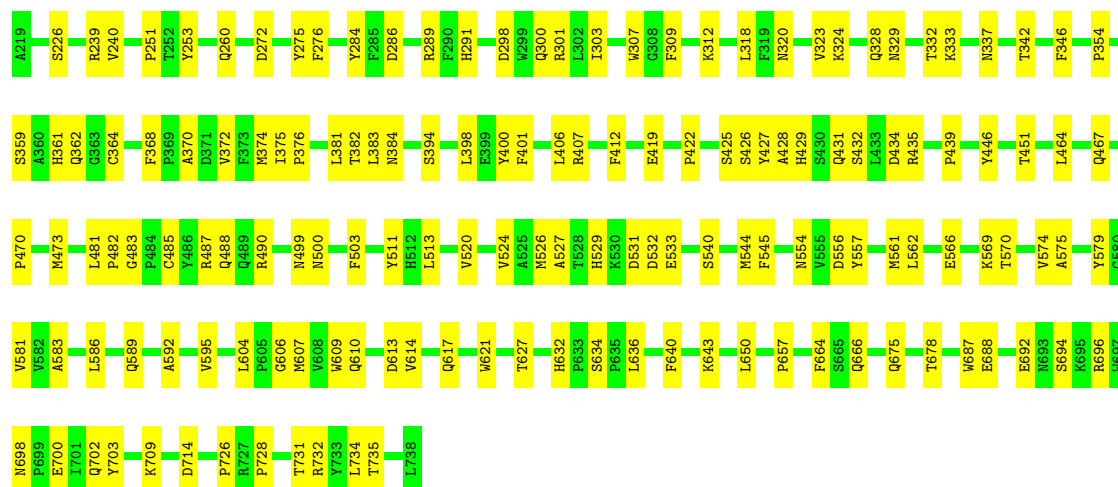
- Molecule 1: Capsid protein VP1





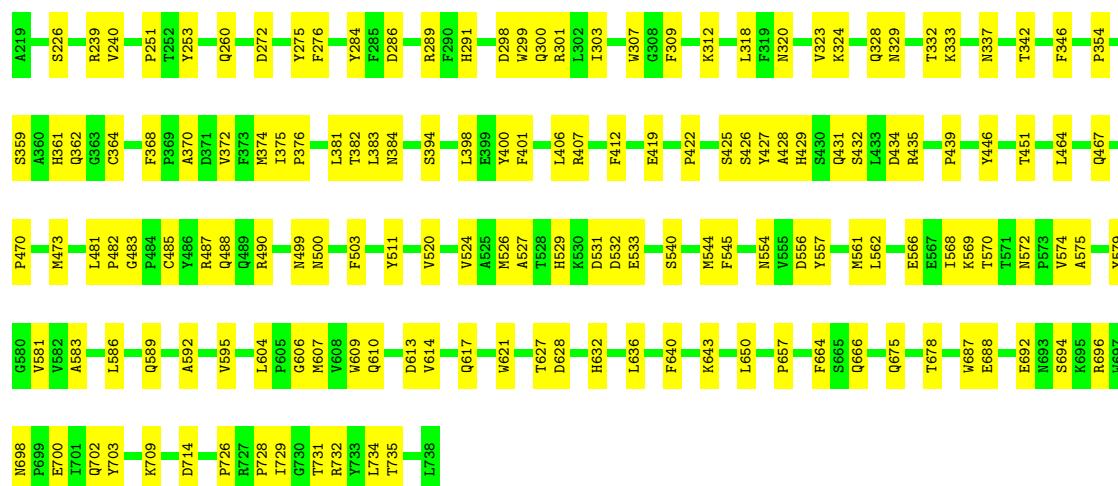
● Molecule 1: Capsid protein VP1

Chain 7: 71% 29%



● Molecule 1: Capsid protein VP1

Chain 8: 71% 29%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	82463	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.56	0/4251	0.54	0/5797
1	2	0.56	0/4251	0.54	0/5797
1	3	0.56	0/4251	0.54	0/5797
1	4	0.56	0/4251	0.54	0/5797
1	5	0.56	0/4251	0.54	0/5797
1	6	0.56	0/4251	0.54	0/5797
1	7	0.56	0/4251	0.54	0/5797
1	8	0.56	0/4251	0.54	0/5797
1	A	0.56	0/4251	0.54	0/5797
1	B	0.56	0/4251	0.54	0/5797
1	C	0.56	0/4251	0.54	0/5797
1	D	0.56	0/4251	0.54	0/5797
1	E	0.56	0/4251	0.54	0/5797
1	F	0.56	0/4251	0.54	0/5797
1	G	0.56	0/4251	0.54	0/5797
1	H	0.56	0/4251	0.54	0/5797
1	I	0.56	0/4251	0.54	0/5797
1	J	0.56	0/4251	0.54	0/5797
1	K	0.56	0/4251	0.54	0/5797
1	L	0.56	0/4251	0.54	0/5797
1	M	0.56	0/4251	0.54	0/5797
1	N	0.56	0/4251	0.54	0/5797
1	O	0.56	0/4251	0.54	0/5797
1	P	0.56	0/4251	0.54	0/5797
1	Q	0.56	0/4251	0.54	0/5797
1	R	0.56	0/4251	0.54	0/5797
1	S	0.56	0/4251	0.54	0/5797
1	T	0.56	0/4251	0.54	0/5797
1	U	0.56	0/4251	0.54	0/5797
1	V	0.56	0/4251	0.54	0/5797
1	W	0.56	0/4251	0.54	0/5797
1	X	0.56	0/4251	0.54	0/5797
1	Y	0.56	0/4251	0.54	0/5797
1	Z	0.56	0/4251	0.54	0/5797

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.56	0/4251	0.54	0/5797
1	b	0.56	0/4251	0.54	0/5797
1	c	0.56	0/4251	0.54	0/5797
1	d	0.56	0/4251	0.54	0/5797
1	e	0.56	0/4251	0.54	0/5797
1	f	0.56	0/4251	0.54	0/5797
1	g	0.56	0/4251	0.54	0/5797
1	h	0.56	0/4251	0.54	0/5797
1	i	0.56	0/4251	0.54	0/5797
1	j	0.56	0/4251	0.54	0/5797
1	k	0.56	0/4251	0.54	0/5797
1	l	0.56	0/4251	0.54	0/5797
1	m	0.56	0/4251	0.54	0/5797
1	n	0.56	0/4251	0.54	0/5797
1	o	0.56	0/4251	0.54	0/5797
1	p	0.56	0/4251	0.54	0/5797
1	q	0.56	0/4251	0.54	0/5797
1	r	0.56	0/4251	0.54	0/5797
1	s	0.56	0/4251	0.54	0/5797
1	t	0.56	0/4251	0.54	0/5797
1	u	0.56	0/4251	0.54	0/5797
1	v	0.56	0/4251	0.54	0/5797
1	w	0.56	0/4251	0.54	0/5797
1	x	0.56	0/4251	0.54	0/5797
1	y	0.56	0/4251	0.54	0/5797
1	z	0.56	0/4251	0.54	0/5797
All	All	0.56	0/255060	0.54	0/347820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	4128	0	3893	138	0
1	2	4128	0	3893	139	0
1	3	4128	0	3893	138	0
1	4	4128	0	3893	136	0
1	5	4128	0	3893	133	0
1	6	4128	0	3893	135	0
1	7	4128	0	3893	134	0
1	8	4128	0	3893	135	0
1	A	4128	0	3893	194	0
1	B	4128	0	3893	188	0
1	C	4128	0	3893	192	0
1	D	4128	0	3893	198	0
1	E	4128	0	3893	193	0
1	F	4128	0	3893	197	0
1	G	4128	0	3893	193	0
1	H	4128	0	3893	194	0
1	I	4128	0	3893	185	0
1	J	4128	0	3893	197	0
1	K	4128	0	3893	196	0
1	L	4128	0	3893	195	0
1	M	4128	0	3893	194	0
1	N	4128	0	3893	195	0
1	O	4128	0	3893	196	0
1	P	4128	0	3893	186	0
1	Q	4128	0	3893	188	0
1	R	4128	0	3893	171	0
1	S	4128	0	3893	175	0
1	T	4128	0	3893	190	0
1	U	4128	0	3893	188	0
1	V	4128	0	3893	191	0
1	W	4128	0	3893	194	0
1	X	4128	0	3893	192	0
1	Y	4128	0	3893	193	0
1	Z	4128	0	3893	196	0
1	a	4128	0	3893	0	0
1	b	4128	0	3893	0	0
1	c	4128	0	3893	0	0
1	d	4128	0	3893	0	0
1	e	4128	0	3893	0	0
1	f	4128	0	3893	0	0
1	g	4128	0	3893	0	0
1	h	4128	0	3893	0	0
1	i	4128	0	3893	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4128	0	3893	0	0
1	k	4128	0	3893	0	0
1	l	4128	0	3893	0	0
1	m	4128	0	3893	0	0
1	n	4128	0	3893	0	0
1	o	4128	0	3893	0	0
1	p	4128	0	3893	0	0
1	q	4128	0	3893	0	0
1	r	4128	0	3893	0	0
1	s	4128	0	3893	0	0
1	t	4128	0	3893	0	0
1	u	4128	0	3893	0	0
1	v	4128	0	3893	0	0
1	w	4128	0	3893	0	0
1	x	4128	0	3893	0	0
1	y	4128	0	3893	0	0
1	z	4128	0	3893	0	0
2	1	16	0	12	1	0
2	2	16	0	12	1	0
2	3	16	0	12	1	0
2	4	16	0	12	1	0
2	5	16	0	12	1	0
2	6	16	0	12	1	0
2	7	16	0	12	1	0
2	8	16	0	12	1	0
2	A	16	0	12	1	0
2	B	16	0	12	1	0
2	C	16	0	12	1	0
2	D	16	0	12	1	0
2	E	16	0	12	1	0
2	F	16	0	12	1	0
2	G	16	0	12	1	0
2	H	16	0	12	1	0
2	I	16	0	12	1	0
2	J	16	0	12	1	0
2	K	16	0	12	1	0
2	L	16	0	12	1	0
2	M	16	0	12	1	0
2	N	16	0	12	1	0
2	O	16	0	12	1	0
2	P	16	0	12	1	0
2	Q	16	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	16	0	12	1	0
2	S	16	0	12	1	0
2	T	16	0	12	1	0
2	U	16	0	12	1	0
2	V	16	0	12	1	0
2	W	16	0	12	1	0
2	X	16	0	12	1	0
2	Y	16	0	12	1	0
2	Z	16	0	12	1	0
2	a	16	0	12	0	0
2	b	16	0	12	0	0
2	c	16	0	12	0	0
2	d	16	0	12	0	0
2	e	16	0	12	0	0
2	f	16	0	12	0	0
2	g	16	0	12	0	0
2	h	16	0	12	0	0
2	i	16	0	12	0	0
2	j	16	0	12	0	0
2	k	16	0	12	0	0
2	l	16	0	12	0	0
2	m	16	0	12	0	0
2	n	16	0	12	0	0
2	o	16	0	12	0	0
2	p	16	0	12	0	0
2	q	16	0	12	0	0
2	r	16	0	12	0	0
2	s	16	0	12	0	0
2	t	16	0	12	0	0
2	u	16	0	12	0	0
2	v	16	0	12	0	0
2	w	16	0	12	0	0
2	x	16	0	12	0	0
2	y	16	0	12	0	0
2	z	16	0	12	0	0
3	1	21	0	12	4	0
3	2	21	0	12	4	0
3	3	21	0	12	3	0
3	4	21	0	12	4	0
3	5	21	0	12	3	0
3	6	21	0	12	3	0
3	7	21	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8	21	0	12	3	0
3	A	21	0	12	4	0
3	B	21	0	12	4	0
3	C	21	0	12	4	0
3	D	21	0	12	4	0
3	E	21	0	12	4	0
3	F	21	0	12	4	0
3	G	21	0	12	4	0
3	H	21	0	12	4	0
3	I	21	0	12	4	0
3	J	21	0	12	4	0
3	K	21	0	12	4	0
3	L	21	0	12	3	0
3	M	21	0	12	4	0
3	N	21	0	12	4	0
3	O	21	0	12	4	0
3	P	21	0	12	3	0
3	Q	21	0	12	4	0
3	R	21	0	12	4	0
3	S	21	0	12	4	0
3	T	21	0	12	4	0
3	U	21	0	12	4	0
3	V	21	0	12	3	0
3	W	21	0	12	4	0
3	X	21	0	12	3	0
3	Y	21	0	12	4	0
3	Z	21	0	12	4	0
3	a	21	0	12	0	0
3	b	21	0	12	0	0
3	c	21	0	12	0	0
3	d	21	0	12	0	0
3	e	21	0	12	0	0
3	f	21	0	12	0	0
3	g	21	0	12	0	0
3	h	21	0	12	0	0
3	i	21	0	12	0	0
3	j	21	0	12	0	0
3	k	21	0	12	0	0
3	l	21	0	12	0	0
3	m	21	0	12	0	0
3	n	21	0	12	0	0
3	o	21	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	p	21	0	12	0	0
3	q	21	0	12	0	0
3	r	21	0	12	0	0
3	s	21	0	12	0	0
3	t	21	0	12	0	0
3	u	21	0	12	0	0
3	v	21	0	12	0	0
3	w	21	0	12	0	0
3	x	21	0	12	0	0
3	y	21	0	12	0	0
3	z	21	0	12	0	0
All	All	249900	0	235020	4470	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4470) 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:C:253:TYR:OH	1:C:375:ILE:O	2.05	0.76
1:L:253:TYR:OH	1:L:375:ILE:O	2.05	0.76
1:R:253:TYR:OH	1:R:375:ILE:O	2.04	0.76
1:T:253:TYR:OH	1:T:375:ILE:O	2.05	0.76
1:V:253:TYR:OH	1:V:375:ILE:O	2.04	0.76
1:Y:253:TYR:OH	1:Y:375:ILE:O	2.04	0.75
1:F:253:TYR:OH	1:F:375:ILE:O	2.05	0.75
1:J:253:TYR:OH	1:J:375:ILE:O	2.05	0.75
1:G:253:TYR:OH	1:G:375:ILE:O	2.04	0.75
1:P:253:TYR:OH	1:P:375:ILE:O	2.04	0.75
1:H:253:TYR:OH	1:H:375:ILE:O	2.05	0.75
1:Z:253:TYR:OH	1:Z:375:ILE:O	2.05	0.75
1:I:253:TYR:OH	1:I:375:ILE:O	2.05	0.75
1:O:253:TYR:OH	1:O:375:ILE:O	2.04	0.75
1:S:253:TYR:OH	1:S:375:ILE:O	2.05	0.75
1:3:253:TYR:OH	1:3:375:ILE:O	2.05	0.75
1:5:253:TYR:OH	1:5:375:ILE:O	2.04	0.74
1:X:253:TYR:OH	1:X:375:ILE:O	2.05	0.74
1:8:253:TYR:OH	1:8:375:ILE:O	2.05	0.74
1:M:253:TYR:OH	1:M:375:ILE:O	2.05	0.74
1:Q:253:TYR:OH	1:Q:375:ILE:O	2.05	0.74
1:A:253:TYR:OH	1:A:375:ILE:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:253:TYR:OH	1:U:375:ILE:O	2.05	0.74
1:D:253:TYR:OH	1:D:375:ILE:O	2.05	0.74
1:K:253:TYR:OH	1:K:375:ILE:O	2.05	0.74
1:N:253:TYR:OH	1:N:375:ILE:O	2.05	0.74
1:4:253:TYR:OH	1:4:375:ILE:O	2.04	0.74
1:E:253:TYR:OH	1:E:375:ILE:O	2.04	0.74
1:W:253:TYR:OH	1:W:375:ILE:O	2.04	0.74
1:7:253:TYR:OH	1:7:375:ILE:O	2.05	0.74
1:B:253:TYR:OH	1:B:375:ILE:O	2.05	0.74
1:1:253:TYR:OH	1:1:375:ILE:O	2.05	0.74
1:2:253:TYR:OH	1:2:375:ILE:O	2.04	0.73
1:6:253:TYR:OH	1:6:375:ILE:O	2.05	0.73
1:B:324:LYS:NZ	1:B:337:ASN:OD1	2.23	0.72
1:W:324:LYS:NZ	1:W:337:ASN:OD1	2.23	0.72
1:E:324:LYS:NZ	1:E:337:ASN:OD1	2.23	0.72
1:F:324:LYS:NZ	1:F:337:ASN:OD1	2.23	0.72
1:H:324:LYS:NZ	1:H:337:ASN:OD1	2.23	0.72
1:J:324:LYS:NZ	1:J:337:ASN:OD1	2.23	0.72
1:S:324:LYS:NZ	1:S:337:ASN:OD1	2.23	0.72
1:C:324:LYS:NZ	1:C:337:ASN:OD1	2.23	0.72
1:I:324:LYS:NZ	1:I:337:ASN:OD1	2.23	0.72
1:V:324:LYS:NZ	1:V:337:ASN:OD1	2.23	0.72
1:M:324:LYS:NZ	1:M:337:ASN:OD1	2.23	0.72
1:Y:324:LYS:NZ	1:Y:337:ASN:OD1	2.23	0.72
1:7:324:LYS:NZ	1:7:337:ASN:OD1	2.23	0.72
1:G:324:LYS:NZ	1:G:337:ASN:OD1	2.23	0.72
1:L:324:LYS:NZ	1:L:337:ASN:OD1	2.23	0.72
1:P:324:LYS:NZ	1:P:337:ASN:OD1	2.23	0.72
1:Z:324:LYS:NZ	1:Z:337:ASN:OD1	2.23	0.72
1:Q:324:LYS:NZ	1:Q:337:ASN:OD1	2.23	0.72
1:X:324:LYS:NZ	1:X:337:ASN:OD1	2.23	0.72
1:4:324:LYS:NZ	1:4:337:ASN:OD1	2.23	0.71
1:5:324:LYS:NZ	1:5:337:ASN:OD1	2.23	0.71
1:R:324:LYS:NZ	1:R:337:ASN:OD1	2.23	0.71
1:T:324:LYS:NZ	1:T:337:ASN:OD1	2.23	0.71
1:N:324:LYS:NZ	1:N:337:ASN:OD1	2.23	0.71
1:1:324:LYS:NZ	1:1:337:ASN:OD1	2.23	0.71
1:6:324:LYS:NZ	1:6:337:ASN:OD1	2.23	0.71
1:A:324:LYS:NZ	1:A:337:ASN:OD1	2.23	0.71
1:U:324:LYS:NZ	1:U:337:ASN:OD1	2.23	0.71
1:O:324:LYS:NZ	1:O:337:ASN:OD1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:324:LYS:NZ	1:K:337:ASN:OD1	2.23	0.71
1:2:324:LYS:NZ	1:2:337:ASN:OD1	2.23	0.71
1:3:324:LYS:NZ	1:3:337:ASN:OD1	2.23	0.71
1:D:324:LYS:NZ	1:D:337:ASN:OD1	2.23	0.71
1:8:324:LYS:NZ	1:8:337:ASN:OD1	2.23	0.70
1:R:303:ILE:HG22	1:R:731:THR:HG23	1.76	0.68
1:G:303:ILE:HG22	1:G:731:THR:HG23	1.76	0.68
1:I:303:ILE:HG22	1:I:731:THR:HG23	1.76	0.68
1:Y:303:ILE:HG22	1:Y:731:THR:HG23	1.76	0.68
1:E:303:ILE:HG22	1:E:731:THR:HG23	1.76	0.68
1:W:303:ILE:HG22	1:W:731:THR:HG23	1.76	0.68
1:2:303:ILE:HG22	1:2:731:THR:HG23	1.76	0.68
1:D:303:ILE:HG22	1:D:731:THR:HG23	1.76	0.68
1:T:427:TYR:H	1:T:732:ARG:HG2	1.59	0.68
1:7:427:TYR:H	1:7:732:ARG:HG2	1.59	0.68
1:E:427:TYR:H	1:E:732:ARG:HG2	1.59	0.68
1:L:427:TYR:H	1:L:732:ARG:HG2	1.59	0.68
1:M:427:TYR:H	1:M:732:ARG:HG2	1.59	0.68
1:P:303:ILE:HG22	1:P:731:THR:HG23	1.76	0.68
1:V:303:ILE:HG22	1:V:731:THR:HG23	1.76	0.68
1:1:427:TYR:H	1:1:732:ARG:HG2	1.59	0.68
1:D:427:TYR:H	1:D:732:ARG:HG2	1.59	0.68
1:J:427:TYR:H	1:J:732:ARG:HG2	1.59	0.68
1:K:427:TYR:H	1:K:732:ARG:HG2	1.59	0.68
1:O:427:TYR:H	1:O:732:ARG:HG2	1.59	0.68
1:Q:303:ILE:HG22	1:Q:731:THR:HG23	1.76	0.68
1:R:427:TYR:H	1:R:732:ARG:HG2	1.59	0.68
1:V:427:TYR:H	1:V:732:ARG:HG2	1.59	0.68
1:Y:427:TYR:H	1:Y:732:ARG:HG2	1.59	0.68
1:Z:427:TYR:H	1:Z:732:ARG:HG2	1.59	0.68
1:5:303:ILE:HG22	1:5:731:THR:HG23	1.76	0.68
1:T:303:ILE:HG22	1:T:731:THR:HG23	1.76	0.68
1:U:303:ILE:HG22	1:U:731:THR:HG23	1.76	0.68
1:3:427:TYR:H	1:3:732:ARG:HG2	1.59	0.68
1:3:303:ILE:HG22	1:3:731:THR:HG23	1.76	0.68
1:4:427:TYR:H	1:4:732:ARG:HG2	1.59	0.68
1:A:427:TYR:H	1:A:732:ARG:HG2	1.59	0.68
1:O:303:ILE:HG22	1:O:731:THR:HG23	1.76	0.68
1:U:427:TYR:H	1:U:732:ARG:HG2	1.59	0.68
1:1:303:ILE:HG22	1:1:731:THR:HG23	1.76	0.68
1:2:427:TYR:H	1:2:732:ARG:HG2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:427:TYR:H	1:8:732:ARG:HG2	1.59	0.68
1:H:303:ILE:HG22	1:H:731:THR:HG23	1.76	0.68
1:N:427:TYR:H	1:N:732:ARG:HG2	1.59	0.68
1:P:427:TYR:H	1:P:732:ARG:HG2	1.59	0.68
1:S:427:TYR:H	1:S:732:ARG:HG2	1.59	0.68
1:B:303:ILE:HG22	1:B:731:THR:HG23	1.76	0.68
1:F:427:TYR:H	1:F:732:ARG:HG2	1.59	0.68
1:H:427:TYR:H	1:H:732:ARG:HG2	1.59	0.68
1:K:303:ILE:HG22	1:K:731:THR:HG23	1.76	0.68
1:X:427:TYR:H	1:X:732:ARG:HG2	1.59	0.68
1:6:427:TYR:H	1:6:732:ARG:HG2	1.59	0.67
1:7:303:ILE:HG22	1:7:731:THR:HG23	1.76	0.67
1:A:303:ILE:HG22	1:A:731:THR:HG23	1.76	0.67
1:S:303:ILE:HG22	1:S:731:THR:HG23	1.76	0.67
1:C:303:ILE:HG22	1:C:731:THR:HG23	1.76	0.67
1:L:303:ILE:HG22	1:L:731:THR:HG23	1.76	0.67
1:W:427:TYR:H	1:W:732:ARG:HG2	1.59	0.67
1:C:427:TYR:H	1:C:732:ARG:HG2	1.59	0.67
1:J:303:ILE:HG22	1:J:731:THR:HG23	1.76	0.67
1:M:303:ILE:HG22	1:M:731:THR:HG23	1.76	0.67
1:N:303:ILE:HG22	1:N:731:THR:HG23	1.76	0.67
1:6:303:ILE:HG22	1:6:731:THR:HG23	1.76	0.67
1:F:303:ILE:HG22	1:F:731:THR:HG23	1.76	0.67
1:I:427:TYR:H	1:I:732:ARG:HG2	1.59	0.67
1:G:427:TYR:H	1:G:732:ARG:HG2	1.59	0.67
1:Z:303:ILE:HG22	1:Z:731:THR:HG23	1.76	0.67
1:8:303:ILE:HG22	1:8:731:THR:HG23	1.76	0.66
1:Q:427:TYR:H	1:Q:732:ARG:HG2	1.59	0.66
1:X:303:ILE:HG22	1:X:731:THR:HG23	1.76	0.66
1:5:427:TYR:H	1:5:732:ARG:HG2	1.59	0.66
1:4:303:ILE:HG22	1:4:731:THR:HG23	1.76	0.66
1:1:589:GLN:HA	1:2:499:ASN:HA	1.77	0.66
1:D:499:ASN:HA	1:T:589:GLN:HA	158.48	0.66
1:D:473:MET:HE1	1:N:275:TYR:HB3	1.78	0.66
1:6:473:MET:HE1	1:7:275:TYR:CD2	2.31	0.66
1:B:427:TYR:H	1:B:732:ARG:HG2	1.59	0.66
1:A:589:GLN:HA	1:G:499:ASN:HA	1.76	0.66
1:A:499:ASN:HA	1:I:589:GLN:HA	1.77	0.65
1:L:531:ASP:OD1	1:L:569:LYS:NZ	2.30	0.65
1:P:531:ASP:OD1	1:P:569:LYS:NZ	2.30	0.65
1:8:531:ASP:OD1	1:8:569:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:531:ASP:OD1	1:F:569:LYS:NZ	2.30	0.65
1:U:531:ASP:OD1	1:U:569:LYS:NZ	2.30	0.65
1:V:531:ASP:OD1	1:V:569:LYS:NZ	2.30	0.65
1:Y:531:ASP:OD1	1:Y:569:LYS:NZ	2.30	0.65
1:Z:531:ASP:OD1	1:Z:569:LYS:NZ	2.30	0.65
1:3:531:ASP:OD1	1:3:569:LYS:NZ	2.30	0.65
1:6:531:ASP:OD1	1:6:569:LYS:NZ	2.30	0.65
1:A:531:ASP:OD1	1:A:569:LYS:NZ	2.30	0.65
1:H:531:ASP:OD1	1:H:569:LYS:NZ	2.30	0.65
1:K:531:ASP:OD1	1:K:569:LYS:NZ	2.30	0.65
1:O:531:ASP:OD1	1:O:569:LYS:NZ	2.30	0.65
1:B:499:ASN:HA	1:C:589:GLN:HA	112.69	0.65
1:I:499:ASN:HA	1:K:589:GLN:HA	131.13	0.65
1:Q:589:GLN:HA	1:R:499:ASN:HA	81.60	0.65
1:W:589:GLN:HA	1:Y:499:ASN:HA	1.79	0.65
1:E:499:ASN:HA	1:V:589:GLN:HA	189.05	0.65
1:G:499:ASN:HA	1:H:589:GLN:HA	81.60	0.65
1:J:589:GLN:HA	1:K:499:ASN:HA	81.60	0.65
1:M:499:ASN:HA	1:O:589:GLN:HA	131.11	0.65
1:R:531:ASP:OD1	1:R:569:LYS:NZ	2.30	0.65
1:W:589:GLN:HA	1:X:499:ASN:HA	81.60	0.65
1:W:499:ASN:HA	1:Y:589:GLN:HA	39.53	0.65
1:Z:589:GLN:HA	1:4:499:ASN:HA	1.79	0.65
1:4:531:ASP:OD1	1:4:569:LYS:NZ	2.30	0.65
1:E:589:GLN:HA	1:X:499:ASN:HA	155.47	0.65
1:F:589:GLN:HA	1:H:499:ASN:HA	160.80	0.65
1:G:589:GLN:HA	1:I:499:ASN:HA	1.79	0.65
1:L:589:GLN:HA	1:T:499:ASN:HA	243.91	0.65
1:T:531:ASP:OD1	1:T:569:LYS:NZ	2.30	0.65
1:X:531:ASP:OD1	1:X:569:LYS:NZ	2.30	0.65
1:Z:589:GLN:HA	1:1:499:ASN:HA	96.12	0.65
1:D:589:GLN:HA	1:L:499:ASN:HA	160.79	0.65
1:B:499:ASN:HA	1:L:589:GLN:HA	1.79	0.65
1:M:589:GLN:HA	1:N:499:ASN:HA	112.70	0.65
1:N:531:ASP:OD1	1:N:569:LYS:NZ	2.30	0.65
1:O:589:GLN:HA	1:P:499:ASN:HA	112.70	0.65
1:Z:499:ASN:HA	1:3:589:GLN:HA	1.79	0.65
1:G:531:ASP:OD1	1:G:569:LYS:NZ	2.30	0.64
1:C:499:ASN:HA	1:P:589:GLN:HA	80.14	0.64
1:S:531:ASP:OD1	1:S:569:LYS:NZ	2.30	0.64
1:5:499:ASN:HA	1:7:589:GLN:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:531:ASP:OD1	1:J:569:LYS:NZ	2.30	0.64
1:J:589:GLN:HA	1:L:499:ASN:HA	1.79	0.64
1:C:499:ASN:HA	1:M:589:GLN:HA	1.79	0.64
1:2:531:ASP:OD1	1:2:569:LYS:NZ	2.30	0.64
1:Q:531:ASP:OD1	1:Q:569:LYS:NZ	2.30	0.64
1:Z:499:ASN:HA	1:2:589:GLN:HA	117.83	0.64
1:D:531:ASP:OD1	1:D:569:LYS:NZ	2.30	0.64
1:M:531:ASP:OD1	1:M:569:LYS:NZ	2.30	0.64
1:C:589:GLN:HA	1:O:499:ASN:HA	155.42	0.64
1:E:589:GLN:HA	1:Q:499:ASN:HA	1.79	0.64
1:Q:499:ASN:HA	1:S:589:GLN:HA	96.01	0.64
1:H:589:GLN:HA	1:W:499:ASN:HA	1.79	0.64
1:N:589:GLN:HA	1:P:499:ASN:HA	1.79	0.64
1:K:499:ASN:HA	1:8:589:GLN:HA	1.79	0.64
1:D:499:ASN:HA	1:P:589:GLN:HA	1.79	0.64
1:A:589:GLN:HA	1:8:499:ASN:HA	179.35	0.64
1:6:589:GLN:HA	1:7:499:ASN:HA	1.79	0.64
1:A:298:ASP:OD2	1:E:400:TYR:OH	2.16	0.64
1:V:400:TYR:OH	1:1:298:ASP:OD2	145.15	0.64
1:E:531:ASP:OD1	1:E:569:LYS:NZ	2.30	0.64
1:O:298:ASP:OD2	1:7:400:TYR:OH	145.15	0.64
1:7:531:ASP:OD1	1:7:569:LYS:NZ	2.30	0.64
1:E:499:ASN:HA	1:F:589:GLN:HA	1.79	0.64
1:F:499:ASN:HA	1:G:589:GLN:HA	96.00	0.64
1:W:531:ASP:OD1	1:W:569:LYS:NZ	2.30	0.64
1:X:589:GLN:HA	1:Y:499:ASN:HA	112.70	0.64
1:H:499:ASN:HA	1:Y:589:GLN:HA	1.79	0.64
1:C:531:ASP:OD1	1:C:569:LYS:NZ	2.30	0.63
1:I:589:GLN:HA	1:J:499:ASN:HA	112.71	0.63
1:R:589:GLN:HA	1:S:499:ASN:HA	1.79	0.63
1:T:298:ASP:OD2	1:U:400:TYR:OH	2.16	0.63
1:V:499:ASN:HA	1:X:589:GLN:HA	1.79	0.63
1:D:589:GLN:HA	1:N:499:ASN:HA	1.79	0.63
1:A:499:ASN:HA	1:K:589:GLN:HA	165.10	0.63
1:F:473:MET:HE1	1:H:275:TYR:CD2	139.18	0.63
1:I:531:ASP:OD1	1:I:569:LYS:NZ	2.30	0.63
1:B:589:GLN:HA	1:J:499:ASN:HA	1.79	0.63
1:F:499:ASN:HA	1:Q:589:GLN:HA	1.79	0.63
1:T:589:GLN:HA	1:U:499:ASN:HA	112.70	0.63
1:S:589:GLN:HA	1:U:499:ASN:HA	1.79	0.63
1:3:499:ASN:HA	1:4:589:GLN:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:589:GLN:HA	1:6:499:ASN:HA	1.80	0.63
1:H:422:PRO:HD3	2:H:901:DC:H4'	1.81	0.63
1:K:400:TYR:OH	1:7:298:ASP:OD2	2.17	0.63
1:B:589:GLN:HA	1:M:499:ASN:HA	132.70	0.63
1:N:589:GLN:HA	1:O:499:ASN:HA	81.60	0.63
1:R:275:TYR:HB3	1:U:473:MET:HE1	1.80	0.63
1:U:589:GLN:HA	1:V:499:ASN:HA	81.60	0.63
1:D:400:TYR:OH	1:E:298:ASP:OD2	2.17	0.63
1:A:473:MET:HE1	1:G:275:TYR:CD2	2.34	0.63
1:K:422:PRO:HD3	2:K:901:DC:H4'	1.81	0.63
1:Y:298:ASP:OD2	1:4:400:TYR:OH	2.17	0.63
1:A:400:TYR:OH	1:J:298:ASP:OD2	63.31	0.63
1:M:298:ASP:OD2	1:N:400:TYR:OH	2.17	0.63
1:N:400:TYR:OH	1:R:298:ASP:OD2	126.61	0.63
1:S:422:PRO:HD3	2:S:901:DC:H4'	1.81	0.63
1:T:275:TYR:HB3	1:V:473:MET:HE1	90.02	0.63
1:1:422:PRO:HD3	2:1:901:DC:H4'	1.81	0.62
1:8:422:PRO:HD3	2:8:901:DC:H4'	1.81	0.62
1:B:422:PRO:HD3	2:B:901:DC:H4'	1.81	0.62
1:C:400:TYR:OH	1:D:298:ASP:OD2	2.17	0.62
1:J:473:MET:HE1	1:K:275:TYR:CD2	55.62	0.62
1:P:422:PRO:HD3	2:P:901:DC:H4'	1.81	0.62
1:J:298:ASP:OD2	1:X:400:TYR:OH	152.19	0.62
1:5:531:ASP:OD1	1:5:569:LYS:NZ	2.30	0.62
1:3:298:ASP:OD2	1:8:400:TYR:OH	2.17	0.62
1:B:531:ASP:OD1	1:B:569:LYS:NZ	2.30	0.62
1:K:298:ASP:OD2	1:L:400:TYR:OH	2.17	0.62
1:O:298:ASP:OD2	1:P:400:TYR:OH	2.17	0.62
1:R:473:MET:HE1	1:S:275:TYR:HB3	1.81	0.62
1:T:422:PRO:HD3	2:T:901:DC:H4'	1.81	0.62
1:U:422:PRO:HD3	2:U:901:DC:H4'	1.81	0.62
1:F:298:ASP:OD2	1:X:400:TYR:OH	126.37	0.62
1:5:422:PRO:HD3	2:5:901:DC:H4'	1.81	0.62
1:C:422:PRO:HD3	2:C:901:DC:H4'	1.81	0.62
1:F:275:TYR:HB3	1:Q:473:MET:HE1	1.81	0.62
1:I:298:ASP:OD2	1:J:400:TYR:OH	2.16	0.62
1:O:422:PRO:HD3	2:O:901:DC:H4'	1.81	0.62
1:V:422:PRO:HD3	2:V:901:DC:H4'	1.81	0.62
1:Y:422:PRO:HD3	2:Y:901:DC:H4'	1.81	0.62
1:3:422:PRO:HD3	2:3:901:DC:H4'	1.81	0.62
1:5:473:MET:HE1	1:6:275:TYR:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASP:OD2	1:Z:400:TYR:OH	124.20	0.62
1:G:422:PRO:HD3	2:G:901:DC:H4'	1.81	0.62
1:L:422:PRO:HD3	2:L:901:DC:H4'	1.81	0.62
1:M:400:TYR:OH	1:N:298:ASP:OD2	71.96	0.62
1:Q:422:PRO:HD3	2:Q:901:DC:H4'	1.81	0.62
1:1:531:ASP:OD1	1:1:569:LYS:NZ	2.30	0.62
1:A:422:PRO:HD3	2:A:901:DC:H4'	1.81	0.62
1:1:473:MET:HE1	1:2:275:TYR:HB3	1.81	0.62
1:E:275:TYR:CD2	1:V:473:MET:HE1	154.33	0.62
1:I:422:PRO:HD3	2:I:901:DC:H4'	1.81	0.62
1:M:298:ASP:OD2	1:S:400:TYR:OH	112.48	0.62
1:N:422:PRO:HD3	2:N:901:DC:H4'	1.81	0.62
1:B:298:ASP:OD2	1:O:400:TYR:OH	152.19	0.62
1:T:499:ASN:HA	1:V:589:GLN:HA	131.13	0.62
1:X:422:PRO:HD3	2:X:901:DC:H4'	1.81	0.62
1:F:400:TYR:OH	1:Z:298:ASP:OD2	126.05	0.62
1:H:400:TYR:OH	1:Z:298:ASP:OD2	2.17	0.62
1:4:422:PRO:HD3	2:4:901:DC:H4'	1.81	0.62
1:P:400:TYR:OH	1:6:298:ASP:OD2	146.79	0.62
1:D:275:TYR:HB3	1:T:473:MET:HE1	127.71	0.62
1:E:298:ASP:OD2	1:H:400:TYR:OH	144.48	0.62
1:E:275:TYR:CD2	1:F:473:MET:HE1	2.35	0.62
1:A:400:TYR:OH	1:B:298:ASP:OD2	2.18	0.62
1:K:400:TYR:OH	1:W:298:ASP:OD2	161.82	0.62
1:J:400:TYR:OH	1:L:298:ASP:OD2	71.64	0.62
1:L:400:TYR:OH	1:N:298:ASP:OD2	144.49	0.62
1:Q:298:ASP:OD2	1:S:400:TYR:OH	2.17	0.62
1:V:298:ASP:OD2	1:W:400:TYR:OH	71.96	0.62
1:Z:400:TYR:OH	1:4:298:ASP:OD2	71.64	0.62
1:U:400:TYR:OH	1:5:298:ASP:OD2	181.61	0.62
1:E:422:PRO:HD3	2:E:901:DC:H4'	1.81	0.62
1:F:298:ASP:OD2	1:G:400:TYR:OH	2.18	0.62
1:R:499:ASN:HA	1:U:589:GLN:HA	1.79	0.62
1:7:422:PRO:HD3	2:7:901:DC:H4'	1.81	0.62
1:E:400:TYR:OH	1:U:298:ASP:OD2	117.36	0.62
1:Z:422:PRO:HD3	2:Z:901:DC:H4'	1.81	0.62
1:2:298:ASP:OD2	1:3:400:TYR:OH	2.17	0.61
1:A:275:TYR:CD2	1:I:473:MET:HE1	2.35	0.61
1:A:275:TYR:CD2	1:K:473:MET:HE1	110.22	0.61
1:J:422:PRO:HD3	2:J:901:DC:H4'	1.81	0.61
1:N:473:MET:HE1	1:P:275:TYR:CD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:298:ASP:OD2	1:2:400:TYR:OH	157.22	0.61
1:D:298:ASP:OD2	1:O:400:TYR:OH	110.39	0.61
1:F:422:PRO:HD3	2:F:901:DC:H4'	1.81	0.61
1:H:298:ASP:OD2	1:I:400:TYR:OH	2.18	0.61
1:I:275:TYR:HB3	1:K:473:MET:HE1	90.02	0.61
1:Q:473:MET:HE1	1:R:275:TYR:CD2	55.62	0.61
1:G:298:ASP:OD2	1:1:400:TYR:OH	146.78	0.61
1:B:406:LEU:HD21	1:B:412:PHE:HB2	1.83	0.61
1:G:400:TYR:OH	1:K:298:ASP:OD2	126.62	0.61
1:L:406:LEU:HD21	1:L:412:PHE:HB2	1.83	0.61
1:R:422:PRO:HD3	2:R:901:DC:H4'	1.81	0.61
1:T:473:MET:HE1	1:U:275:TYR:HB3	57.18	0.61
1:U:473:MET:HE1	1:V:275:TYR:CD2	55.63	0.61
1:C:406:LEU:HD21	1:C:412:PHE:HB2	1.83	0.61
1:D:422:PRO:HD3	2:D:901:DC:H4'	1.81	0.61
1:J:406:LEU:HD21	1:J:412:PHE:HB2	1.83	0.61
1:M:406:LEU:HD21	1:M:412:PHE:HB2	1.83	0.61
1:D:400:TYR:OH	1:S:298:ASP:OD2	97.40	0.61
1:I:298:ASP:OD2	1:T:400:TYR:OH	180.73	0.61
1:T:406:LEU:HD21	1:T:412:PHE:HB2	1.83	0.61
1:W:406:LEU:HD21	1:W:412:PHE:HB2	1.83	0.61
1:Z:406:LEU:HD21	1:Z:412:PHE:HB2	1.83	0.61
1:A:473:MET:HE1	1:8:275:TYR:CD2	169.73	0.61
1:F:400:TYR:OH	1:R:298:ASP:OD2	2.17	0.61
1:G:298:ASP:OD2	1:W:400:TYR:OH	2.17	0.61
1:Q:406:LEU:HD21	1:Q:412:PHE:HB2	1.83	0.61
1:T:298:ASP:OD2	1:6:400:TYR:OH	177.59	0.61
1:W:275:TYR:CD2	1:Y:473:MET:HE1	53.04	0.61
1:1:406:LEU:HD21	1:1:412:PHE:HB2	1.83	0.61
1:B:473:MET:HE1	1:M:275:TYR:CD2	137.55	0.61
1:B:473:MET:HE1	1:J:275:TYR:CD2	2.35	0.61
1:O:473:MET:HE1	1:P:275:TYR:CD2	58.55	0.61
1:B:400:TYR:OH	1:C:298:ASP:OD2	2.18	0.61
1:C:298:ASP:OD2	1:M:400:TYR:OH	71.64	0.61
1:M:422:PRO:HD3	2:M:901:DC:H4'	1.81	0.61
1:P:298:ASP:OD2	1:Q:400:TYR:OH	2.18	0.61
1:W:422:PRO:HD3	2:W:901:DC:H4'	1.81	0.61
1:5:400:TYR:OH	1:8:298:ASP:OD2	2.18	0.61
1:R:406:LEU:HD21	1:R:412:PHE:HB2	1.83	0.61
1:B:400:TYR:OH	1:L:298:ASP:OD2	28.09	0.61
1:F:406:LEU:HD21	1:F:412:PHE:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:406:LEU:HD21	1:N:412:PHE:HB2	1.83	0.61
1:W:473:MET:HE1	1:Y:275:TYR:CD2	2.36	0.61
1:X:298:ASP:OD2	1:Y:400:TYR:OH	2.18	0.61
1:2:422:PRO:HD3	2:2:901:DC:H4'	1.81	0.61
1:4:406:LEU:HD21	1:4:412:PHE:HB2	1.83	0.61
1:G:406:LEU:HD21	1:G:412:PHE:HB2	1.83	0.61
1:T:400:TYR:OH	1:Y:298:ASP:OD2	151.67	0.61
1:Y:406:LEU:HD21	1:Y:412:PHE:HB2	1.83	0.61
1:6:422:PRO:HD3	2:6:901:DC:H4'	1.81	0.60
1:P:406:LEU:HD21	1:P:412:PHE:HB2	1.83	0.60
1:R:400:TYR:OH	1:X:298:ASP:OD2	62.32	0.60
1:A:406:LEU:HD21	1:A:412:PHE:HB2	1.83	0.60
1:B:275:TYR:CD2	1:L:473:MET:HE1	2.36	0.60
1:U:406:LEU:HD21	1:U:412:PHE:HB2	1.83	0.60
1:V:406:LEU:HD21	1:V:412:PHE:HB2	1.83	0.60
1:B:275:TYR:CD2	1:C:473:MET:HE1	58.58	0.60
1:R:400:TYR:OH	1:V:298:ASP:OD2	2.18	0.60
1:V:400:TYR:OH	1:W:298:ASP:OD2	2.17	0.60
1:3:275:TYR:HB3	1:4:473:MET:HE1	1.84	0.60
1:G:275:TYR:HB3	1:H:473:MET:HE1	56.60	0.60
1:H:499:ASN:OD1	1:H:500:ASN:N	2.35	0.60
1:N:473:MET:HE1	1:O:275:TYR:HB3	56.61	0.60
1:Q:298:ASP:OD2	1:Y:400:TYR:OH	118.26	0.60
1:S:499:ASN:OD1	1:S:500:ASN:N	2.35	0.60
1:U:499:ASN:OD1	1:U:500:ASN:N	2.35	0.60
1:V:499:ASN:OD1	1:V:500:ASN:N	2.35	0.60
1:2:406:LEU:HD21	1:2:412:PHE:HB2	1.83	0.60
1:3:556:ASP:OD1	1:3:557:TYR:N	2.35	0.60
1:5:406:LEU:HD21	1:5:412:PHE:HB2	1.83	0.60
1:L:499:ASN:OD1	1:L:500:ASN:N	2.35	0.60
1:O:556:ASP:OD1	1:O:557:TYR:N	2.35	0.60
1:P:499:ASN:OD1	1:P:500:ASN:N	2.35	0.60
1:R:556:ASP:OD1	1:R:557:TYR:N	2.35	0.60
1:Y:556:ASP:OD1	1:Y:557:TYR:N	2.35	0.60
1:Z:473:MET:HE1	1:1:275:TYR:HB3	103.00	0.60
1:D:406:LEU:HD21	1:D:412:PHE:HB2	1.83	0.60
1:L:473:MET:HE1	1:T:275:TYR:HB3	216.69	0.60
1:Y:499:ASN:OD1	1:Y:500:ASN:N	2.35	0.60
1:1:499:ASN:OD1	1:1:500:ASN:N	2.35	0.60
1:8:499:ASN:OD1	1:8:500:ASN:N	2.35	0.60
1:A:657:PRO:HD2	1:J:678:THR:HG21	83.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:406:LEU:HD21	1:O:412:PHE:HB2	1.83	0.60
1:C:400:TYR:OH	1:S:298:ASP:OD2	126.37	0.60
1:X:406:LEU:HD21	1:X:412:PHE:HB2	1.83	0.60
1:2:499:ASN:OD1	1:2:500:ASN:N	2.35	0.60
1:7:406:LEU:HD21	1:7:412:PHE:HB2	1.83	0.60
1:C:275:TYR:CD2	1:M:473:MET:HE1	2.36	0.60
1:G:499:ASN:OD1	1:G:500:ASN:N	2.35	0.60
1:I:499:ASN:OD1	1:I:500:ASN:N	2.35	0.60
1:J:473:MET:HE1	1:L:275:TYR:CD2	2.36	0.60
1:K:499:ASN:OD1	1:K:500:ASN:N	2.35	0.60
1:T:499:ASN:OD1	1:T:500:ASN:N	2.35	0.60
1:Z:499:ASN:OD1	1:Z:500:ASN:N	2.35	0.60
1:4:499:ASN:OD1	1:4:500:ASN:N	2.35	0.60
1:7:556:ASP:OD1	1:7:557:TYR:N	2.35	0.60
1:B:499:ASN:OD1	1:B:500:ASN:N	2.35	0.60
1:D:499:ASN:OD1	1:D:500:ASN:N	2.35	0.60
1:I:406:LEU:HD21	1:I:412:PHE:HB2	1.83	0.60
1:N:499:ASN:OD1	1:N:500:ASN:N	2.35	0.60
1:W:499:ASN:OD1	1:W:500:ASN:N	2.35	0.60
1:X:499:ASN:OD1	1:X:500:ASN:N	2.35	0.60
1:X:556:ASP:OD1	1:X:557:TYR:N	2.35	0.60
1:3:406:LEU:HD21	1:3:412:PHE:HB2	1.83	0.59
1:E:406:LEU:HD21	1:E:412:PHE:HB2	1.83	0.59
1:E:556:ASP:OD1	1:E:557:TYR:N	2.35	0.59
1:K:406:LEU:HD21	1:K:412:PHE:HB2	1.83	0.59
1:M:678:THR:HG21	1:N:657:PRO:HD2	1.84	0.59
1:N:556:ASP:OD1	1:N:557:TYR:N	2.35	0.59
1:O:499:ASN:OD1	1:O:500:ASN:N	2.35	0.59
1:Q:499:ASN:OD1	1:Q:500:ASN:N	2.35	0.59
1:S:556:ASP:OD1	1:S:557:TYR:N	2.35	0.59
1:U:556:ASP:OD1	1:U:557:TYR:N	2.35	0.59
1:H:657:PRO:HD2	1:Z:678:THR:HG21	1.84	0.59
1:2:678:THR:HG21	1:3:657:PRO:HD2	1.84	0.59
1:4:556:ASP:OD1	1:4:557:TYR:N	2.35	0.59
1:5:499:ASN:OD1	1:5:500:ASN:N	2.35	0.59
1:6:406:LEU:HD21	1:6:412:PHE:HB2	1.83	0.59
1:6:499:ASN:OD1	1:6:500:ASN:N	2.35	0.59
1:A:499:ASN:OD1	1:A:500:ASN:N	2.35	0.59
1:B:556:ASP:OD1	1:B:557:TYR:N	2.35	0.59
1:E:499:ASN:OD1	1:E:500:ASN:N	2.35	0.59
1:E:678:THR:HG21	1:H:657:PRO:HD2	132.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:657:PRO:HD2	1:K:678:THR:HG21	165.88	0.59
1:K:657:PRO:HD2	1:W:678:THR:HG21	180.60	0.59
1:R:657:PRO:HD2	1:V:678:THR:HG21	1.84	0.59
1:T:657:PRO:HD2	1:Y:678:THR:HG21	131.28	0.59
1:S:473:MET:HE1	1:U:275:TYR:CD2	2.36	0.59
1:W:473:MET:HE1	1:X:275:TYR:CD2	55.62	0.59
1:8:406:LEU:HD21	1:8:412:PHE:HB2	1.83	0.59
1:D:678:THR:HG21	1:O:657:PRO:HD2	115.10	0.59
1:F:499:ASN:OD1	1:F:500:ASN:N	2.35	0.59
1:H:406:LEU:HD21	1:H:412:PHE:HB2	1.83	0.59
1:H:678:THR:HG21	1:I:657:PRO:HD2	1.85	0.59
1:L:556:ASP:OD1	1:L:557:TYR:N	2.35	0.59
1:C:473:MET:HE1	1:O:275:TYR:CD2	169.46	0.59
1:M:678:THR:HG21	1:S:657:PRO:HD2	119.32	0.59
1:V:275:TYR:HB3	1:X:473:MET:HE1	1.84	0.59
1:E:473:MET:HE1	1:X:275:TYR:CD2	169.99	0.59
1:T:678:THR:HG21	1:6:657:PRO:HD2	179.82	0.59
1:D:275:TYR:HB3	1:P:473:MET:HE1	1.84	0.59
1:S:406:LEU:HD21	1:S:412:PHE:HB2	1.83	0.59
1:T:556:ASP:OD1	1:T:557:TYR:N	2.35	0.59
1:X:473:MET:HE1	1:Y:275:TYR:HB3	57.20	0.59
1:H:275:TYR:HB3	1:Y:473:MET:HE1	1.84	0.59
1:Z:556:ASP:OD1	1:Z:557:TYR:N	2.35	0.59
1:B:657:PRO:HD2	1:C:678:THR:HG21	1.84	0.59
1:B:657:PRO:HD2	1:L:678:THR:HG21	78.37	0.59
1:C:499:ASN:OD1	1:C:500:ASN:N	2.35	0.59
1:F:657:PRO:HD2	1:R:678:THR:HG21	1.84	0.59
1:G:556:ASP:OD1	1:G:557:TYR:N	2.35	0.59
1:H:556:ASP:OD1	1:H:557:TYR:N	2.35	0.59
1:I:678:THR:HG21	1:T:657:PRO:HD2	186.99	0.59
1:G:678:THR:HG21	1:1:657:PRO:HD2	173.74	0.59
1:3:678:THR:HG21	1:8:657:PRO:HD2	1.84	0.59
1:F:678:THR:HG21	1:X:657:PRO:HD2	125.00	0.59
1:J:499:ASN:OD1	1:J:500:ASN:N	2.35	0.59
1:J:678:THR:HG21	1:X:657:PRO:HD2	138.98	0.59
1:K:678:THR:HG21	1:L:657:PRO:HD2	1.85	0.59
1:C:657:PRO:HD2	1:S:678:THR:HG21	113.78	0.59
1:Z:275:TYR:CD2	1:2:473:MET:HE1	96.71	0.59
1:Z:473:MET:HE1	1:4:275:TYR:CD2	2.37	0.59
1:7:499:ASN:OD1	1:7:500:ASN:N	2.35	0.59
1:P:556:ASP:OD1	1:P:557:TYR:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:499:ASN:OD1	1:R:500:ASN:N	2.35	0.59
1:A:678:THR:HG21	1:E:657:PRO:HD2	1.85	0.59
1:C:657:PRO:HD2	1:D:678:THR:HG21	1.85	0.59
1:F:678:THR:HG21	1:G:657:PRO:HD2	1.84	0.59
1:M:473:MET:HE1	1:N:275:TYR:CD2	58.58	0.59
1:O:678:THR:HG21	1:P:657:PRO:HD2	1.84	0.59
1:Q:381:LEU:HD21	1:S:439:PRO:HB3	103.68	0.59
1:D:657:PRO:HD2	1:S:678:THR:HG21	103.28	0.59
1:V:657:PRO:HD2	1:W:678:THR:HG21	1.84	0.59
1:H:439:PRO:HB3	1:W:381:LEU:HD21	1.85	0.59
1:1:439:PRO:HB3	1:2:381:LEU:HD21	1.85	0.59
1:3:499:ASN:OD1	1:3:500:ASN:N	2.35	0.59
1:D:381:LEU:HD21	1:T:439:PRO:HB3	122.16	0.59
1:F:275:TYR:CD2	1:G:473:MET:HE1	104.16	0.59
1:I:473:MET:HE1	1:J:275:TYR:CD2	58.55	0.59
1:M:499:ASN:OD1	1:M:500:ASN:N	2.35	0.59
1:Q:678:THR:HG21	1:Y:657:PRO:HD2	160.70	0.59
1:V:657:PRO:HD2	1:1:678:THR:HG21	168.97	0.59
1:5:381:LEU:HD21	1:7:439:PRO:HB3	1.85	0.59
1:A:556:ASP:OD1	1:A:557:TYR:N	2.35	0.59
1:F:556:ASP:OD1	1:F:557:TYR:N	2.35	0.59
1:G:473:MET:HE1	1:I:275:TYR:CD2	2.38	0.59
1:J:556:ASP:OD1	1:J:557:TYR:N	2.35	0.59
1:M:275:TYR:HB3	1:O:473:MET:HE1	90.03	0.59
1:P:657:PRO:HD2	1:6:678:THR:HG21	173.74	0.59
1:T:678:THR:HG21	1:U:657:PRO:HD2	1.85	0.59
1:V:714:ASP:HB3	1:V:726:PRO:HG2	1.85	0.59
1:W:439:PRO:HB3	1:Y:381:LEU:HD21	1.85	0.59
1:U:678:THR:HG21	1:2:657:PRO:HD2	178.21	0.58
1:2:714:ASP:HB3	1:2:726:PRO:HG2	1.85	0.58
1:3:511:TYR:HD2	1:3:520:VAL:HG22	1.68	0.58
1:A:657:PRO:HD2	1:B:678:THR:HG21	1.84	0.58
1:B:511:TYR:HD2	1:B:520:VAL:HG22	1.69	0.58
1:C:556:ASP:OD1	1:C:557:TYR:N	2.35	0.58
1:H:511:TYR:HD2	1:H:520:VAL:HG22	1.68	0.58
1:I:511:TYR:HD2	1:I:520:VAL:HG22	1.68	0.58
1:I:632:HIS:CE1	3:I:902:DA:H8	2.22	0.58
1:K:511:TYR:HD2	1:K:520:VAL:HG22	1.68	0.58
1:N:439:PRO:HB3	1:O:381:LEU:HD21	50.96	0.58
1:O:439:PRO:HB3	1:P:381:LEU:HD21	57.06	0.58
1:E:439:PRO:HB3	1:Q:381:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:381:LEU:HD21	1:Q:439:PRO:HB3	1.85	0.58
1:Q:439:PRO:HB3	1:R:381:LEU:HD21	50.96	0.58
1:T:511:TYR:HD2	1:T:520:VAL:HG22	1.68	0.58
1:X:511:TYR:HD2	1:X:520:VAL:HG22	1.68	0.58
1:Y:511:TYR:HD2	1:Y:520:VAL:HG22	1.68	0.58
1:X:678:THR:HG21	1:Y:657:PRO:HD2	1.84	0.58
1:I:511:TYR:HD2	1:I:520:VAL:HG22	1.68	0.58
1:Z:275:TYR:HB3	1:3:473:MET:HE1	1.85	0.58
1:5:657:PRO:HD2	1:8:678:THR:HG21	1.84	0.58
1:A:632:HIS:CE1	3:A:902:DA:H8	2.22	0.58
1:A:714:ASP:HB3	1:A:726:PRO:HG2	1.85	0.58
1:C:381:LEU:HD21	1:P:439:PRO:HB3	49.16	0.58
1:C:714:ASP:HB3	1:C:726:PRO:HG2	1.86	0.58
1:D:714:ASP:HB3	1:D:726:PRO:HG2	1.85	0.58
1:G:511:TYR:HD2	1:G:520:VAL:HG22	1.68	0.58
1:G:381:LEU:HD21	1:H:439:PRO:HB3	50.96	0.58
1:I:556:ASP:OD1	1:I:557:TYR:N	2.35	0.58
1:J:657:PRO:HD2	1:L:678:THR:HG21	97.85	0.58
1:L:632:HIS:CE1	3:L:902:DA:H8	2.21	0.58
1:N:714:ASP:HB3	1:N:726:PRO:HG2	1.85	0.58
1:O:511:TYR:HD2	1:O:520:VAL:HG22	1.68	0.58
1:O:632:HIS:CE1	3:O:902:DA:H8	2.21	0.58
1:P:678:THR:HG21	1:Q:657:PRO:HD2	1.84	0.58
1:R:511:TYR:HD2	1:R:520:VAL:HG22	1.68	0.58
1:R:632:HIS:CE1	3:R:902:DA:H8	2.22	0.58
1:R:657:PRO:HD2	1:X:678:THR:HG21	85.59	0.58
1:T:632:HIS:CE1	3:T:902:DA:H8	2.22	0.58
1:Y:714:ASP:HB3	1:Y:726:PRO:HG2	1.85	0.58
1:F:657:PRO:HD2	1:Z:678:THR:HG21	126.59	0.58
1:3:381:LEU:HD21	1:4:439:PRO:HB3	1.85	0.58
1:U:657:PRO:HD2	1:5:678:THR:HG21	191.25	0.58
1:5:439:PRO:HB3	1:6:381:LEU:HD21	1.85	0.58
1:D:632:HIS:CE1	3:D:902:DA:H8	2.22	0.58
1:E:632:HIS:CE1	3:E:902:DA:H8	2.22	0.58
1:E:714:ASP:HB3	1:E:726:PRO:HG2	1.86	0.58
1:A:431:GLN:HE22	1:G:354:PRO:HB3	1.68	0.58
1:G:632:HIS:CE1	3:G:902:DA:H8	2.22	0.58
1:I:714:ASP:HB3	1:I:726:PRO:HG2	1.86	0.58
1:B:439:PRO:HB3	1:J:381:LEU:HD21	1.85	0.58
1:J:511:TYR:HD2	1:J:520:VAL:HG22	1.68	0.58
1:I:381:LEU:HD21	1:K:439:PRO:HB3	81.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:PRO:HB3	1:M:381:LEU:HD21	135.98	0.58
1:M:556:ASP:OD1	1:M:557:TYR:N	2.35	0.58
1:M:714:ASP:HB3	1:M:726:PRO:HG2	1.86	0.58
1:N:511:TYR:HD2	1:N:520:VAL:HG22	1.68	0.58
1:B:678:THR:HG21	1:O:657:PRO:HD2	138.98	0.58
1:Q:678:THR:HG21	1:S:657:PRO:HD2	1.84	0.58
1:Q:275:TYR:CD2	1:S:473:MET:HE1	104.21	0.58
1:R:381:LEU:HD21	1:U:439:PRO:HB3	1.85	0.58
1:U:511:TYR:HD2	1:U:520:VAL:HG22	1.68	0.58
1:V:511:TYR:HD2	1:V:520:VAL:HG22	1.68	0.58
1:X:714:ASP:HB3	1:X:726:PRO:HG2	1.86	0.58
1:Z:714:ASP:HB3	1:Z:726:PRO:HG2	1.86	0.58
1:2:632:HIS:CE1	3:2:902:DA:H8	2.22	0.58
1:7:632:HIS:CE1	3:7:902:DA:H8	2.22	0.58
1:K:657:PRO:HD2	1:7:678:THR:HG21	1.84	0.58
1:8:511:TYR:HD2	1:8:520:VAL:HG22	1.68	0.58
1:C:511:TYR:HD2	1:C:520:VAL:HG22	1.68	0.58
1:C:632:HIS:CE1	3:C:902:DA:H8	2.22	0.58
1:D:473:MET:HE1	1:L:275:TYR:CD2	139.05	0.58
1:D:657:PRO:HD2	1:E:678:THR:HG21	1.84	0.58
1:K:275:TYR:CD2	1:8:473:MET:HE1	2.38	0.58
1:L:657:PRO:HD2	1:N:678:THR:HG21	132.66	0.58
1:M:511:TYR:HD2	1:M:520:VAL:HG22	1.68	0.58
1:Q:511:TYR:HD2	1:Q:520:VAL:HG22	1.69	0.58
1:T:381:LEU:HD21	1:V:439:PRO:HB3	81.34	0.58
1:V:632:HIS:CE1	3:V:902:DA:H8	2.22	0.58
1:W:381:LEU:HD21	1:Y:439:PRO:HB3	54.21	0.58
1:W:632:HIS:CE1	3:W:902:DA:H8	2.22	0.58
1:Y:678:THR:HG21	1:4:657:PRO:HD2	1.84	0.58
1:Z:657:PRO:HD2	1:4:678:THR:HG21	97.85	0.58
1:4:511:TYR:HD2	1:4:520:VAL:HG22	1.69	0.58
1:6:632:HIS:CE1	3:6:902:DA:H8	2.22	0.58
1:7:714:ASP:HB3	1:7:726:PRO:HG2	1.86	0.58
1:C:381:LEU:HD21	1:M:439:PRO:HB3	1.85	0.58
1:O:678:THR:HG21	1:7:657:PRO:HD2	170.78	0.58
1:P:511:TYR:HD2	1:P:520:VAL:HG22	1.68	0.58
1:U:632:HIS:CE1	3:U:902:DA:H8	2.22	0.58
1:E:381:LEU:HD21	1:V:439:PRO:HB3	149.81	0.58
1:V:556:ASP:OD1	1:V:557:TYR:N	2.35	0.58
1:H:473:MET:HE1	1:W:275:TYR:HB3	1.85	0.58
1:W:511:TYR:HD2	1:W:520:VAL:HG22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:714:ASP:HB3	1:W:726:PRO:HG2	1.86	0.58
1:2:511:TYR:HD2	1:2:520:VAL:HG22	1.69	0.58
1:5:275:TYR:CD2	1:7:473:MET:HE1	2.39	0.58
1:K:275:TYR:HB3	1:8:473:MET:HE1	1.85	0.58
1:E:473:MET:HE1	1:Q:275:TYR:CD2	2.39	0.58
1:F:632:HIS:CE1	3:F:902:DA:H8	2.22	0.58
1:H:632:HIS:CE1	3:H:902:DA:H8	2.22	0.58
1:J:714:ASP:HB3	1:J:726:PRO:HG2	1.86	0.58
1:K:556:ASP:OD1	1:K:557:TYR:N	2.35	0.58
1:L:714:ASP:HB3	1:L:726:PRO:HG2	1.86	0.58
1:N:657:PRO:HD2	1:R:678:THR:HG21	165.88	0.58
1:S:632:HIS:CE1	3:S:902:DA:H8	2.22	0.58
1:5:714:ASP:HB3	1:5:726:PRO:HG2	1.86	0.58
1:D:511:TYR:HD2	1:D:520:VAL:HG22	1.68	0.58
1:K:714:ASP:HB3	1:K:726:PRO:HG2	1.85	0.58
1:J:439:PRO:HB3	1:L:381:LEU:HD21	1.85	0.58
1:D:439:PRO:HB3	1:N:381:LEU:HD21	1.85	0.58
1:Q:714:ASP:HB3	1:Q:726:PRO:HG2	1.86	0.58
1:S:714:ASP:HB3	1:S:726:PRO:HG2	1.86	0.58
1:E:657:PRO:HD2	1:U:678:THR:HG21	159.79	0.58
1:Z:632:HIS:CE1	3:Z:902:DA:H8	2.21	0.58
1:1:714:ASP:HB3	1:1:726:PRO:HG2	1.86	0.58
1:6:473:MET:HE1	1:7:275:TYR:HD2	1.68	0.58
1:6:714:ASP:HB3	1:6:726:PRO:HG2	1.86	0.58
1:8:632:HIS:CE1	3:8:902:DA:H8	2.22	0.58
1:B:632:HIS:CE1	3:B:902:DA:H8	2.21	0.58
1:D:556:ASP:OD1	1:D:557:TYR:N	2.35	0.58
1:E:473:MET:HE1	1:X:275:TYR:HB3	167.77	0.58
1:E:511:TYR:HD2	1:E:520:VAL:HG22	1.68	0.58
1:F:714:ASP:HB3	1:F:726:PRO:HG2	1.85	0.58
1:K:632:HIS:CE1	3:K:902:DA:H8	2.22	0.58
1:L:511:TYR:HD2	1:L:520:VAL:HG22	1.68	0.58
1:O:714:ASP:HB3	1:O:726:PRO:HG2	1.86	0.58
1:S:511:TYR:HD2	1:S:520:VAL:HG22	1.68	0.58
1:V:678:THR:HG21	1:W:657:PRO:HD2	35.19	0.58
1:W:473:MET:HE1	1:X:275:TYR:HB3	56.61	0.58
1:6:439:PRO:HB3	1:7:381:LEU:HD21	1.85	0.58
1:7:511:TYR:HD2	1:7:520:VAL:HG22	1.68	0.58
1:8:556:ASP:OD1	1:8:557:TYR:N	2.35	0.58
1:B:714:ASP:HB3	1:B:726:PRO:HG2	1.86	0.58
1:F:275:TYR:HB3	1:G:473:MET:HE1	104.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:714:ASP:HB3	1:H:726:PRO:HG2	1.86	0.58
1:A:381:LEU:HD21	1:K:439:PRO:HB3	103.24	0.58
1:P:632:HIS:CE1	3:P:902:DA:H8	2.22	0.58
1:T:714:ASP:HB3	1:T:726:PRO:HG2	1.85	0.58
1:X:632:HIS:CE1	3:X:902:DA:H8	2.22	0.58
1:Y:632:HIS:CE1	3:Y:902:DA:H8	2.22	0.58
1:Z:511:TYR:HD2	1:Z:520:VAL:HG22	1.68	0.58
1:1:473:MET:HE1	1:2:275:TYR:CD2	2.39	0.58
1:1:556:ASP:OD1	1:1:557:TYR:N	2.35	0.58
1:A:511:TYR:HD2	1:A:520:VAL:HG22	1.68	0.58
1:E:381:LEU:HD21	1:F:439:PRO:HB3	1.85	0.58
1:I:473:MET:HE1	1:J:275:TYR:HB3	57.22	0.58
1:M:657:PRO:HD2	1:N:678:THR:HG21	35.19	0.58
1:S:439:PRO:HB3	1:U:381:LEU:HD21	1.85	0.58
1:D:275:TYR:CD2	1:T:473:MET:HE1	130.11	0.58
1:A:678:THR:HG21	1:Z:657:PRO:HD2	113.87	0.58
1:B:381:LEU:HD21	1:C:439:PRO:HB3	57.06	0.57
1:G:714:ASP:HB3	1:G:726:PRO:HG2	1.86	0.57
1:A:275:TYR:HB3	1:I:473:MET:HE1	1.86	0.57
1:J:632:HIS:CE1	3:J:902:DA:H8	2.21	0.57
1:C:275:TYR:HB3	1:P:473:MET:HE1	54.11	0.57
1:P:714:ASP:HB3	1:P:726:PRO:HG2	1.85	0.57
1:Q:632:HIS:CE1	3:Q:902:DA:H8	2.22	0.57
1:U:439:PRO:HB3	1:V:381:LEU:HD21	50.97	0.57
1:3:275:TYR:CD2	1:4:473:MET:HE1	2.39	0.57
1:4:714:ASP:HB3	1:4:726:PRO:HG2	1.86	0.57
1:5:632:HIS:CE1	3:5:902:DA:H8	2.22	0.57
1:D:381:LEU:HD21	1:P:439:PRO:HB3	1.85	0.57
1:G:678:THR:HG21	1:W:657:PRO:HD2	1.84	0.57
1:H:473:MET:HE1	1:W:275:TYR:CD2	2.38	0.57
1:K:381:LEU:HD21	1:8:439:PRO:HB3	1.85	0.57
1:B:381:LEU:HD21	1:L:439:PRO:HB3	1.85	0.57
1:C:678:THR:HG21	1:M:657:PRO:HD2	97.85	0.57
1:N:473:MET:HE1	1:O:275:TYR:CD2	55.62	0.57
1:Z:275:TYR:CD2	1:3:473:MET:HE1	2.39	0.57
1:A:431:GLN:NE2	1:G:354:PRO:HB3	2.20	0.57
1:C:275:TYR:CD2	1:P:473:MET:HE1	53.39	0.57
1:8:714:ASP:HB3	1:8:726:PRO:HG2	1.85	0.57
1:A:464:LEU:HD23	1:G:554:ASN:HB3	1.86	0.57
1:H:381:LEU:HD21	1:Y:439:PRO:HB3	1.85	0.57
1:M:632:HIS:CE1	3:M:902:DA:H8	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:275:TYR:CD2	1:O:473:MET:HE1	88.58	0.57
1:Q:556:ASP:OD1	1:Q:557:TYR:N	2.35	0.57
1:3:342:THR:HG22	1:3:407:ARG:HG3	1.87	0.57
1:4:632:HIS:CE1	3:4:902:DA:H8	2.22	0.57
1:5:342:THR:HG22	1:5:407:ARG:HG3	1.87	0.57
1:A:342:THR:HG22	1:A:407:ARG:HG3	1.87	0.57
1:D:275:TYR:CD2	1:P:473:MET:HE1	2.39	0.57
1:I:342:THR:HG22	1:I:407:ARG:HG3	1.87	0.57
1:I:678:THR:HG21	1:J:657:PRO:HD2	1.85	0.57
1:O:342:THR:HG22	1:O:407:ARG:HG3	1.87	0.57
1:Q:342:THR:HG22	1:Q:407:ARG:HG3	1.87	0.57
1:R:439:PRO:HB3	1:S:381:LEU:HD21	1.85	0.57
1:1:342:THR:HG22	1:1:407:ARG:HG3	1.87	0.57
1:5:275:TYR:HB3	1:7:473:MET:HE1	1.85	0.57
1:A:439:PRO:HB3	1:8:381:LEU:HD21	165.19	0.57
1:A:439:PRO:HB3	1:G:381:LEU:HD21	1.87	0.57
1:E:346:PHE:HZ	1:E:398:LEU:HD22	1.70	0.57
1:F:439:PRO:HB3	1:H:381:LEU:HD21	133.92	0.57
1:G:342:THR:HG22	1:G:407:ARG:HG3	1.87	0.57
1:G:439:PRO:HB3	1:I:381:LEU:HD21	1.87	0.57
1:N:632:HIS:CE1	3:N:902:DA:H8	2.22	0.57
1:O:346:PHE:HZ	1:O:398:LEU:HD22	1.70	0.57
1:R:714:ASP:HB3	1:R:726:PRO:HG2	1.86	0.57
1:U:307:TRP:O	1:U:426:SER:OG	2.22	0.57
1:W:556:ASP:OD1	1:W:557:TYR:N	2.35	0.57
1:1:431:GLN:HE22	1:2:354:PRO:HB3	1.69	0.57
1:1:632:HIS:CE1	3:1:902:DA:H8	2.21	0.57
1:5:346:PHE:HZ	1:5:398:LEU:HD22	1.70	0.57
1:J:439:PRO:HB3	1:K:381:LEU:HD21	50.97	0.57
1:L:307:TRP:O	1:L:426:SER:OG	2.22	0.57
1:L:346:PHE:HZ	1:L:398:LEU:HD22	1.70	0.57
1:M:307:TRP:O	1:M:426:SER:OG	2.22	0.57
1:Q:275:TYR:HB3	1:S:473:MET:HE1	104.80	0.57
1:Q:346:PHE:HZ	1:Q:398:LEU:HD22	1.70	0.57
1:R:342:THR:HG22	1:R:407:ARG:HG3	1.87	0.57
1:T:342:THR:HG22	1:T:407:ARG:HG3	1.87	0.57
1:T:439:PRO:HB3	1:U:381:LEU:HD21	57.04	0.57
1:W:342:THR:HG22	1:W:407:ARG:HG3	1.87	0.57
1:Y:342:THR:HG22	1:Y:407:ARG:HG3	1.87	0.57
1:Z:307:TRP:O	1:Z:426:SER:OG	2.22	0.57
1:Z:346:PHE:HZ	1:Z:398:LEU:HD22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:381:LEU:HD21	1:3:439:PRO:HB3	1.85	0.57
1:Z:439:PRO:HB3	1:1:381:LEU:HD21	100.74	0.57
1:5:511:TYR:HD2	1:5:520:VAL:HG22	1.68	0.57
1:6:307:TRP:O	1:6:426:SER:OG	2.22	0.57
1:6:346:PHE:HZ	1:6:398:LEU:HD22	1.70	0.57
1:A:346:PHE:HZ	1:A:398:LEU:HD22	1.70	0.57
1:C:346:PHE:HZ	1:C:398:LEU:HD22	1.70	0.57
1:D:342:THR:HG22	1:D:407:ARG:HG3	1.87	0.57
1:E:473:MET:HE1	1:Q:275:TYR:HB3	1.85	0.57
1:F:346:PHE:HZ	1:F:398:LEU:HD22	1.70	0.57
1:H:307:TRP:O	1:H:426:SER:OG	2.22	0.57
1:J:307:TRP:O	1:J:426:SER:OG	2.22	0.57
1:K:346:PHE:HZ	1:K:398:LEU:HD22	1.70	0.57
1:N:439:PRO:HB3	1:P:381:LEU:HD21	1.85	0.57
1:R:307:TRP:O	1:R:426:SER:OG	2.22	0.57
1:S:307:TRP:O	1:S:426:SER:OG	2.22	0.57
1:L:439:PRO:HB3	1:T:381:LEU:HD21	208.71	0.57
1:D:354:PRO:HB3	1:T:431:GLN:HE22	115.10	0.57
1:U:342:THR:HG22	1:U:407:ARG:HG3	1.87	0.57
1:W:346:PHE:HZ	1:W:398:LEU:HD22	1.70	0.57
1:X:307:TRP:O	1:X:426:SER:OG	2.22	0.57
1:V:381:LEU:HD21	1:X:439:PRO:HB3	1.85	0.57
1:X:439:PRO:HB3	1:Y:381:LEU:HD21	57.06	0.57
1:3:632:HIS:CE1	3:3:902:DA:H8	2.22	0.57
1:Z:473:MET:HE1	1:4:275:TYR:HB3	1.87	0.57
1:A:307:TRP:O	1:A:426:SER:OG	2.22	0.57
1:B:307:TRP:O	1:B:426:SER:OG	2.22	0.57
1:C:307:TRP:O	1:C:426:SER:OG	2.22	0.57
1:C:342:THR:HG22	1:C:407:ARG:HG3	1.87	0.57
1:D:346:PHE:HZ	1:D:398:LEU:HD22	1.70	0.57
1:E:342:THR:HG22	1:E:407:ARG:HG3	1.87	0.57
1:E:439:PRO:HB3	1:X:381:LEU:HD21	164.84	0.57
1:F:307:TRP:O	1:F:426:SER:OG	2.22	0.57
1:F:342:THR:HG22	1:F:407:ARG:HG3	1.87	0.57
1:H:346:PHE:HZ	1:H:398:LEU:HD22	1.70	0.57
1:G:275:TYR:CD2	1:H:473:MET:HE1	55.62	0.57
1:I:439:PRO:HB3	1:J:381:LEU:HD21	57.05	0.57
1:R:473:MET:HE1	1:S:275:TYR:CD2	2.42	0.57
1:S:342:THR:HG22	1:S:407:ARG:HG3	1.87	0.57
1:T:307:TRP:O	1:T:426:SER:OG	2.22	0.57
1:U:714:ASP:HB3	1:U:726:PRO:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:439:PRO:HB3	1:X:381:LEU:HD21	50.97	0.57
1:Z:439:PRO:HB3	1:4:381:LEU:HD21	1.85	0.57
1:4:307:TRP:O	1:4:426:SER:OG	2.22	0.57
1:7:346:PHE:HZ	1:7:398:LEU:HD22	1.70	0.57
1:B:342:THR:HG22	1:B:407:ARG:HG3	1.87	0.57
1:C:473:MET:HE1	1:O:275:TYR:HB3	168.46	0.57
1:F:381:LEU:HD21	1:G:439:PRO:HB3	103.68	0.57
1:H:275:TYR:CD2	1:Y:473:MET:HE1	2.40	0.57
1:J:342:THR:HG22	1:J:407:ARG:HG3	1.87	0.57
1:M:381:LEU:HD21	1:O:439:PRO:HB3	81.32	0.57
1:M:473:MET:HE1	1:N:275:TYR:HB3	57.25	0.57
1:M:439:PRO:HB3	1:N:381:LEU:HD21	57.06	0.57
1:O:307:TRP:O	1:O:426:SER:OG	2.22	0.57
1:O:431:GLN:HE22	1:P:354:PRO:HB3	48.21	0.57
1:P:342:THR:HG22	1:P:407:ARG:HG3	1.87	0.57
1:Z:342:THR:HG22	1:Z:407:ARG:HG3	1.87	0.57
1:3:714:ASP:HB3	1:3:726:PRO:HG2	1.85	0.56
1:6:342:THR:HG22	1:6:407:ARG:HG3	1.87	0.56
1:7:342:THR:HG22	1:7:407:ARG:HG3	1.87	0.56
1:D:473:MET:HE1	1:L:275:TYR:HB3	138.73	0.56
1:K:342:THR:HG22	1:K:407:ARG:HG3	1.87	0.56
1:M:346:PHE:HZ	1:M:398:LEU:HD22	1.70	0.56
1:M:342:THR:HG22	1:M:407:ARG:HG3	1.87	0.56
1:N:307:TRP:O	1:N:426:SER:OG	2.22	0.56
1:8:342:THR:HG22	1:8:407:ARG:HG3	1.87	0.56
1:I:346:PHE:HZ	1:I:398:LEU:HD22	1.70	0.56
1:D:439:PRO:HB3	1:L:381:LEU:HD21	133.93	0.56
1:V:275:TYR:CD2	1:X:473:MET:HE1	2.39	0.56
1:Z:381:LEU:HD21	1:2:439:PRO:HB3	92.70	0.56
1:3:346:PHE:HZ	1:3:398:LEU:HD22	1.70	0.56
1:6:511:TYR:HD2	1:6:520:VAL:HG22	1.69	0.56
1:F:511:TYR:HD2	1:F:520:VAL:HG22	1.69	0.56
1:G:473:MET:HE1	1:I:275:TYR:HB3	1.86	0.56
1:O:473:MET:HE1	1:P:275:TYR:HB3	57.21	0.56
1:V:346:PHE:HZ	1:V:398:LEU:HD22	1.70	0.56
1:X:473:MET:HE1	1:Y:275:TYR:CD2	58.54	0.56
1:8:307:TRP:O	1:8:426:SER:OG	2.22	0.56
1:P:307:TRP:O	1:P:426:SER:OG	2.22	0.56
1:R:346:PHE:HZ	1:R:398:LEU:HD22	1.70	0.56
1:S:346:PHE:HZ	1:S:398:LEU:HD22	1.70	0.56
1:T:346:PHE:HZ	1:T:398:LEU:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:346:PHE:HZ	1:U:398:LEU:HD22	1.70	0.56
1:1:346:PHE:HZ	1:1:398:LEU:HD22	1.70	0.56
1:2:346:PHE:HZ	1:2:398:LEU:HD22	1.70	0.56
1:5:556:ASP:OD1	1:5:557:TYR:N	2.35	0.56
1:V:342:THR:HG22	1:V:407:ARG:HG3	1.87	0.56
1:I:275:TYR:CD2	1:K:473:MET:HE1	88.57	0.56
1:6:556:ASP:OD1	1:6:557:TYR:N	2.35	0.56
1:8:346:PHE:HZ	1:8:398:LEU:HD22	1.70	0.56
1:G:346:PHE:HZ	1:G:398:LEU:HD22	1.70	0.56
1:H:342:THR:HG22	1:H:407:ARG:HG3	1.87	0.56
1:A:381:LEU:HD21	1:I:439:PRO:HB3	1.86	0.56
1:B:346:PHE:HZ	1:B:398:LEU:HD22	1.70	0.56
1:J:346:PHE:HZ	1:J:398:LEU:HD22	1.70	0.56
1:P:346:PHE:HZ	1:P:398:LEU:HD22	1.70	0.56
1:2:556:ASP:OD1	1:2:557:TYR:N	2.35	0.56
1:4:342:THR:HG22	1:4:407:ARG:HG3	1.87	0.56
1:A:473:MET:HE1	1:G:275:TYR:HB3	1.86	0.56
1:H:526:MET:HE2	1:H:575:ALA:HA	1.88	0.56
1:J:431:GLN:HE22	1:L:354:PRO:HB3	1.71	0.56
1:N:342:THR:HG22	1:N:407:ARG:HG3	1.87	0.56
1:S:526:MET:HE2	1:S:575:ALA:HA	1.95	0.56
1:Y:307:TRP:O	1:Y:426:SER:OG	2.22	0.56
1:2:342:THR:HG22	1:2:407:ARG:HG3	1.87	0.56
1:Z:431:GLN:HE22	1:4:354:PRO:HB3	1.71	0.56
1:C:354:PRO:HB3	1:M:431:GLN:HE22	1.71	0.56
1:M:431:GLN:HE22	1:N:354:PRO:HB3	48.21	0.56
1:S:473:MET:HE1	1:U:275:TYR:HB3	1.88	0.56
1:F:354:PRO:HB3	1:G:431:GLN:HE22	93.47	0.56
1:L:342:THR:HG22	1:L:407:ARG:HG3	1.87	0.56
1:N:431:GLN:HE22	1:O:354:PRO:HB3	50.44	0.56
1:O:464:LEU:HD23	1:P:554:ASN:HB3	100.46	0.56
1:X:342:THR:HG22	1:X:407:ARG:HG3	1.87	0.56
1:W:354:PRO:HB3	1:Y:431:GLN:HE22	46.96	0.56
1:Z:275:TYR:HB3	1:2:473:MET:HE1	94.44	0.56
1:1:464:LEU:HD23	1:2:554:ASN:HB3	1.88	0.55
1:3:354:PRO:HB3	1:4:431:GLN:HE22	1.71	0.55
1:B:431:GLN:HE22	1:M:354:PRO:HB3	121.34	0.55
1:D:554:ASN:HB3	1:T:464:LEU:HD23	148.09	0.55
1:I:431:GLN:HE22	1:J:354:PRO:HB3	48.19	0.55
1:N:346:PHE:HZ	1:N:398:LEU:HD22	1.70	0.55
1:Q:431:GLN:HE22	1:R:354:PRO:HB3	50.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:431:GLN:HE22	1:X:354:PRO:HB3	50.44	0.55
1:E:431:GLN:HE22	1:X:354:PRO:HB3	152.41	0.55
1:A:526:MET:HE2	1:A:575:ALA:HA	1.88	0.55
1:E:354:PRO:HB3	1:V:431:GLN:HE22	134.44	0.55
1:E:307:TRP:O	1:E:426:SER:OG	2.22	0.55
1:A:554:ASN:HB3	1:I:464:LEU:HD23	1.88	0.55
1:Z:473:MET:HE1	1:I:275:TYR:CD2	105.60	0.55
1:A:354:PRO:HB3	1:I:431:GLN:HE22	1.70	0.55
1:B:431:GLN:HE22	1:J:354:PRO:HB3	1.72	0.55
1:L:473:MET:HE1	1:T:275:TYR:CD2	218.15	0.55
1:C:275:TYR:HB3	1:M:473:MET:HE1	1.88	0.55
1:O:431:GLN:NE2	1:P:354:PRO:HB3	47.69	0.55
1:W:431:GLN:HE22	1:Y:354:PRO:HB3	1.72	0.55
1:X:346:PHE:HZ	1:X:398:LEU:HD22	1.70	0.55
1:Y:346:PHE:HZ	1:Y:398:LEU:HD22	1.70	0.55
1:4:346:PHE:HZ	1:4:398:LEU:HD22	1.70	0.55
1:B:354:PRO:HB3	1:C:431:GLN:HE22	48.21	0.55
1:F:431:GLN:HE22	1:H:354:PRO:HB3	123.58	0.55
1:G:354:PRO:HB3	1:H:431:GLN:HE22	50.44	0.55
1:J:431:GLN:HE22	1:K:354:PRO:HB3	50.45	0.55
1:K:354:PRO:HB3	1:8:431:GLN:HE22	1.71	0.55
1:J:473:MET:HE1	1:L:275:TYR:HB3	1.88	0.55
1:C:439:PRO:HB3	1:O:381:LEU:HD21	165.95	0.55
1:F:275:TYR:CD2	1:Q:473:MET:HE1	2.41	0.55
1:I:431:GLN:NE2	1:2:354:PRO:HB3	2.22	0.55
1:7:307:TRP:O	1:7:426:SER:OG	2.22	0.55
1:5:354:PRO:HB3	1:7:431:GLN:HE22	1.72	0.55
1:B:354:PRO:HB3	1:L:431:GLN:HE22	1.72	0.55
1:D:354:PRO:HB3	1:P:431:GLN:HE22	1.71	0.55
1:E:431:GLN:HE22	1:Q:354:PRO:HB3	1.72	0.55
1:I:354:PRO:HB3	1:K:431:GLN:HE22	80.87	0.55
1:5:473:MET:HE1	1:6:275:TYR:CD2	2.41	0.55
1:D:354:PRO:HB3	1:T:431:GLN:NE2	115.75	0.55
1:H:354:PRO:HB3	1:Y:431:GLN:HE22	1.71	0.55
1:I:307:TRP:O	1:I:426:SER:OG	2.22	0.55
1:T:473:MET:HE1	1:U:275:TYR:CD2	58.51	0.55
1:G:307:TRP:O	1:G:426:SER:OG	2.22	0.55
1:D:431:GLN:HE22	1:N:354:PRO:HB3	1.71	0.55
1:M:354:PRO:HB3	1:O:431:GLN:HE22	80.87	0.55
1:R:431:GLN:HE22	1:S:354:PRO:HB3	1.72	0.55
1:Z:354:PRO:HB3	1:3:431:GLN:HE22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:431:GLN:HE22	1:1:354:PRO:HB3	94.63	0.55
1:A:354:PRO:HB3	1:K:431:GLN:HE22	95.65	0.55
1:A:431:GLN:HE22	1:8:354:PRO:HB3	150.60	0.55
1:L:431:GLN:HE22	1:T:354:PRO:HB3	194.97	0.55
1:N:473:MET:HE1	1:P:275:TYR:HD2	1.72	0.55
1:V:526:MET:HE2	1:V:575:ALA:HA	1.89	0.55
1:W:473:MET:HE1	1:Y:275:TYR:HB3	1.89	0.55
1:F:431:GLN:NE2	1:H:354:PRO:HB3	123.41	0.54
1:J:431:GLN:NE2	1:K:354:PRO:HB3	50.40	0.54
1:C:431:GLN:HE22	1:O:354:PRO:HB3	151.96	0.54
1:N:431:GLN:HE22	1:P:354:PRO:HB3	1.72	0.54
1:W:307:TRP:O	1:W:426:SER:OG	2.22	0.54
1:Z:354:PRO:HB3	1:2:431:GLN:HE22	83.87	0.54
1:A:473:MET:HE1	1:8:275:TYR:HD2	169.82	0.54
1:D:431:GLN:HE22	1:L:354:PRO:HB3	123.58	0.54
1:A:354:PRO:HB3	1:I:431:GLN:NE2	2.23	0.54
1:G:431:GLN:HE22	1:I:354:PRO:HB3	1.72	0.54
1:R:431:GLN:NE2	1:S:354:PRO:HB3	2.23	0.54
1:L:431:GLN:NE2	1:T:354:PRO:HB3	195.60	0.54
1:R:354:PRO:HB3	1:U:431:GLN:HE22	1.72	0.54
1:U:431:GLN:HE22	1:V:354:PRO:HB3	50.44	0.54
1:Z:431:GLN:NE2	1:1:354:PRO:HB3	95.48	0.54
1:A:431:GLN:NE2	1:8:354:PRO:HB3	151.15	0.54
1:B:275:TYR:HB3	1:C:473:MET:HE1	57.24	0.54
1:E:354:PRO:HB3	1:F:431:GLN:NE2	2.23	0.54
1:H:354:PRO:HB3	1:Y:431:GLN:NE2	2.23	0.54
1:H:431:GLN:NE2	1:W:354:PRO:HB3	2.23	0.54
1:J:431:GLN:NE2	1:L:354:PRO:HB3	2.23	0.54
1:B:275:TYR:HB3	1:L:473:MET:HE1	1.88	0.54
1:C:431:GLN:NE2	1:O:354:PRO:HB3	152.29	0.54
1:Q:354:PRO:HB3	1:S:431:GLN:NE2	93.29	0.54
1:T:431:GLN:NE2	1:U:354:PRO:HB3	47.67	0.54
1:S:431:GLN:HE22	1:U:354:PRO:HB3	1.72	0.54
1:V:354:PRO:HB3	1:X:431:GLN:HE22	1.71	0.54
1:E:354:PRO:HB3	1:F:431:GLN:HE22	1.72	0.54
1:F:473:MET:HE1	1:H:275:TYR:HD2	139.23	0.54
1:C:354:PRO:HB3	1:M:431:GLN:NE2	2.23	0.54
1:N:431:GLN:NE2	1:P:354:PRO:HB3	2.23	0.54
1:C:354:PRO:HB3	1:P:431:GLN:HE22	49.27	0.54
1:D:354:PRO:HB3	1:P:431:GLN:NE2	2.23	0.54
1:R:275:TYR:CD2	1:U:473:MET:HE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:354:PRO:HB3	1:V:431:GLN:HE22	80.87	0.54
1:T:275:TYR:CD2	1:V:473:MET:HE1	88.57	0.54
1:5:307:TRP:O	1:5:426:SER:OG	2.22	0.54
1:6:431:GLN:NE2	1:7:354:PRO:HB3	2.23	0.54
1:K:354:PRO:HB3	1:8:431:GLN:NE2	2.23	0.54
1:A:354:PRO:HB3	1:K:431:GLN:NE2	95.75	0.54
1:N:431:GLN:NE2	1:O:354:PRO:HB3	50.40	0.54
1:Q:354:PRO:HB3	1:S:431:GLN:HE22	93.47	0.54
1:T:431:GLN:HE22	1:U:354:PRO:HB3	48.19	0.54
1:X:431:GLN:HE22	1:Y:354:PRO:HB3	48.21	0.54
1:V:354:PRO:HB3	1:X:431:GLN:NE2	2.23	0.54
1:X:431:GLN:NE2	1:Y:354:PRO:HB3	47.69	0.54
1:Z:354:PRO:HB3	1:2:431:GLN:NE2	83.62	0.54
1:3:354:PRO:HB3	1:4:431:GLN:NE2	2.23	0.54
1:5:354:PRO:HB3	1:7:431:GLN:NE2	2.23	0.54
1:6:431:GLN:HE22	1:7:354:PRO:HB3	1.72	0.54
1:B:526:MET:HE2	1:B:575:ALA:HA	1.91	0.54
1:F:354:PRO:HB3	1:G:431:GLN:NE2	93.29	0.54
1:F:354:PRO:HB3	1:Q:431:GLN:HE22	1.71	0.54
1:I:431:GLN:NE2	1:J:354:PRO:HB3	47.67	0.54
1:D:431:GLN:NE2	1:N:354:PRO:HB3	2.23	0.54
1:E:431:GLN:NE2	1:Q:354:PRO:HB3	2.23	0.54
1:Z:354:PRO:HB3	1:3:431:GLN:NE2	2.23	0.54
1:M:354:PRO:HB3	1:O:431:GLN:NE2	81.29	0.54
1:C:354:PRO:HB3	1:P:431:GLN:NE2	50.06	0.54
1:U:289:ARG:HH21	1:U:617:GLN:HB3	1.73	0.54
1:U:473:MET:HE1	1:V:275:TYR:HD2	55.76	0.54
1:H:431:GLN:HE22	1:W:354:PRO:HB3	1.71	0.54
1:5:431:GLN:HE22	1:6:354:PRO:HB3	1.71	0.54
1:R:289:ARG:HH21	1:R:617:GLN:HB3	1.74	0.54
1:S:289:ARG:HH21	1:S:617:GLN:HB3	1.73	0.54
1:E:275:TYR:HD2	1:V:473:MET:HE1	154.17	0.54
1:B:431:GLN:NE2	1:M:354:PRO:HB3	121.44	0.53
1:F:354:PRO:HB3	1:Q:431:GLN:NE2	2.23	0.53
1:G:431:GLN:NE2	1:I:354:PRO:HB3	2.23	0.53
1:D:431:GLN:NE2	1:L:354:PRO:HB3	123.41	0.53
1:T:289:ARG:HH21	1:T:617:GLN:HB3	1.74	0.53
1:S:431:GLN:NE2	1:U:354:PRO:HB3	2.23	0.53
1:U:431:GLN:NE2	1:V:354:PRO:HB3	50.40	0.53
1:Y:289:ARG:HH21	1:Y:617:GLN:HB3	1.74	0.53
1:6:289:ARG:HH21	1:6:617:GLN:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ARG:HH21	1:C:617:GLN:HB3	1.73	0.53
1:F:289:ARG:HH21	1:F:617:GLN:HB3	1.73	0.53
1:G:354:PRO:HB3	1:H:431:GLN:NE2	50.40	0.53
1:L:289:ARG:HH21	1:L:617:GLN:HB3	1.73	0.53
1:M:289:ARG:HH21	1:M:617:GLN:HB3	1.74	0.53
1:Z:289:ARG:HH21	1:Z:617:GLN:HB3	1.73	0.53
1:5:431:GLN:NE2	1:6:354:PRO:HB3	2.23	0.53
1:8:300:GLN:NE2	1:8:703:TYR:O	2.41	0.53
1:A:289:ARG:HH21	1:A:617:GLN:HB3	1.74	0.53
1:E:275:TYR:HD2	1:F:473:MET:HE1	1.73	0.53
1:J:289:ARG:HH21	1:J:617:GLN:HB3	1.73	0.53
1:N:289:ARG:HH21	1:N:617:GLN:HB3	1.74	0.53
1:R:354:PRO:HB3	1:U:431:GLN:NE2	2.23	0.53
1:V:307:TRP:O	1:V:426:SER:OG	2.22	0.53
1:T:354:PRO:HB3	1:V:431:GLN:NE2	81.30	0.53
1:W:289:ARG:HH21	1:W:617:GLN:HB3	1.74	0.53
1:E:289:ARG:HH21	1:E:617:GLN:HB3	1.73	0.53
1:B:431:GLN:NE2	1:J:354:PRO:HB3	2.23	0.53
1:I:354:PRO:HB3	1:K:431:GLN:NE2	81.29	0.53
1:M:431:GLN:NE2	1:N:354:PRO:HB3	47.69	0.53
1:N:526:MET:HE2	1:N:575:ALA:HA	2.00	0.53
1:Q:473:MET:HE1	1:R:275:TYR:HB3	56.61	0.53
1:U:473:MET:HE1	1:V:275:TYR:HB3	56.61	0.53
1:F:483:GLY:HA3	1:F:609:TRP:HB3	1.91	0.53
1:H:483:GLY:HA3	1:H:609:TRP:HB3	1.91	0.53
1:K:300:GLN:NE2	1:K:703:TYR:O	2.41	0.53
1:K:483:GLY:HA3	1:K:609:TRP:HB3	1.91	0.53
1:O:289:ARG:HH21	1:O:617:GLN:HB3	1.74	0.53
1:W:275:TYR:HD2	1:Y:473:MET:HE1	52.51	0.53
1:7:289:ARG:HH21	1:7:617:GLN:HB3	1.73	0.53
1:A:490:ARG:NH1	1:I:586:LEU:HD23	2.24	0.53
1:D:289:ARG:HH21	1:D:617:GLN:HB3	1.73	0.53
1:E:464:LEU:HD23	1:X:554:ASN:HB3	168.38	0.53
1:G:483:GLY:HA3	1:G:609:TRP:HB3	1.91	0.53
1:H:300:GLN:NE2	1:H:703:TYR:O	2.41	0.53
1:I:289:ARG:HH21	1:I:617:GLN:HB3	1.73	0.53
1:J:483:GLY:HA3	1:J:609:TRP:HB3	1.91	0.53
1:P:483:GLY:HA3	1:P:609:TRP:HB3	1.91	0.53
1:W:431:GLN:NE2	1:X:354:PRO:HB3	50.40	0.53
1:W:464:LEU:HD23	1:X:554:ASN:HB3	59.37	0.53
1:Z:431:GLN:NE2	1:4:354:PRO:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:289:ARG:HH21	1:2:617:GLN:HB3	1.73	0.53
1:8:226:SER:HB2	1:8:320:ASN:H	1.74	0.53
1:A:604:LEU:HD23	1:G:524:VAL:HG11	1.89	0.53
1:G:226:SER:HB2	1:G:320:ASN:H	1.74	0.53
1:K:289:ARG:HH21	1:K:617:GLN:HB3	1.73	0.53
1:B:354:PRO:HB3	1:L:431:GLN:NE2	2.23	0.53
1:M:483:GLY:HA3	1:M:609:TRP:HB3	1.91	0.53
1:P:226:SER:HB2	1:P:320:ASN:H	1.74	0.53
1:P:289:ARG:HH21	1:P:617:GLN:HB3	1.73	0.53
1:Q:526:MET:HE2	1:Q:575:ALA:HA	1.89	0.53
1:V:483:GLY:HA3	1:V:609:TRP:HB3	1.91	0.53
1:B:483:GLY:HA3	1:B:609:TRP:HB3	1.91	0.53
1:E:275:TYR:HB3	1:F:473:MET:HE1	1.91	0.53
1:E:431:GLN:NE2	1:X:354:PRO:HB3	153.14	0.53
1:F:226:SER:HB2	1:F:320:ASN:H	1.74	0.53
1:G:289:ARG:HH21	1:G:617:GLN:HB3	1.74	0.53
1:G:300:GLN:NE2	1:G:703:TYR:O	2.41	0.53
1:G:554:ASN:HB3	1:H:464:LEU:HD23	59.36	0.53
1:I:554:ASN:HB3	1:K:464:LEU:HD23	95.46	0.53
1:L:483:GLY:HA3	1:L:609:TRP:HB3	1.91	0.53
1:P:300:GLN:NE2	1:P:703:TYR:O	2.41	0.53
1:Q:289:ARG:HH21	1:Q:617:GLN:HB3	1.74	0.53
1:R:226:SER:HB2	1:R:320:ASN:H	1.74	0.53
1:R:300:GLN:NE2	1:R:703:TYR:O	2.41	0.53
1:S:483:GLY:HA3	1:S:609:TRP:HB3	1.91	0.53
1:U:226:SER:HB2	1:U:320:ASN:H	1.74	0.53
1:X:226:SER:HB2	1:X:320:ASN:H	1.74	0.53
1:Y:226:SER:HB2	1:Y:320:ASN:H	1.74	0.53
1:W:354:PRO:HB3	1:Y:431:GLN:NE2	47.35	0.53
1:Y:483:GLY:HA3	1:Y:609:TRP:HB3	1.91	0.53
1:Y:300:GLN:NE2	1:Y:703:TYR:O	2.41	0.53
1:1:483:GLY:HA3	1:1:609:TRP:HB3	1.91	0.53
1:5:289:ARG:HH21	1:5:617:GLN:HB3	1.74	0.53
1:K:554:ASN:HB3	1:8:464:LEU:HD23	1.91	0.53
1:B:354:PRO:HB3	1:C:431:GLN:NE2	47.69	0.53
1:C:483:GLY:HA3	1:C:609:TRP:HB3	1.91	0.53
1:J:226:SER:HB2	1:J:320:ASN:H	1.74	0.53
1:J:464:LEU:HD23	1:L:554:ASN:HB3	1.91	0.53
1:J:473:MET:HE1	1:K:275:TYR:HD2	55.75	0.53
1:T:226:SER:HB2	1:T:320:ASN:H	1.74	0.53
1:T:483:GLY:HA3	1:T:609:TRP:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:226:SER:HB2	1:V:320:ASN:H	1.74	0.53
1:3:483:GLY:HA3	1:3:609:TRP:HB3	1.91	0.53
1:4:289:ARG:HH21	1:4:617:GLN:HB3	1.74	0.53
1:5:545:PHE:O	1:5:561:MET:N	2.27	0.53
1:6:483:GLY:HA3	1:6:609:TRP:HB3	1.91	0.53
1:D:483:GLY:HA3	1:D:609:TRP:HB3	1.91	0.53
1:E:354:PRO:HB3	1:V:431:GLN:NE2	134.25	0.53
1:O:483:GLY:HA3	1:O:609:TRP:HB3	1.91	0.53
1:Q:307:TRP:O	1:Q:426:SER:OG	2.22	0.53
1:R:483:GLY:HA3	1:R:609:TRP:HB3	1.91	0.53
1:U:545:PHE:O	1:U:561:MET:N	2.27	0.53
1:U:483:GLY:HA3	1:U:609:TRP:HB3	1.91	0.53
1:5:554:ASN:HB3	1:7:464:LEU:HD23	1.91	0.52
1:6:464:LEU:HD23	1:7:554:ASN:HB3	1.91	0.52
1:A:300:GLN:NE2	1:A:703:TYR:O	2.41	0.52
1:B:554:ASN:HB3	1:L:464:LEU:HD23	1.91	0.52
1:C:464:LEU:HD23	1:O:554:ASN:HB3	168.14	0.52
1:F:554:ASN:HB3	1:Q:464:LEU:HD23	1.91	0.52
1:C:554:ASN:HB3	1:M:464:LEU:HD23	1.91	0.52
1:D:473:MET:HE1	1:N:275:TYR:CD2	2.45	0.52
1:D:554:ASN:HB3	1:P:464:LEU:HD23	1.91	0.52
1:Q:464:LEU:HD23	1:R:554:ASN:HB3	59.37	0.52
1:T:464:LEU:HD23	1:U:554:ASN:HB3	100.45	0.52
1:W:464:LEU:HD23	1:Y:554:ASN:HB3	1.91	0.52
1:2:226:SER:HB2	1:2:320:ASN:H	1.74	0.52
1:5:464:LEU:HD23	1:6:554:ASN:HB3	1.91	0.52
1:A:275:TYR:HD2	1:I:473:MET:HE1	1.74	0.52
1:B:554:ASN:HB3	1:C:464:LEU:HD23	100.46	0.52
1:D:226:SER:HB2	1:D:320:ASN:H	1.74	0.52
1:D:307:TRP:O	1:D:426:SER:OG	2.22	0.52
1:D:464:LEU:HD23	1:N:554:ASN:HB3	1.91	0.52
1:D:487:ARG:HG2	1:D:488:GLN:N	2.25	0.52
1:E:554:ASN:HB3	1:F:464:LEU:HD23	1.91	0.52
1:F:464:LEU:HD23	1:H:554:ASN:HB3	152.11	0.52
1:G:487:ARG:HG2	1:G:488:GLN:N	2.25	0.52
1:K:307:TRP:O	1:K:426:SER:OG	2.22	0.52
1:K:226:SER:HB2	1:K:320:ASN:H	1.74	0.52
1:L:300:GLN:NE2	1:L:703:TYR:O	2.41	0.52
1:M:226:SER:HB2	1:M:320:ASN:H	1.74	0.52
1:N:300:GLN:NE2	1:N:703:TYR:O	2.41	0.52
1:E:464:LEU:HD23	1:Q:554:ASN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:431:GLN:NE2	1:R:354:PRO:HB3	50.40	0.52
1:R:464:LEU:HD23	1:S:554:ASN:HB3	1.91	0.52
1:W:431:GLN:NE2	1:Y:354:PRO:HB3	2.23	0.52
1:Z:464:LEU:HD23	1:1:554:ASN:HB3	104.29	0.52
1:1:289:ARG:HH21	1:1:617:GLN:HB3	1.73	0.52
1:3:487:ARG:HG2	1:3:488:GLN:N	2.25	0.52
1:4:487:ARG:HG2	1:4:488:GLN:N	2.25	0.52
1:7:487:ARG:HG2	1:7:488:GLN:N	2.25	0.52
1:A:487:ARG:HG2	1:A:488:GLN:N	2.25	0.52
1:E:487:ARG:HG2	1:E:488:GLN:N	2.25	0.52
1:F:487:ARG:HG2	1:F:488:GLN:N	2.25	0.52
1:A:586:LEU:HD23	1:G:490:ARG:NH1	2.23	0.52
1:H:487:ARG:HG2	1:H:488:GLN:N	2.25	0.52
1:J:464:LEU:HD23	1:K:554:ASN:HB3	59.37	0.52
1:K:487:ARG:HG2	1:K:488:GLN:N	2.25	0.52
1:M:487:ARG:HG2	1:M:488:GLN:N	2.25	0.52
1:M:554:ASN:HB3	1:O:464:LEU:HD23	95.44	0.52
1:N:464:LEU:HD23	1:P:554:ASN:HB3	1.91	0.52
1:N:487:ARG:HG2	1:N:488:GLN:N	2.25	0.52
1:P:487:ARG:HG2	1:P:488:GLN:N	2.25	0.52
1:S:226:SER:HB2	1:S:320:ASN:H	1.74	0.52
1:V:289:ARG:HH21	1:V:617:GLN:HB3	1.74	0.52
1:W:487:ARG:HG2	1:W:488:GLN:N	2.25	0.52
1:X:483:GLY:HA3	1:X:609:TRP:HB3	1.91	0.52
1:W:275:TYR:HB3	1:Y:473:MET:HE1	50.58	0.52
1:Z:554:ASN:HB3	1:3:464:LEU:HD23	1.91	0.52
1:1:487:ARG:HG2	1:1:488:GLN:N	2.25	0.52
1:2:483:GLY:HA3	1:2:609:TRP:HB3	1.91	0.52
1:3:226:SER:HB2	1:3:320:ASN:H	1.74	0.52
1:5:226:SER:HB2	1:5:320:ASN:H	1.74	0.52
1:6:226:SER:HB2	1:6:320:ASN:H	1.74	0.52
1:6:487:ARG:HG2	1:6:488:GLN:N	2.25	0.52
1:A:464:LEU:HD23	1:8:554:ASN:HB3	186.87	0.52
1:A:554:ASN:HB3	1:K:464:LEU:HD23	146.45	0.52
1:B:289:ARG:HH21	1:B:617:GLN:HB3	1.73	0.52
1:J:487:ARG:HG2	1:J:488:GLN:N	2.25	0.52
1:O:487:ARG:HG2	1:O:488:GLN:N	2.25	0.52
1:Q:226:SER:HB2	1:Q:320:ASN:H	1.74	0.52
1:Q:487:ARG:HG2	1:Q:488:GLN:N	2.25	0.52
1:S:464:LEU:HD23	1:U:554:ASN:HB3	1.91	0.52
1:S:487:ARG:HG2	1:S:488:GLN:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:487:ARG:HG2	1:T:488:GLN:N	2.25	0.52
1:L:464:LEU:HD23	1:T:554:ASN:HB3	228.29	0.52
1:X:289:ARG:HH21	1:X:617:GLN:HB3	1.74	0.52
1:X:464:LEU:HD23	1:Y:554:ASN:HB3	100.46	0.52
1:W:554:ASN:HB3	1:Y:464:LEU:HD23	59.64	0.52
1:Z:526:MET:HE2	1:Z:575:ALA:HA	1.91	0.52
1:Z:300:GLN:NE2	1:Z:703:TYR:O	2.41	0.52
1:3:300:GLN:NE2	1:3:703:TYR:O	2.41	0.52
1:8:289:ARG:HH21	1:8:617:GLN:HB3	1.73	0.52
1:8:545:PHE:O	1:8:561:MET:N	2.27	0.52
1:A:524:VAL:HG11	1:I:604:LEU:HD23	1.92	0.52
1:A:583:ALA:O	1:G:487:ARG:HD2	2.09	0.52
1:H:425:SER:HB2	1:H:427:TYR:CZ	2.45	0.52
1:I:483:GLY:HA3	1:I:609:TRP:HB3	1.91	0.52
1:D:464:LEU:HD23	1:L:554:ASN:HB3	152.10	0.52
1:O:226:SER:HB2	1:O:320:ASN:H	1.74	0.52
1:U:464:LEU:HD23	1:V:554:ASN:HB3	59.37	0.52
1:E:554:ASN:HB3	1:V:464:LEU:HD23	188.09	0.52
1:V:554:ASN:HB3	1:X:464:LEU:HD23	1.91	0.52
1:8:483:GLY:HA3	1:8:609:TRP:HB3	1.91	0.52
1:A:425:SER:HB2	1:A:427:TYR:CZ	2.45	0.52
1:J:425:SER:HB2	1:J:427:TYR:CZ	2.45	0.52
1:K:425:SER:HB2	1:K:427:TYR:CZ	2.45	0.52
1:L:487:ARG:HG2	1:L:488:GLN:N	2.25	0.52
1:O:425:SER:HB2	1:O:427:TYR:CZ	2.45	0.52
1:O:300:GLN:NE2	1:O:703:TYR:O	2.41	0.52
1:Q:425:SER:HB2	1:Q:427:TYR:CZ	2.45	0.52
1:Q:545:PHE:O	1:Q:561:MET:N	2.27	0.52
1:Q:554:ASN:HB3	1:S:464:LEU:HD23	103.69	0.52
1:S:425:SER:HB2	1:S:427:TYR:CZ	2.45	0.52
1:T:425:SER:HB2	1:T:427:TYR:CZ	2.45	0.52
1:W:425:SER:HB2	1:W:427:TYR:CZ	2.45	0.52
1:H:464:LEU:HD23	1:W:554:ASN:HB3	1.91	0.52
1:Z:487:ARG:HG2	1:Z:488:GLN:N	2.25	0.52
1:1:425:SER:HB2	1:1:427:TYR:CZ	2.45	0.52
1:Z:554:ASN:HB3	1:2:464:LEU:HD23	117.32	0.52
1:3:425:SER:HB2	1:3:427:TYR:CZ	2.45	0.52
1:A:473:MET:HE1	1:8:275:TYR:HB3	167.39	0.52
1:C:425:SER:HB2	1:C:427:TYR:CZ	2.45	0.52
1:D:425:SER:HB2	1:D:427:TYR:CZ	2.45	0.52
1:E:425:SER:HB2	1:E:427:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:554:ASN:HB3	1:G:464:LEU:HD23	103.68	0.52
1:H:289:ARG:HH21	1:H:617:GLN:HB3	1.73	0.52
1:I:487:ARG:HG2	1:I:488:GLN:N	2.25	0.52
1:L:425:SER:HB2	1:L:427:TYR:CZ	2.45	0.52
1:P:425:SER:HB2	1:P:427:TYR:CZ	2.45	0.52
1:R:425:SER:HB2	1:R:427:TYR:CZ	2.45	0.52
1:R:487:ARG:HG2	1:R:488:GLN:N	2.25	0.52
1:U:425:SER:HB2	1:U:427:TYR:CZ	2.45	0.52
1:U:487:ARG:HG2	1:U:488:GLN:N	2.25	0.52
1:V:425:SER:HB2	1:V:427:TYR:CZ	2.45	0.52
1:V:487:ARG:HG2	1:V:488:GLN:N	2.25	0.52
1:1:307:TRP:O	1:1:426:SER:OG	2.22	0.52
1:2:300:GLN:NE2	1:2:703:TYR:O	2.41	0.52
1:4:483:GLY:HA3	1:4:609:TRP:HB3	1.91	0.52
1:8:425:SER:HB2	1:8:427:TYR:CZ	2.45	0.52
1:A:657:PRO:HG3	1:B:372:VAL:HG11	1.92	0.52
1:B:425:SER:HB2	1:B:427:TYR:CZ	2.45	0.52
1:E:483:GLY:HA3	1:E:609:TRP:HB3	1.91	0.52
1:F:425:SER:HB2	1:F:427:TYR:CZ	2.45	0.52
1:I:464:LEU:HD23	1:J:554:ASN:HB3	100.46	0.52
1:N:483:GLY:HA3	1:N:609:TRP:HB3	1.91	0.52
1:B:372:VAL:HG11	1:O:657:PRO:HG3	145.28	0.52
1:T:300:GLN:NE2	1:T:703:TYR:O	2.41	0.52
1:V:545:PHE:O	1:V:561:MET:N	2.27	0.52
1:X:425:SER:HB2	1:X:427:TYR:CZ	2.45	0.52
1:1:226:SER:HB2	1:1:320:ASN:H	1.74	0.52
1:2:307:TRP:O	1:2:426:SER:OG	2.22	0.52
1:2:487:ARG:HG2	1:2:488:GLN:N	2.25	0.52
1:3:289:ARG:HH21	1:3:617:GLN:HB3	1.73	0.52
1:3:307:TRP:O	1:3:426:SER:OG	2.22	0.52
1:5:483:GLY:HA3	1:5:609:TRP:HB3	1.91	0.52
1:7:483:GLY:HA3	1:7:609:TRP:HB3	1.91	0.52
1:8:487:ARG:HG2	1:8:488:GLN:N	2.25	0.52
1:G:464:LEU:HD23	1:I:554:ASN:HB3	1.91	0.52
1:H:226:SER:HB2	1:H:320:ASN:H	1.74	0.52
1:N:473:MET:HE1	1:P:275:TYR:HB3	1.92	0.52
1:Q:483:GLY:HA3	1:Q:609:TRP:HB3	1.91	0.52
1:Y:487:ARG:HG2	1:Y:488:GLN:N	2.25	0.52
1:1:300:GLN:NE2	1:1:703:TYR:O	2.41	0.52
1:4:526:MET:HE2	1:4:575:ALA:HA	1.92	0.52
1:7:425:SER:HB2	1:7:427:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ARG:HG2	1:C:488:GLN:N	2.25	0.52
1:D:300:GLN:NE2	1:D:703:TYR:O	2.41	0.52
1:G:362:GLN:NE2	1:1:666:GLN:OE1	187.23	0.52
1:J:473:MET:HE1	1:K:275:TYR:HB3	56.61	0.52
1:C:275:TYR:HD2	1:M:473:MET:HE1	1.75	0.52
1:P:545:PHE:O	1:P:561:MET:N	2.27	0.52
1:Y:425:SER:HB2	1:Y:427:TYR:CZ	2.45	0.52
1:Z:226:SER:HB2	1:Z:320:ASN:H	1.74	0.52
1:4:300:GLN:NE2	1:4:703:TYR:O	2.41	0.51
1:A:226:SER:HB2	1:A:320:ASN:H	1.74	0.51
1:E:226:SER:HB2	1:E:320:ASN:H	1.74	0.51
1:E:527:ALA:HB1	1:E:569:LYS:HG2	1.93	0.51
1:F:527:ALA:HB1	1:F:569:LYS:HG2	1.92	0.51
1:I:362:GLN:NE2	1:T:666:GLN:OE1	208.63	0.51
1:J:473:MET:HE1	1:L:275:TYR:HD2	1.75	0.51
1:J:527:ALA:HB1	1:J:569:LYS:HG2	1.93	0.51
1:B:473:MET:HE1	1:M:275:TYR:HB3	135.05	0.51
1:N:226:SER:HB2	1:N:320:ASN:H	1.74	0.51
1:N:425:SER:HB2	1:N:427:TYR:CZ	2.45	0.51
1:S:473:MET:HE1	1:U:275:TYR:HD2	1.75	0.51
1:D:524:VAL:HG11	1:T:604:LEU:HD23	130.33	0.51
1:W:226:SER:HB2	1:W:320:ASN:H	1.74	0.51
1:W:483:GLY:HA3	1:W:609:TRP:HB3	1.91	0.51
1:W:527:ALA:HB1	1:W:569:LYS:HG2	1.93	0.51
1:X:487:ARG:HG2	1:X:488:GLN:N	2.25	0.51
1:1:604:LEU:HD23	1:2:524:VAL:HG11	1.91	0.51
1:2:425:SER:HB2	1:2:427:TYR:CZ	2.45	0.51
1:4:425:SER:HB2	1:4:427:TYR:CZ	2.45	0.51
1:7:226:SER:HB2	1:7:320:ASN:H	1.74	0.51
1:K:657:PRO:HG3	1:7:372:VAL:HG11	1.93	0.51
1:B:473:MET:HE1	1:J:275:TYR:HB3	1.91	0.51
1:B:527:ALA:HB1	1:B:569:LYS:HG2	1.93	0.51
1:G:425:SER:HB2	1:G:427:TYR:CZ	2.45	0.51
1:H:362:GLN:NE2	1:I:666:GLN:OE1	2.43	0.51
1:L:606:GLY:HA3	1:T:636:LEU:HD21	195.87	0.51
1:O:586:LEU:HD23	1:P:490:ARG:NH1	114.11	0.51
1:T:554:ASN:HB3	1:V:464:LEU:HD23	95.46	0.51
1:Z:425:SER:HB2	1:Z:427:TYR:CZ	2.45	0.51
1:Z:483:GLY:HA3	1:Z:609:TRP:HB3	1.91	0.51
1:1:586:LEU:HD23	1:2:490:ARG:NH1	2.25	0.51
1:3:527:ALA:HB1	1:3:569:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:527:ALA:HB1	1:5:569:LYS:HG2	1.93	0.51
1:B:226:SER:HB2	1:B:320:ASN:H	1.74	0.51
1:D:527:ALA:HB1	1:D:569:LYS:HG2	1.93	0.51
1:D:657:PRO:HG3	1:E:372:VAL:HG11	1.93	0.51
1:I:425:SER:HB2	1:I:427:TYR:CZ	2.45	0.51
1:A:275:TYR:HD2	1:K:473:MET:HE1	110.45	0.51
1:M:425:SER:HB2	1:M:427:TYR:CZ	2.45	0.51
1:N:527:ALA:HB1	1:N:569:LYS:HG2	1.93	0.51
1:O:527:ALA:HB1	1:O:569:LYS:HG2	1.93	0.51
1:D:490:ARG:NH1	1:T:586:LEU:HD23	150.93	0.51
1:E:657:PRO:HG3	1:U:372:VAL:HG11	157.58	0.51
1:V:372:VAL:HG11	1:W:657:PRO:HG3	42.95	0.51
1:Y:545:PHE:O	1:Y:561:MET:N	2.27	0.51
1:Z:606:GLY:HA3	1:1:636:LEU:HD21	80.85	0.51
1:4:226:SER:HB2	1:4:320:ASN:H	1.74	0.51
1:Z:464:LEU:HD23	1:4:554:ASN:HB3	1.91	0.51
1:5:425:SER:HB2	1:5:427:TYR:CZ	2.45	0.51
1:6:527:ALA:HB1	1:6:569:LYS:HG2	1.93	0.51
1:A:275:TYR:HB3	1:K:473:MET:HE1	108.49	0.51
1:A:473:MET:HE1	1:G:275:TYR:HD2	1.74	0.51
1:A:527:ALA:HB1	1:A:569:LYS:HG2	1.93	0.51
1:A:483:GLY:HA3	1:A:609:TRP:HB3	1.91	0.51
1:A:666:GLN:OE1	1:J:362:GLN:NE2	62.26	0.51
1:C:527:ALA:HB1	1:C:569:LYS:HG2	1.93	0.51
1:K:526:MET:HE2	1:K:575:ALA:HA	1.92	0.51
1:M:464:LEU:HD23	1:N:554:ASN:HB3	100.46	0.51
1:M:351:TYR:OH	1:M:645:PRO:O	2.26	0.51
1:N:464:LEU:HD23	1:O:554:ASN:HB3	59.37	0.51
1:O:604:LEU:HD23	1:P:524:VAL:HG11	80.74	0.51
1:R:554:ASN:HB3	1:U:464:LEU:HD23	1.91	0.51
1:T:527:ALA:HB1	1:T:569:LYS:HG2	1.93	0.51
1:V:527:ALA:HB1	1:V:569:LYS:HG2	1.92	0.51
1:H:554:ASN:HB3	1:Y:464:LEU:HD23	1.92	0.51
1:Y:527:ALA:HB1	1:Y:569:LYS:HG2	1.93	0.51
1:1:527:ALA:HB1	1:1:569:LYS:HG2	1.93	0.51
1:2:527:ALA:HB1	1:2:569:LYS:HG2	1.93	0.51
1:3:554:ASN:HB3	1:4:464:LEU:HD23	1.91	0.51
1:4:527:ALA:HB1	1:4:569:LYS:HG2	1.93	0.51
1:C:226:SER:HB2	1:C:320:ASN:H	1.74	0.51
1:G:527:ALA:HB1	1:G:569:LYS:HG2	1.93	0.51
1:I:527:ALA:HB1	1:I:569:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ASN:HD22	1:I:592:ALA:HA	1.76	0.51
1:L:226:SER:HB2	1:L:320:ASN:H	1.74	0.51
1:Q:527:ALA:HB1	1:Q:569:LYS:HG2	1.93	0.51
1:T:526:MET:HE2	1:T:575:ALA:HA	1.95	0.51
1:1:583:ALA:O	1:2:487:ARG:HD2	2.11	0.51
1:H:372:VAL:HG11	1:I:657:PRO:HG3	1.92	0.51
1:I:226:SER:HB2	1:I:320:ASN:H	1.74	0.51
1:B:464:LEU:HD23	1:M:554:ASN:HB3	152.28	0.51
1:M:362:GLN:NE2	1:N:666:GLN:OE1	2.44	0.51
1:R:527:ALA:HB1	1:R:569:LYS:HG2	1.93	0.51
1:S:527:ALA:HB1	1:S:569:LYS:HG2	1.93	0.51
1:D:487:ARG:HD2	1:T:583:ALA:O	145.03	0.51
1:2:372:VAL:HG11	1:3:657:PRO:HG3	1.93	0.51
1:T:362:GLN:NE2	1:6:666:GLN:OE1	194.51	0.51
1:B:464:LEU:HD23	1:J:554:ASN:HB3	1.92	0.51
1:E:300:GLN:NE2	1:E:703:TYR:O	2.41	0.51
1:L:527:ALA:HB1	1:L:569:LYS:HG2	1.93	0.51
1:Q:362:GLN:NE2	1:Y:666:GLN:OE1	156.99	0.51
1:T:636:LEU:HD21	1:V:606:GLY:HA3	105.07	0.51
1:U:527:ALA:HB1	1:U:569:LYS:HG2	1.93	0.51
1:R:636:LEU:HD21	1:U:606:GLY:HA3	1.93	0.51
1:V:666:GLN:OE1	1:W:362:GLN:NE2	2.44	0.51
1:E:606:GLY:HA3	1:X:636:LEU:HD21	129.59	0.51
1:W:606:GLY:HA3	1:X:636:LEU:HD21	64.08	0.51
1:F:362:GLN:NE2	1:X:666:GLN:OE1	156.38	0.51
1:Z:527:ALA:HB1	1:Z:569:LYS:HG2	1.93	0.51
1:Z:636:LEU:HD21	1:3:606:GLY:HA3	1.93	0.51
1:K:636:LEU:HD21	1:8:606:GLY:HA3	1.93	0.51
1:C:526:MET:HE2	1:C:575:ALA:HA	1.92	0.51
1:D:372:VAL:HG11	1:O:657:PRO:HG3	117.40	0.51
1:G:362:GLN:NE2	1:W:666:GLN:OE1	2.44	0.51
1:F:606:GLY:HA3	1:H:636:LEU:HD21	123.87	0.51
1:J:362:GLN:NE2	1:X:666:GLN:OE1	177.99	0.51
1:L:526:MET:HE2	1:L:575:ALA:HA	1.92	0.51
1:C:606:GLY:HA3	1:O:636:LEU:HD21	128.83	0.51
1:F:666:GLN:OE1	1:R:362:GLN:NE2	2.44	0.51
1:E:275:TYR:HB3	1:V:473:MET:HE1	151.76	0.51
1:G:372:VAL:HG11	1:W:657:PRO:HG3	1.93	0.51
1:Y:526:MET:HE2	1:Y:575:ALA:HA	2.01	0.51
1:Z:545:PHE:O	1:Z:561:MET:N	2.27	0.51
1:3:636:LEU:HD21	1:4:606:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:657:PRO:HG3	1:6:372:VAL:HG11	174.64	0.51
1:5:636:LEU:HD21	1:7:606:GLY:HA3	1.93	0.51
1:B:487:ARG:HG2	1:B:488:GLN:N	2.25	0.51
1:C:554:ASN:HB3	1:P:464:LEU:HD23	58.41	0.51
1:D:636:LEU:HD21	1:P:606:GLY:HA3	1.93	0.51
1:G:606:GLY:HA3	1:I:636:LEU:HD21	1.93	0.51
1:B:606:GLY:HA3	1:J:636:LEU:HD21	1.93	0.51
1:A:636:LEU:HD21	1:K:606:GLY:HA3	120.26	0.51
1:J:606:GLY:HA3	1:K:636:LEU:HD21	64.08	0.51
1:M:527:ALA:HB1	1:M:569:LYS:HG2	1.93	0.51
1:O:473:MET:HE1	1:P:275:TYR:HD2	58.77	0.51
1:O:583:ALA:O	1:P:487:ARG:HD2	94.35	0.51
1:P:372:VAL:HG11	1:Q:657:PRO:HG3	1.93	0.51
1:T:372:VAL:HG11	1:U:657:PRO:HG3	1.93	0.51
1:U:666:GLN:OE1	1:5:362:GLN:NE2	216.26	0.51
1:V:657:PRO:HG3	1:1:372:VAL:HG11	170.70	0.51
1:W:300:GLN:NE2	1:W:703:TYR:O	2.41	0.51
1:Y:362:GLN:NE2	1:4:666:GLN:OE1	2.44	0.51
1:B:606:GLY:HA3	1:M:636:LEU:HD21	96.96	0.51
1:D:545:PHE:O	1:D:561:MET:N	2.27	0.51
1:F:524:VAL:HG11	1:G:604:LEU:HD23	79.06	0.51
1:H:329:ASN:O	1:H:332:THR:HG22	2.12	0.51
1:A:499:ASN:ND2	1:I:592:ALA:HA	2.26	0.51
1:I:604:LEU:HD23	1:J:524:VAL:HG11	80.73	0.51
1:I:606:GLY:HA3	1:J:636:LEU:HD21	73.00	0.51
1:G:657:PRO:HG3	1:K:372:VAL:HG11	163.90	0.51
1:D:606:GLY:HA3	1:N:636:LEU:HD21	1.93	0.51
1:M:636:LEU:HD21	1:O:606:GLY:HA3	105.08	0.51
1:N:606:GLY:HA3	1:O:636:LEU:HD21	64.07	0.51
1:Q:362:GLN:NE2	1:S:666:GLN:OE1	2.44	0.51
1:E:606:GLY:HA3	1:Q:636:LEU:HD21	1.93	0.51
1:P:362:GLN:NE2	1:Q:666:GLN:OE1	2.45	0.51
1:U:632:HIS:HA	3:U:902:DA:H2"	1.94	0.51
1:V:657:PRO:HG3	1:W:372:VAL:HG11	1.93	0.51
1:W:636:LEU:HD21	1:Y:606:GLY:HA3	20.79	0.51
1:X:527:ALA:HB1	1:X:569:LYS:HG2	1.93	0.51
1:Z:524:VAL:HG11	1:2:604:LEU:HD23	87.15	0.50
1:3:524:VAL:HG11	1:4:604:LEU:HD23	1.93	0.50
1:Z:604:LEU:HD23	1:4:524:VAL:HG11	1.93	0.50
1:5:487:ARG:HG2	1:5:488:GLN:N	2.25	0.50
1:6:425:SER:HB2	1:6:427:TYR:CZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:636:LEU:HD21	1:M:606:GLY:HA3	1.93	0.50
1:D:604:LEU:HD23	1:L:524:VAL:HG11	129.64	0.50
1:D:657:PRO:HG3	1:S:372:VAL:HG11	106.91	0.50
1:E:329:ASN:O	1:E:332:THR:HG22	2.12	0.50
1:F:636:LEU:HD21	1:G:606:GLY:HA3	78.87	0.50
1:F:473:MET:HE1	1:H:275:TYR:HB3	138.86	0.50
1:N:666:GLN:OE1	1:R:362:GLN:NE2	176.22	0.50
1:N:604:LEU:HD23	1:O:524:VAL:HG11	71.58	0.50
1:Q:473:MET:HE1	1:R:275:TYR:HD2	55.75	0.50
1:S:632:HIS:HA	3:S:902:DA:H2''	1.94	0.50
1:U:372:VAL:HG11	1:2:657:PRO:HG3	180.07	0.50
1:E:636:LEU:HD21	1:V:606:GLY:HA3	135.38	0.50
1:R:657:PRO:HG3	1:X:372:VAL:HG11	81.64	0.50
1:X:372:VAL:HG11	1:Y:657:PRO:HG3	1.94	0.50
1:Q:372:VAL:HG11	1:Y:657:PRO:HG3	157.96	0.50
1:3:329:ASN:O	1:3:332:THR:HG22	2.12	0.50
1:6:300:GLN:NE2	1:6:703:TYR:O	2.41	0.50
1:7:329:ASN:O	1:7:332:THR:HG22	2.12	0.50
1:8:632:HIS:HA	3:8:902:DA:H2''	1.94	0.50
1:A:666:GLN:OE1	1:B:362:GLN:NE2	2.43	0.50
1:B:362:GLN:NE2	1:O:666:GLN:OE1	177.99	0.50
1:B:666:GLN:OE1	1:C:362:GLN:NE2	2.44	0.50
1:F:300:GLN:NE2	1:F:703:TYR:O	2.41	0.50
1:G:329:ASN:O	1:G:332:THR:HG22	2.12	0.50
1:G:632:HIS:HA	3:G:902:DA:H2''	1.93	0.50
1:H:545:PHE:O	1:H:561:MET:N	2.27	0.50
1:B:666:GLN:OE1	1:L:362:GLN:NE2	62.12	0.50
1:J:606:GLY:HA3	1:L:636:LEU:HD21	1.93	0.50
1:M:300:GLN:NE2	1:M:703:TYR:O	2.41	0.50
1:M:604:LEU:HD23	1:N:524:VAL:HG11	80.74	0.50
1:O:329:ASN:O	1:O:332:THR:HG22	2.12	0.50
1:P:329:ASN:O	1:P:332:THR:HG22	2.12	0.50
1:P:632:HIS:HA	3:P:902:DA:H2''	1.94	0.50
1:R:632:HIS:HA	3:R:902:DA:H2''	1.93	0.50
1:S:329:ASN:O	1:S:332:THR:HG22	2.12	0.50
1:U:362:GLN:NE2	1:2:666:GLN:OE1	200.67	0.50
1:2:632:HIS:HA	3:2:902:DA:H2''	1.93	0.50
1:A:636:LEU:HD21	1:I:606:GLY:HA3	1.93	0.50
1:B:604:LEU:HD23	1:M:524:VAL:HG11	94.31	0.50
1:B:636:LEU:HD21	1:C:606:GLY:HA3	73.01	0.50
1:C:300:GLN:NE2	1:C:703:TYR:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:GLN:NE2	1:M:666:GLN:OE1	94.63	0.50
1:C:632:HIS:HA	3:C:902:DA:H2"	1.93	0.50
1:D:606:GLY:HA3	1:L:636:LEU:HD21	123.87	0.50
1:D:632:HIS:HA	3:D:902:DA:H2"	1.93	0.50
1:F:372:VAL:HG11	1:G:657:PRO:HG3	1.93	0.50
1:G:524:VAL:HG11	1:H:604:LEU:HD23	71.57	0.50
1:F:362:GLN:NE2	1:G:666:GLN:OE1	2.44	0.50
1:I:632:HIS:HA	3:I:902:DA:H2"	1.93	0.50
1:I:524:VAL:HG11	1:K:604:LEU:HD23	116.84	0.50
1:J:657:PRO:HG3	1:L:372:VAL:HG11	97.01	0.50
1:L:657:PRO:HG3	1:N:372:VAL:HG11	139.41	0.50
1:Q:329:ASN:O	1:Q:332:THR:HG22	2.12	0.50
1:Q:300:GLN:NE2	1:Q:703:TYR:O	2.41	0.50
1:Q:604:LEU:HD23	1:R:524:VAL:HG11	71.58	0.50
1:R:666:GLN:OE1	1:V:362:GLN:NE2	2.45	0.50
1:C:666:GLN:OE1	1:S:362:GLN:NE2	127.28	0.50
1:R:604:LEU:HD23	1:S:524:VAL:HG11	1.94	0.50
1:V:632:HIS:HA	3:V:902:DA:H2"	1.93	0.50
1:W:604:LEU:HD23	1:Y:524:VAL:HG11	1.93	0.50
1:Y:632:HIS:HA	3:Y:902:DA:H2"	1.94	0.50
1:Z:657:PRO:HG3	1:4:372:VAL:HG11	97.01	0.50
1:Z:632:HIS:HA	3:Z:902:DA:H2"	1.93	0.50
1:2:362:GLN:NE2	1:3:666:GLN:OE1	2.44	0.50
1:3:632:HIS:HA	3:3:902:DA:H2"	1.93	0.50
1:B:636:LEU:HD21	1:L:606:GLY:HA3	1.93	0.50
1:D:362:GLN:NE2	1:O:666:GLN:OE1	127.51	0.50
1:C:657:PRO:HG3	1:D:372:VAL:HG11	1.93	0.50
1:D:666:GLN:OE1	1:S:362:GLN:NE2	105.29	0.50
1:F:604:LEU:HD23	1:H:524:VAL:HG11	129.64	0.50
1:G:586:LEU:HD23	1:I:490:ARG:NH1	2.26	0.50
1:H:524:VAL:HG11	1:Y:604:LEU:HD23	1.94	0.50
1:J:604:LEU:HD23	1:K:524:VAL:HG11	71.58	0.50
1:L:632:HIS:HA	3:L:902:DA:H2"	1.93	0.50
1:M:545:PHE:O	1:M:561:MET:N	2.27	0.50
1:O:632:HIS:HA	3:O:902:DA:H2"	1.93	0.50
1:F:636:LEU:HD21	1:Q:606:GLY:HA3	1.93	0.50
1:R:329:ASN:O	1:R:332:THR:HG22	2.12	0.50
1:R:606:GLY:HA3	1:S:636:LEU:HD21	1.93	0.50
1:W:329:ASN:O	1:W:332:THR:HG22	2.12	0.50
1:F:657:PRO:HG3	1:Z:372:VAL:HG11	128.41	0.50
1:Z:275:TYR:HD2	1:2:473:MET:HE1	96.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:636:LEU:HD21	1:2:606:GLY:HA3	83.42	0.50
1:4:329:ASN:O	1:4:332:THR:HG22	2.12	0.50
1:5:300:GLN:NE2	1:5:703:TYR:O	2.41	0.50
1:5:606:GLY:HA3	1:6:636:LEU:HD21	1.93	0.50
1:7:632:HIS:HA	3:7:902:DA:H2"	1.93	0.50
1:B:604:LEU:HD23	1:J:524:VAL:HG11	1.93	0.50
1:E:632:HIS:HA	3:E:902:DA:H2"	1.94	0.50
1:H:666:GLN:OE1	1:Z:362:GLN:NE2	2.44	0.50
1:K:372:VAL:HG11	1:L:657:PRO:HG3	1.93	0.50
1:K:524:VAL:HG11	1:8:604:LEU:HD23	1.93	0.50
1:N:329:ASN:O	1:N:332:THR:HG22	2.12	0.50
1:O:372:VAL:HG11	1:7:657:PRO:HG3	170.02	0.50
1:O:372:VAL:HG11	1:P:657:PRO:HG3	1.93	0.50
1:Q:372:VAL:HG11	1:S:657:PRO:HG3	1.93	0.50
1:T:666:GLN:OE1	1:Y:362:GLN:NE2	160.34	0.50
1:U:329:ASN:O	1:U:332:THR:HG22	2.12	0.50
1:T:606:GLY:HA3	1:U:636:LEU:HD21	73.00	0.50
1:U:604:LEU:HD23	1:V:524:VAL:HG11	71.58	0.50
1:E:604:LEU:HD23	1:X:524:VAL:HG11	130.75	0.50
1:W:604:LEU:HD23	1:X:524:VAL:HG11	71.58	0.50
1:Y:329:ASN:O	1:Y:332:THR:HG22	2.12	0.50
1:U:657:PRO:HG3	1:5:372:VAL:HG11	194.50	0.50
1:6:604:LEU:HD23	1:7:524:VAL:HG11	1.93	0.50
1:6:606:GLY:HA3	1:7:636:LEU:HD21	1.93	0.50
1:3:372:VAL:HG11	1:8:657:PRO:HG3	1.93	0.50
1:A:425:SER:HB2	1:A:427:TYR:CE2	2.47	0.50
1:A:632:HIS:HA	3:A:902:DA:H2"	1.93	0.50
1:B:300:GLN:NE2	1:B:703:TYR:O	2.41	0.50
1:C:329:ASN:O	1:C:332:THR:HG22	2.12	0.50
1:C:473:MET:HE1	1:O:275:TYR:HD2	169.46	0.50
1:C:636:LEU:HD21	1:P:606:GLY:HA3	66.37	0.50
1:C:666:GLN:OE1	1:D:362:GLN:NE2	2.45	0.50
1:E:425:SER:HB2	1:E:427:TYR:CE2	2.47	0.50
1:F:425:SER:HB2	1:F:427:TYR:CE2	2.47	0.50
1:F:545:PHE:O	1:F:561:MET:N	2.27	0.50
1:G:666:GLN:OE1	1:K:362:GLN:NE2	176.23	0.50
1:H:696:ARG:NE	1:H:698:ASN:OD1	2.42	0.50
1:I:329:ASN:O	1:I:332:THR:HG22	2.12	0.50
1:I:372:VAL:HG11	1:T:657:PRO:HG3	191.44	0.50
1:J:329:ASN:O	1:J:332:THR:HG22	2.12	0.50
1:K:362:GLN:NE2	1:L:666:GLN:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:362:GLN:NE2	1:S:666:GLN:OE1	134.68	0.50
1:M:632:HIS:HA	3:M:902:DA:H2"	1.93	0.50
1:N:425:SER:HB2	1:N:427:TYR:CE2	2.47	0.50
1:Q:275:TYR:HD2	1:S:473:MET:HE1	104.43	0.50
1:T:329:ASN:O	1:T:332:THR:HG22	2.12	0.50
1:V:300:GLN:NE2	1:V:703:TYR:O	2.41	0.50
1:X:632:HIS:HA	3:X:902:DA:H2"	1.93	0.50
1:G:372:VAL:HG11	1:1:657:PRO:HG3	174.65	0.50
1:Z:666:GLN:OE1	1:4:362:GLN:NE2	94.63	0.50
1:P:666:GLN:OE1	1:6:362:GLN:NE2	187.24	0.50
1:6:425:SER:HB2	1:6:427:TYR:CE2	2.47	0.50
1:6:545:PHE:O	1:6:561:MET:N	2.27	0.50
1:K:666:GLN:OE1	1:7:362:GLN:NE2	2.44	0.50
1:A:606:GLY:HA3	1:8:636:LEU:HD21	137.82	0.50
1:A:329:ASN:O	1:A:332:THR:HG22	2.12	0.50
1:A:383:LEU:HD11	1:I:429:HIS:O	2.12	0.50
1:B:329:ASN:O	1:B:332:THR:HG22	2.12	0.50
1:B:524:VAL:HG11	1:C:604:LEU:HD23	80.74	0.50
1:B:657:PRO:HG3	1:L:372:VAL:HG11	71.98	0.50
1:C:545:PHE:O	1:C:561:MET:N	2.27	0.50
1:E:524:VAL:HG11	1:F:604:LEU:HD23	1.94	0.50
1:E:636:LEU:HD21	1:F:606:GLY:HA3	1.93	0.50
1:F:329:ASN:O	1:F:332:THR:HG22	2.12	0.50
1:A:592:ALA:HA	1:G:499:ASN:HD22	1.77	0.50
1:H:606:GLY:HA3	1:W:636:LEU:HD21	1.93	0.50
1:H:632:HIS:HA	3:H:902:DA:H2"	1.93	0.50
1:J:372:VAL:HG11	1:X:657:PRO:HG3	145.28	0.50
1:J:425:SER:HB2	1:J:427:TYR:CE2	2.47	0.50
1:J:632:HIS:HA	3:J:902:DA:H2"	1.93	0.50
1:K:527:ALA:HB1	1:K:569:LYS:HG2	1.93	0.50
1:L:329:ASN:O	1:L:332:THR:HG22	2.12	0.50
1:L:545:PHE:O	1:L:561:MET:N	2.27	0.50
1:B:524:VAL:HG11	1:L:604:LEU:HD23	1.94	0.50
1:L:604:LEU:HD23	1:T:524:VAL:HG11	205.89	0.50
1:M:329:ASN:O	1:M:332:THR:HG22	2.12	0.50
1:M:425:SER:HB2	1:M:427:TYR:CE2	2.47	0.50
1:N:657:PRO:HG3	1:R:372:VAL:HG11	163.90	0.50
1:N:632:HIS:HA	3:N:902:DA:H2"	1.94	0.50
1:O:425:SER:HB2	1:O:427:TYR:CE2	2.47	0.50
1:P:526:MET:HE2	1:P:575:ALA:HA	1.95	0.50
1:D:524:VAL:HG11	1:P:604:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:606:GLY:HA3	1:P:636:LEU:HD21	1.93	0.50
1:R:526:MET:HE2	1:R:575:ALA:HA	1.93	0.50
1:S:545:PHE:O	1:S:561:MET:N	2.27	0.50
1:T:632:HIS:HA	3:T:902:DA:H2"	1.94	0.50
1:S:604:LEU:HD23	1:U:524:VAL:HG11	1.94	0.50
1:V:329:ASN:O	1:V:332:THR:HG22	2.12	0.50
1:F:372:VAL:HG11	1:X:657:PRO:HG3	129.73	0.50
1:Y:372:VAL:HG11	1:4:657:PRO:HG3	1.93	0.50
1:X:604:LEU:HD23	1:Y:524:VAL:HG11	80.74	0.50
1:X:362:GLN:NE2	1:Y:666:GLN:OE1	2.45	0.50
1:Z:425:SER:HB2	1:Z:427:TYR:CE2	2.47	0.50
1:Z:428:ALA:O	1:Z:735:THR:HA	2.12	0.50
1:1:482:PRO:O	1:1:607:MET:HG3	2.12	0.50
1:2:425:SER:HB2	1:2:427:TYR:CE2	2.47	0.50
1:3:425:SER:HB2	1:3:427:TYR:CE2	2.47	0.50
1:7:425:SER:HB2	1:7:427:TYR:CE2	2.47	0.50
1:A:657:PRO:HG3	1:J:372:VAL:HG11	82.54	0.50
1:B:632:HIS:HA	3:B:902:DA:H2"	1.94	0.50
1:C:425:SER:HB2	1:C:427:TYR:CE2	2.47	0.50
1:C:604:LEU:HD23	1:O:524:VAL:HG11	129.67	0.50
1:D:425:SER:HB2	1:D:427:TYR:CE2	2.47	0.50
1:F:428:ALA:O	1:F:735:THR:HA	2.12	0.50
1:F:657:PRO:HG3	1:R:372:VAL:HG11	1.93	0.50
1:G:428:ALA:O	1:G:735:THR:HA	2.12	0.50
1:H:527:ALA:HB1	1:H:569:LYS:HG2	1.93	0.50
1:J:666:GLN:OE1	1:L:362:GLN:NE2	94.63	0.50
1:K:425:SER:HB2	1:K:427:TYR:CE2	2.47	0.50
1:K:428:ALA:O	1:K:735:THR:HA	2.12	0.50
1:L:425:SER:HB2	1:L:427:TYR:CE2	2.47	0.50
1:L:586:LEU:HD23	1:T:490:ARG:NH1	228.81	0.50
1:M:473:MET:HE1	1:N:275:TYR:HD2	58.80	0.50
1:L:666:GLN:OE1	1:N:362:GLN:NE2	162.68	0.50
1:C:586:LEU:HD23	1:O:490:ARG:NH1	133.49	0.50
1:P:527:ALA:HB1	1:P:569:LYS:HG2	1.93	0.50
1:Q:636:LEU:HD21	1:S:606:GLY:HA3	78.87	0.50
1:T:372:VAL:HG11	1:6:657:PRO:HG3	184.36	0.50
1:T:482:PRO:O	1:T:607:MET:HG3	2.12	0.50
1:U:526:MET:HE2	1:U:575:ALA:HA	1.96	0.50
1:R:666:GLN:OE1	1:X:362:GLN:NE2	63.52	0.50
1:T:657:PRO:HG3	1:Y:372:VAL:HG11	138.84	0.50
1:Y:482:PRO:O	1:Y:607:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:329:ASN:O	1:Z:332:THR:HG22	2.12	0.50
1:Z:473:MET:HE1	1:4:275:TYR:HD2	1.76	0.50
1:1:632:HIS:HA	3:1:902:DA:H2"	1.93	0.50
1:5:425:SER:HB2	1:5:427:TYR:CE2	2.47	0.50
1:5:524:VAL:HG11	1:7:604:LEU:HD23	1.93	0.50
1:5:666:GLN:OE1	1:8:362:GLN:NE2	2.45	0.50
1:6:482:PRO:O	1:6:607:MET:HG3	2.12	0.50
1:7:482:PRO:O	1:7:607:MET:HG3	2.12	0.50
1:7:696:ARG:NE	1:7:698:ASN:OD1	2.42	0.50
1:B:657:PRO:HG3	1:C:372:VAL:HG11	1.94	0.50
1:C:657:PRO:HG3	1:S:372:VAL:HG11	119.69	0.50
1:D:666:GLN:OE1	1:E:362:GLN:NE2	2.44	0.50
1:E:524:VAL:HG11	1:V:604:LEU:HD23	140.29	0.50
1:E:482:PRO:O	1:E:607:MET:HG3	2.12	0.50
1:A:362:GLN:NE2	1:E:666:GLN:OE1	2.45	0.50
1:F:482:PRO:O	1:F:607:MET:HG3	2.12	0.50
1:H:425:SER:HB2	1:H:427:TYR:CE2	2.47	0.50
1:E:362:GLN:NE2	1:H:666:GLN:OE1	162.67	0.50
1:I:372:VAL:HG11	1:J:657:PRO:HG3	1.93	0.50
1:I:636:LEU:HD21	1:K:606:GLY:HA3	105.07	0.50
1:K:329:ASN:O	1:K:332:THR:HG22	2.11	0.50
1:L:428:ALA:O	1:L:735:THR:HA	2.12	0.50
1:C:372:VAL:HG11	1:M:657:PRO:HG3	97.01	0.50
1:O:362:GLN:NE2	1:P:666:GLN:OE1	2.44	0.50
1:O:428:ALA:O	1:O:735:THR:HA	2.12	0.50
1:P:428:ALA:O	1:P:735:THR:HA	2.12	0.50
1:Q:482:PRO:O	1:Q:607:MET:HG3	2.12	0.50
1:S:696:ARG:NE	1:S:698:ASN:OD1	2.42	0.50
1:E:666:GLN:OE1	1:U:362:GLN:NE2	155.51	0.50
1:U:425:SER:HB2	1:U:427:TYR:CE2	2.47	0.50
1:U:482:PRO:O	1:U:607:MET:HG3	2.12	0.50
1:S:606:GLY:HA3	1:U:636:LEU:HD21	1.93	0.50
1:R:657:PRO:HG3	1:V:372:VAL:HG11	1.93	0.50
1:V:425:SER:HB2	1:V:427:TYR:CE2	2.47	0.50
1:V:482:PRO:O	1:V:607:MET:HG3	2.12	0.50
1:W:482:PRO:O	1:W:607:MET:HG3	2.12	0.50
1:V:362:GLN:NE2	1:W:666:GLN:OE1	72.58	0.50
1:X:425:SER:HB2	1:X:427:TYR:CE2	2.47	0.50
1:V:524:VAL:HG11	1:X:604:LEU:HD23	1.93	0.50
1:Y:428:ALA:O	1:Y:735:THR:HA	2.12	0.50
1:X:606:GLY:HA3	1:Y:636:LEU:HD21	73.02	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:425:SER:HB2	1:1:427:TYR:CE2	2.47	0.49
1:Z:586:LEU:HD23	1:1:490:ARG:NH1	84.75	0.49
1:3:428:ALA:O	1:3:735:THR:HA	2.12	0.49
1:3:545:PHE:O	1:3:561:MET:N	2.27	0.49
1:6:329:ASN:O	1:6:332:THR:HG22	2.12	0.49
1:8:329:ASN:O	1:8:332:THR:HG22	2.12	0.49
1:8:526:MET:HE2	1:8:575:ALA:HA	1.93	0.49
1:3:362:GLN:NE2	1:8:666:GLN:OE1	2.44	0.49
1:B:482:PRO:O	1:B:607:MET:HG3	2.12	0.49
1:D:428:ALA:O	1:D:735:THR:HA	2.12	0.49
1:E:604:LEU:HD23	1:Q:524:VAL:HG11	1.94	0.49
1:E:696:ARG:NE	1:E:698:ASN:OD1	2.42	0.49
1:G:636:LEU:HD21	1:H:606:GLY:HA3	64.07	0.49
1:I:526:MET:HE2	1:I:575:ALA:HA	1.96	0.49
1:I:545:PHE:O	1:I:561:MET:N	2.27	0.49
1:J:482:PRO:O	1:J:607:MET:HG3	2.12	0.49
1:J:428:ALA:O	1:J:735:THR:HA	2.12	0.49
1:K:482:PRO:O	1:K:607:MET:HG3	2.12	0.49
1:K:666:GLN:OE1	1:W:362:GLN:NE2	195.33	0.49
1:K:632:HIS:HA	3:K:902:DA:H2"	1.93	0.49
1:Q:425:SER:HB2	1:Q:427:TYR:CE2	2.47	0.49
1:S:300:GLN:NE2	1:S:703:TYR:O	2.41	0.49
1:T:425:SER:HB2	1:T:427:TYR:CE2	2.47	0.49
1:T:604:LEU:HD23	1:U:524:VAL:HG11	80.73	0.49
1:V:428:ALA:O	1:V:735:THR:HA	2.12	0.49
1:H:636:LEU:HD21	1:Y:606:GLY:HA3	1.93	0.49
1:F:666:GLN:OE1	1:Z:362:GLN:NE2	157.16	0.49
1:Z:604:LEU:HD23	1:1:524:VAL:HG11	81.88	0.49
1:Z:482:PRO:O	1:Z:607:MET:HG3	2.12	0.49
1:4:428:ALA:O	1:4:735:THR:HA	2.12	0.49
1:6:632:HIS:HA	3:6:902:DA:H2"	1.94	0.49
1:7:428:ALA:O	1:7:735:THR:HA	2.12	0.49
1:8:527:ALA:HB1	1:8:569:LYS:HG2	1.93	0.49
1:A:372:VAL:HG11	1:E:657:PRO:HG3	1.93	0.49
1:A:372:VAL:HG11	1:Z:657:PRO:HG3	117.84	0.49
1:A:428:ALA:O	1:A:735:THR:HA	2.12	0.49
1:B:473:MET:HE1	1:J:275:TYR:HD2	1.74	0.49
1:C:482:PRO:O	1:C:607:MET:HG3	2.12	0.49
1:D:482:PRO:O	1:D:607:MET:HG3	2.12	0.49
1:E:428:ALA:O	1:E:735:THR:HA	2.12	0.49
1:F:632:HIS:HA	3:F:902:DA:H2"	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:526:MET:HE2	1:G:575:ALA:HA	1.95	0.49
1:I:425:SER:HB2	1:I:427:TYR:CE2	2.47	0.49
1:L:482:PRO:O	1:L:607:MET:HG3	2.12	0.49
1:M:482:PRO:O	1:M:607:MET:HG3	2.12	0.49
1:N:428:ALA:O	1:N:735:THR:HA	2.12	0.49
1:N:482:PRO:O	1:N:607:MET:HG3	2.12	0.49
1:M:372:VAL:HG11	1:N:657:PRO:HG3	1.93	0.49
1:U:606:GLY:HA3	1:V:636:LEU:HD21	64.07	0.49
1:W:524:VAL:HG11	1:Y:604:LEU:HD23	15.28	0.49
1:W:526:MET:HE2	1:W:575:ALA:HA	1.98	0.49
1:6:435:ARG:NH2	1:7:272:ASP:O	2.46	0.49
1:O:362:GLN:NE2	1:7:666:GLN:OE1	172.29	0.49
1:A:487:ARG:HD2	1:I:583:ALA:O	2.12	0.49
1:B:275:TYR:HD2	1:L:473:MET:HE1	1.75	0.49
1:C:435:ARG:NH2	1:O:272:ASP:O	165.89	0.49
1:H:428:ALA:O	1:H:735:THR:HA	2.12	0.49
1:A:272:ASP:O	1:I:435:ARG:NH2	2.45	0.49
1:I:482:PRO:O	1:I:607:MET:HG3	2.12	0.49
1:J:604:LEU:HD23	1:L:524:VAL:HG11	1.94	0.49
1:O:251:PRO:HG3	1:O:374:MET:HE3	1.94	0.49
1:P:696:ARG:NE	1:P:698:ASN:OD1	2.42	0.49
1:R:434:ASP:OD1	1:R:434:ASP:N	2.46	0.49
1:R:428:ALA:O	1:R:735:THR:HA	2.12	0.49
1:U:428:ALA:O	1:U:735:THR:HA	2.12	0.49
1:V:636:LEU:HD21	1:X:606:GLY:HA3	1.93	0.49
1:W:473:MET:HE1	1:Y:275:TYR:HD2	1.75	0.49
1:W:428:ALA:O	1:W:735:THR:HA	2.12	0.49
1:X:428:ALA:O	1:X:735:THR:HA	2.12	0.49
1:Y:434:ASP:OD1	1:Y:434:ASP:N	2.45	0.49
1:V:666:GLN:OE1	1:1:362:GLN:NE2	170.73	0.49
1:4:425:SER:HB2	1:4:427:TYR:CE2	2.47	0.49
1:5:482:PRO:O	1:5:607:MET:HG3	2.12	0.49
1:A:482:PRO:O	1:A:607:MET:HG3	2.12	0.49
1:B:275:TYR:HD2	1:C:473:MET:HE1	58.80	0.49
1:E:272:ASP:O	1:F:435:ARG:NH2	2.46	0.49
1:E:372:VAL:HG11	1:H:657:PRO:HG3	139.40	0.49
1:I:300:GLN:NE2	1:I:703:TYR:O	2.41	0.49
1:K:657:PRO:HG3	1:W:372:VAL:HG11	183.41	0.49
1:M:428:ALA:O	1:M:735:THR:HA	2.12	0.49
1:M:657:PRO:HG3	1:N:372:VAL:HG11	42.95	0.49
1:N:604:LEU:HD23	1:P:524:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:419:GLU:OE2	1:O:643:LYS:N	2.44	0.49
1:Q:428:ALA:O	1:Q:735:THR:HA	2.12	0.49
1:R:425:SER:HB2	1:R:427:TYR:CE2	2.47	0.49
1:S:428:ALA:O	1:S:735:THR:HA	2.12	0.49
1:T:362:GLN:NE2	1:U:666:GLN:OE1	2.46	0.49
1:X:329:ASN:O	1:X:332:THR:HG22	2.12	0.49
1:3:419:GLU:OE2	1:3:643:LYS:N	2.44	0.49
1:5:428:ALA:O	1:5:735:THR:HA	2.12	0.49
1:7:527:ALA:HB1	1:7:569:LYS:HG2	1.93	0.49
1:5:657:PRO:HG3	1:8:372:VAL:HG11	1.93	0.49
1:8:425:SER:HB2	1:8:427:TYR:CE2	2.47	0.49
1:8:428:ALA:O	1:8:735:THR:HA	2.12	0.49
1:A:524:VAL:HG11	1:K:604:LEU:HD23	129.90	0.49
1:B:425:SER:HB2	1:B:427:TYR:CE2	2.47	0.49
1:B:473:MET:HE1	1:M:275:TYR:HD2	137.18	0.49
1:B:428:ALA:O	1:B:735:THR:HA	2.12	0.49
1:C:524:VAL:HG11	1:M:604:LEU:HD23	1.94	0.49
1:E:526:MET:HE2	1:E:575:ALA:HA	1.94	0.49
1:H:657:PRO:HG3	1:Z:372:VAL:HG11	1.93	0.49
1:D:435:ARG:NH2	1:L:272:ASP:O	139.23	0.49
1:M:434:ASP:OD1	1:M:434:ASP:N	2.45	0.49
1:M:606:GLY:HA3	1:N:636:LEU:HD21	73.02	0.49
1:Q:606:GLY:HA3	1:R:636:LEU:HD21	64.08	0.49
1:W:606:GLY:HA3	1:Y:636:LEU:HD21	1.93	0.49
1:Z:606:GLY:HA3	1:4:636:LEU:HD21	1.93	0.49
1:1:329:ASN:O	1:1:332:THR:HG22	2.12	0.49
1:2:329:ASN:O	1:2:332:THR:HG22	2.12	0.49
1:5:329:ASN:O	1:5:332:THR:HG22	2.12	0.49
1:A:604:LEU:HD23	1:8:524:VAL:HG11	139.23	0.49
1:D:329:ASN:O	1:D:332:THR:HG22	2.12	0.49
1:F:275:TYR:HD2	1:G:473:MET:HE1	104.39	0.49
1:G:604:LEU:HD23	1:I:524:VAL:HG11	1.94	0.49
1:J:434:ASP:OD1	1:J:434:ASP:N	2.45	0.49
1:O:545:PHE:O	1:O:561:MET:N	2.27	0.49
1:O:482:PRO:O	1:O:607:MET:HG3	2.12	0.49
1:P:425:SER:HB2	1:P:427:TYR:CE2	2.47	0.49
1:C:524:VAL:HG11	1:P:604:LEU:HD23	73.27	0.49
1:P:482:PRO:O	1:P:607:MET:HG3	2.12	0.49
1:O:606:GLY:HA3	1:P:636:LEU:HD21	73.02	0.49
1:R:524:VAL:HG11	1:U:604:LEU:HD23	1.93	0.49
1:S:425:SER:HB2	1:S:427:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:372:VAL:HG11	1:S:657:PRO:HG3	119.87	0.49
1:Z:272:ASP:O	1:2:435:ARG:NH2	92.19	0.49
1:A:362:GLN:NE2	1:Z:666:GLN:OE1	125.29	0.49
1:Z:524:VAL:HG11	1:3:604:LEU:HD23	1.93	0.49
1:3:272:ASP:O	1:4:435:ARG:NH2	2.46	0.49
1:4:482:PRO:O	1:4:607:MET:HG3	2.12	0.49
1:5:490:ARG:NH1	1:7:586:LEU:HD23	2.28	0.49
1:C:434:ASP:OD1	1:C:434:ASP:N	2.45	0.49
1:D:604:LEU:HD23	1:N:524:VAL:HG11	1.93	0.49
1:E:566:GLU:OE2	1:E:569:LYS:NZ	2.45	0.49
1:G:425:SER:HB2	1:G:427:TYR:CE2	2.47	0.49
1:G:482:PRO:O	1:G:607:MET:HG3	2.12	0.49
1:H:473:MET:HE1	1:W:275:TYR:HD2	1.78	0.49
1:I:434:ASP:OD1	1:I:434:ASP:N	2.45	0.49
1:G:592:ALA:HA	1:I:499:ASN:ND2	2.28	0.49
1:M:435:ARG:NH2	1:N:272:ASP:O	58.98	0.49
1:M:272:ASP:O	1:O:435:ARG:NH2	98.08	0.49
1:S:482:PRO:O	1:S:607:MET:HG3	2.12	0.49
1:T:434:ASP:OD1	1:T:434:ASP:N	2.45	0.49
1:T:524:VAL:HG11	1:V:604:LEU:HD23	116.84	0.49
1:W:566:GLU:OE2	1:W:569:LYS:NZ	2.45	0.49
1:Y:425:SER:HB2	1:Y:427:TYR:CE2	2.47	0.49
1:Z:435:ARG:NH2	1:4:272:ASP:O	2.46	0.49
1:1:434:ASP:OD1	1:1:434:ASP:N	2.45	0.49
1:1:606:GLY:HA3	1:2:636:LEU:HD21	1.95	0.49
1:4:632:HIS:HA	3:4:902:DA:H2"	1.94	0.49
1:6:586:LEU:HD23	1:7:490:ARG:NH1	2.28	0.49
1:C:286:ASP:O	1:C:364:CYS:HA	2.13	0.49
1:D:286:ASP:O	1:D:364:CYS:HA	2.13	0.49
1:E:586:LEU:HD23	1:Q:490:ARG:NH1	2.28	0.49
1:E:490:ARG:NH1	1:F:586:LEU:HD23	2.28	0.49
1:G:435:ARG:NH2	1:I:272:ASP:O	2.45	0.49
1:I:473:MET:HE1	1:J:275:TYR:HD2	58.77	0.49
1:L:286:ASP:O	1:L:364:CYS:HA	2.13	0.49
1:M:524:VAL:HG11	1:O:604:LEU:HD23	116.84	0.49
1:M:666:GLN:OE1	1:N:362:GLN:NE2	72.58	0.49
1:N:419:GLU:OE2	1:N:643:LYS:N	2.44	0.49
1:N:435:ARG:NH2	1:O:272:ASP:O	60.17	0.49
1:N:586:LEU:HD23	1:P:490:ARG:NH1	2.28	0.49
1:C:490:ARG:NH1	1:P:586:LEU:HD23	85.14	0.49
1:Q:632:HIS:HA	3:Q:902:DA:H2"	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:286:ASP:O	1:S:364:CYS:HA	2.13	0.49
1:T:286:ASP:O	1:T:364:CYS:HA	2.13	0.49
1:D:636:LEU:HD21	1:T:606:GLY:HA3	123.30	0.49
1:W:632:HIS:HA	3:W:902:DA:H2''	1.94	0.49
1:X:434:ASP:OD1	1:X:434:ASP:N	2.45	0.49
1:2:482:PRO:O	1:2:607:MET:HG3	2.12	0.49
1:3:482:PRO:O	1:3:607:MET:HG3	2.12	0.49
1:4:286:ASP:O	1:4:364:CYS:HA	2.13	0.49
1:A:586:LEU:HD23	1:8:490:ARG:NH1	161.43	0.49
1:A:434:ASP:N	1:A:434:ASP:OD1	2.45	0.49
1:E:545:PHE:O	1:E:561:MET:N	2.27	0.49
1:F:286:ASP:O	1:F:364:CYS:HA	2.13	0.49
1:F:524:VAL:HG11	1:Q:604:LEU:HD23	1.93	0.49
1:G:286:ASP:O	1:G:364:CYS:HA	2.13	0.49
1:H:586:LEU:HD23	1:W:490:ARG:NH1	2.28	0.49
1:J:286:ASP:O	1:J:364:CYS:HA	2.13	0.49
1:N:286:ASP:O	1:N:364:CYS:HA	2.13	0.49
1:O:434:ASP:N	1:O:434:ASP:OD1	2.45	0.49
1:P:286:ASP:O	1:P:364:CYS:HA	2.13	0.49
1:Q:286:ASP:O	1:Q:364:CYS:HA	2.13	0.49
1:R:286:ASP:O	1:R:364:CYS:HA	2.13	0.49
1:Q:490:ARG:NH1	1:S:586:LEU:HD23	81.09	0.49
1:T:428:ALA:O	1:T:735:THR:HA	2.12	0.49
1:W:286:ASP:O	1:W:364:CYS:HA	2.13	0.49
1:W:425:SER:HB2	1:W:427:TYR:CE2	2.47	0.49
1:X:482:PRO:O	1:X:607:MET:HG3	2.12	0.49
1:Z:272:ASP:O	1:3:435:ARG:NH2	2.46	0.49
1:1:286:ASP:O	1:1:364:CYS:HA	2.13	0.49
1:2:286:ASP:O	1:2:364:CYS:HA	2.13	0.49
1:2:526:MET:HE2	1:2:575:ALA:HA	1.93	0.49
1:3:696:ARG:NE	1:3:698:ASN:OD1	2.42	0.49
1:4:419:GLU:OE2	1:4:643:LYS:N	2.44	0.49
1:5:632:HIS:HA	3:5:902:DA:H2''	1.94	0.49
1:A:490:ARG:NH1	1:K:586:LEU:HD23	162.47	0.49
1:C:566:GLU:OE2	1:C:569:LYS:NZ	2.45	0.49
1:D:473:MET:HE1	1:L:275:TYR:HD2	139.10	0.49
1:D:526:MET:HE2	1:D:575:ALA:HA	1.98	0.49
1:H:286:ASP:O	1:H:364:CYS:HA	2.13	0.49
1:H:490:ARG:NH1	1:Y:586:LEU:HD23	2.28	0.49
1:J:526:MET:HE2	1:J:575:ALA:HA	1.95	0.49
1:I:362:GLN:NE2	1:J:666:GLN:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:286:ASP:O	1:M:364:CYS:HA	2.13	0.49
1:M:419:GLU:OE2	1:M:643:LYS:N	2.44	0.49
1:M:566:GLU:OE2	1:M:569:LYS:NZ	2.45	0.49
1:N:586:LEU:HD23	1:O:490:ARG:NH1	82.06	0.49
1:Q:435:ARG:NH2	1:R:272:ASP:O	60.17	0.49
1:Q:566:GLU:OE2	1:Q:569:LYS:NZ	2.45	0.49
1:R:586:LEU:HD23	1:S:490:ARG:NH1	2.28	0.49
1:S:434:ASP:OD1	1:S:434:ASP:N	2.45	0.49
1:R:490:ARG:NH1	1:U:586:LEU:HD23	2.28	0.49
1:T:490:ARG:NH1	1:V:586:LEU:HD23	134.67	0.49
1:X:286:ASP:O	1:X:364:CYS:HA	2.13	0.49
1:W:435:ARG:NH2	1:Y:272:ASP:O	2.46	0.49
1:Y:286:ASP:O	1:Y:364:CYS:HA	2.13	0.49
1:5:272:ASP:O	1:7:435:ARG:NH2	2.46	0.48
1:A:606:GLY:HA3	1:G:636:LEU:HD21	1.95	0.48
1:D:435:ARG:NH2	1:N:272:ASP:O	2.46	0.48
1:G:592:ALA:HA	1:I:499:ASN:HD22	1.78	0.48
1:H:258:TYR:OH	1:H:399:GLU:OE1	2.28	0.48
1:H:482:PRO:O	1:H:607:MET:HG3	2.12	0.48
1:A:272:ASP:O	1:K:435:ARG:NH2	113.68	0.48
1:M:526:MET:HE2	1:M:575:ALA:HA	1.95	0.48
1:N:434:ASP:N	1:N:434:ASP:OD1	2.45	0.48
1:O:592:ALA:HA	1:P:499:ASN:HD22	104.37	0.48
1:E:473:MET:HE1	1:Q:275:TYR:HD2	1.78	0.48
1:R:435:ARG:NH2	1:S:272:ASP:O	2.46	0.48
1:Q:524:VAL:HG11	1:S:604:LEU:HD23	79.06	0.48
1:U:434:ASP:N	1:U:434:ASP:OD1	2.45	0.48
1:V:286:ASP:O	1:V:364:CYS:HA	2.13	0.48
1:W:272:ASP:O	1:Y:435:ARG:NH2	44.64	0.48
1:H:604:LEU:HD23	1:W:524:VAL:HG11	1.94	0.48
1:Z:419:GLU:OE2	1:Z:643:LYS:N	2.44	0.48
1:Z:435:ARG:NH2	1:1:272:ASP:O	102.56	0.48
1:1:696:ARG:NE	1:1:698:ASN:OD1	2.42	0.48
1:3:490:ARG:NH1	1:4:586:LEU:HD23	2.28	0.48
1:Z:490:ARG:NH1	1:3:586:LEU:HD23	2.28	0.48
1:4:434:ASP:OD1	1:4:434:ASP:N	2.46	0.48
1:8:286:ASP:O	1:8:364:CYS:HA	2.13	0.48
1:B:696:ARG:NE	1:B:698:ASN:OD1	2.42	0.48
1:C:592:ALA:HA	1:O:499:ASN:ND2	157.37	0.48
1:E:272:ASP:O	1:V:435:ARG:NH2	149.99	0.48
1:E:490:ARG:NH1	1:V:586:LEU:HD23	175.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:ARG:NH1	1:G:586:LEU:HD23	81.08	0.48
1:G:434:ASP:OD1	1:G:434:ASP:N	2.45	0.48
1:H:272:ASP:O	1:Y:435:ARG:NH2	2.46	0.48
1:G:490:ARG:NH1	1:H:586:LEU:HD23	82.06	0.48
1:I:586:LEU:HD23	1:J:490:ARG:NH1	114.11	0.48
1:K:286:ASP:O	1:K:364:CYS:HA	2.13	0.48
1:I:490:ARG:NH1	1:K:586:LEU:HD23	134.67	0.48
1:D:586:LEU:HD23	1:N:490:ARG:NH1	2.28	0.48
1:M:490:ARG:NH1	1:O:586:LEU:HD23	134.67	0.48
1:E:435:ARG:NH2	1:Q:272:ASP:O	2.46	0.48
1:S:258:TYR:OH	1:S:399:GLU:OE1	2.28	0.48
1:T:586:LEU:HD23	1:U:490:ARG:NH1	114.10	0.48
1:U:286:ASP:O	1:U:364:CYS:HA	2.13	0.48
1:Z:286:ASP:O	1:Z:364:CYS:HA	2.13	0.48
1:5:275:TYR:HD2	1:7:473:MET:HE1	1.78	0.48
1:6:428:ALA:O	1:6:735:THR:HA	2.12	0.48
1:6:526:MET:HE2	1:6:575:ALA:HA	1.95	0.48
1:A:286:ASP:O	1:A:364:CYS:HA	2.13	0.48
1:B:490:ARG:NH1	1:L:586:LEU:HD23	2.28	0.48
1:C:428:ALA:O	1:C:735:THR:HA	2.12	0.48
1:B:490:ARG:NH1	1:C:586:LEU:HD23	114.10	0.48
1:D:566:GLU:OE2	1:D:569:LYS:NZ	2.45	0.48
1:F:526:MET:HE2	1:F:575:ALA:HA	1.95	0.48
1:B:435:ARG:NH2	1:J:272:ASP:O	2.46	0.48
1:B:435:ARG:NH2	1:M:272:ASP:O	129.42	0.48
1:N:435:ARG:NH2	1:P:272:ASP:O	2.46	0.48
1:O:696:ARG:NE	1:O:698:ASN:OD1	2.42	0.48
1:Q:586:LEU:HD23	1:R:490:ARG:NH1	82.06	0.48
1:L:435:ARG:NH2	1:T:272:ASP:O	219.95	0.48
1:2:566:GLU:OE2	1:2:569:LYS:NZ	2.45	0.48
1:3:529:HIS:ND1	1:3:533:GLU:O	2.47	0.48
1:Z:586:LEU:HD23	1:4:490:ARG:NH1	2.28	0.48
1:6:286:ASP:O	1:6:364:CYS:HA	2.13	0.48
1:B:286:ASP:O	1:B:364:CYS:HA	2.13	0.48
1:C:592:ALA:HA	1:O:499:ASN:HD22	156.89	0.48
1:E:286:ASP:O	1:E:364:CYS:HA	2.13	0.48
1:I:428:ALA:O	1:I:735:THR:HA	2.12	0.48
1:J:300:GLN:NE2	1:J:703:TYR:O	2.41	0.48
1:M:586:LEU:HD23	1:N:490:ARG:NH1	114.11	0.48
1:O:286:ASP:O	1:O:364:CYS:HA	2.13	0.48
1:R:482:PRO:O	1:R:607:MET:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:696:ARG:NE	1:T:698:ASN:OD1	2.42	0.48
1:U:696:ARG:NE	1:U:698:ASN:OD1	2.42	0.48
1:V:529:HIS:ND1	1:V:533:GLU:O	2.47	0.48
1:W:529:HIS:ND1	1:W:533:GLU:O	2.47	0.48
1:W:586:LEU:HD23	1:Y:490:ARG:NH1	2.28	0.48
1:W:490:ARG:NH1	1:Y:586:LEU:HD23	33.84	0.48
1:1:529:HIS:ND1	1:1:533:GLU:O	2.47	0.48
1:Z:490:ARG:NH1	1:2:586:LEU:HD23	108.92	0.48
1:2:428:ALA:O	1:2:735:THR:HA	2.12	0.48
1:3:526:MET:HE2	1:3:575:ALA:HA	1.95	0.48
1:5:604:LEU:HD23	1:6:524:VAL:HG11	1.94	0.48
1:7:545:PHE:O	1:7:561:MET:N	2.27	0.48
1:8:482:PRO:O	1:8:607:MET:HG3	2.12	0.48
1:A:435:ARG:NH2	1:8:272:ASP:O	166.50	0.48
1:B:586:LEU:HD23	1:M:490:ARG:NH1	113.22	0.48
1:D:529:HIS:ND1	1:D:533:GLU:O	2.47	0.48
1:D:586:LEU:HD23	1:L:490:ARG:NH1	147.86	0.48
1:E:529:HIS:ND1	1:E:533:GLU:O	2.47	0.48
1:G:529:HIS:ND1	1:G:533:GLU:O	2.47	0.48
1:I:566:GLU:OE2	1:I:569:LYS:NZ	2.45	0.48
1:O:526:MET:HE2	1:O:575:ALA:HA	1.95	0.48
1:O:351:TYR:OH	1:O:645:PRO:O	2.26	0.48
1:P:434:ASP:OD1	1:P:434:ASP:N	2.45	0.48
1:Q:529:HIS:ND1	1:Q:533:GLU:O	2.47	0.48
1:T:529:HIS:ND1	1:T:533:GLU:O	2.47	0.48
1:U:529:HIS:ND1	1:U:533:GLU:O	2.47	0.48
1:U:586:LEU:HD23	1:V:490:ARG:NH1	82.06	0.48
1:7:286:ASP:O	1:7:364:CYS:HA	2.13	0.48
1:B:434:ASP:OD1	1:B:434:ASP:N	2.45	0.48
1:C:251:PRO:HG3	1:C:374:MET:HE3	1.99	0.48
1:I:529:HIS:ND1	1:I:533:GLU:O	2.47	0.48
1:J:529:HIS:ND1	1:J:533:GLU:O	2.47	0.48
1:K:529:HIS:ND1	1:K:533:GLU:O	2.47	0.48
1:M:529:HIS:ND1	1:M:533:GLU:O	2.47	0.48
1:O:529:HIS:ND1	1:O:533:GLU:O	2.47	0.48
1:P:419:GLU:OE2	1:P:643:LYS:N	2.44	0.48
1:R:566:GLU:OE2	1:R:569:LYS:NZ	2.45	0.48
1:L:592:ALA:HA	1:T:499:ASN:HD22	245.24	0.48
1:T:566:GLU:OE2	1:T:569:LYS:NZ	2.45	0.48
1:S:586:LEU:HD23	1:U:490:ARG:NH1	2.28	0.48
1:Z:592:ALA:HA	1:1:499:ASN:HD22	98.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASP:O	1:P:435:ARG:NH2	61.42	0.48
1:E:435:ARG:NH2	1:X:272:ASP:O	165.92	0.48
1:G:566:GLU:OE2	1:G:569:LYS:NZ	2.45	0.48
1:J:419:GLU:OE2	1:J:643:LYS:N	2.44	0.48
1:J:586:LEU:HD23	1:L:490:ARG:NH1	2.29	0.48
1:L:529:HIS:ND1	1:L:533:GLU:O	2.47	0.48
1:Q:434:ASP:OD1	1:Q:434:ASP:N	2.46	0.48
1:F:272:ASP:O	1:Q:435:ARG:NH2	2.46	0.48
1:Q:272:ASP:O	1:S:435:ARG:NH2	102.51	0.48
1:H:435:ARG:NH2	1:W:272:ASP:O	2.46	0.48
1:X:435:ARG:NH2	1:Y:272:ASP:O	58.98	0.48
1:Y:529:HIS:ND1	1:Y:533:GLU:O	2.47	0.48
1:Z:529:HIS:ND1	1:Z:533:GLU:O	2.47	0.48
1:3:434:ASP:N	1:3:434:ASP:OD1	2.46	0.48
1:C:490:ARG:NH1	1:M:586:LEU:HD23	2.29	0.48
1:E:419:GLU:OE2	1:E:643:LYS:N	2.44	0.48
1:F:434:ASP:N	1:F:434:ASP:OD1	2.46	0.48
1:F:451:THR:HG21	1:H:503:PHE:CZ	153.29	0.48
1:I:435:ARG:NH2	1:J:272:ASP:O	58.98	0.48
1:B:586:LEU:HD23	1:J:490:ARG:NH1	2.28	0.48
1:B:272:ASP:O	1:L:435:ARG:NH2	2.46	0.48
1:S:529:HIS:ND1	1:S:533:GLU:O	2.47	0.48
1:W:419:GLU:OE2	1:W:643:LYS:N	2.44	0.48
1:W:434:ASP:OD1	1:W:434:ASP:N	2.45	0.48
1:W:586:LEU:HD23	1:X:490:ARG:NH1	82.06	0.48
1:W:435:ARG:NH2	1:X:272:ASP:O	60.17	0.48
1:E:586:LEU:HD23	1:X:490:ARG:NH1	134.89	0.48
1:X:586:LEU:HD23	1:Y:490:ARG:NH1	114.11	0.48
1:Z:583:ALA:O	1:1:487:ARG:HD2	88.59	0.48
1:1:428:ALA:O	1:1:735:THR:HA	2.12	0.48
1:2:529:HIS:ND1	1:2:533:GLU:O	2.47	0.48
1:4:545:PHE:O	1:4:561:MET:N	2.27	0.48
1:5:286:ASP:O	1:5:364:CYS:HA	2.13	0.48
1:5:435:ARG:NH2	1:6:272:ASP:O	2.46	0.48
1:6:434:ASP:OD1	1:6:434:ASP:N	2.46	0.48
1:B:272:ASP:O	1:C:435:ARG:NH2	58.98	0.48
1:B:529:HIS:ND1	1:B:533:GLU:O	2.47	0.48
1:B:566:GLU:OE2	1:B:569:LYS:NZ	2.45	0.48
1:F:490:ARG:NH1	1:Q:586:LEU:HD23	2.28	0.48
1:G:419:GLU:OE2	1:G:643:LYS:N	2.44	0.48
1:F:272:ASP:O	1:G:435:ARG:NH2	102.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:529:HIS:ND1	1:H:533:GLU:O	2.47	0.48
1:G:429:HIS:O	1:I:383:LEU:HD11	2.14	0.48
1:J:451:THR:HG21	1:K:503:PHE:CZ	73.97	0.48
1:L:583:ALA:O	1:T:487:ARG:HD2	227.83	0.48
1:C:272:ASP:O	1:M:435:ARG:NH2	2.46	0.48
1:C:429:HIS:O	1:O:383:LEU:HD11	158.56	0.48
1:T:435:ARG:NH2	1:U:272:ASP:O	58.97	0.48
1:R:272:ASP:O	1:U:435:ARG:NH2	2.46	0.48
1:V:272:ASP:O	1:X:435:ARG:NH2	2.46	0.48
1:X:529:HIS:ND1	1:X:533:GLU:O	2.47	0.48
1:1:526:MET:HE2	1:1:575:ALA:HA	1.95	0.48
1:3:286:ASP:O	1:3:364:CYS:HA	2.13	0.48
1:5:586:LEU:HD23	1:6:490:ARG:NH1	2.28	0.48
1:C:696:ARG:NE	1:C:698:ASN:OD1	2.42	0.48
1:E:251:PRO:HG3	1:E:374:MET:HE3	1.96	0.48
1:F:503:PHE:CZ	1:G:451:THR:HG21	97.37	0.48
1:I:286:ASP:O	1:I:364:CYS:HA	2.13	0.48
1:I:451:THR:HG21	1:J:503:PHE:CZ	102.52	0.48
1:K:487:ARG:HD2	1:8:583:ALA:O	2.14	0.48
1:K:566:GLU:OE2	1:K:569:LYS:NZ	2.45	0.48
1:M:275:TYR:HD2	1:O:473:MET:HE1	89.23	0.48
1:D:503:PHE:CZ	1:P:451:THR:HG21	2.49	0.48
1:T:272:ASP:O	1:V:435:ARG:NH2	98.10	0.48
1:V:490:ARG:NH1	1:X:586:LEU:HD23	2.28	0.48
1:Z:487:ARG:HD2	1:3:583:ALA:O	2.14	0.47
1:5:529:HIS:ND1	1:5:533:GLU:O	2.47	0.47
1:8:529:HIS:ND1	1:8:533:GLU:O	2.47	0.47
1:D:487:ARG:HD2	1:P:583:ALA:O	2.15	0.47
1:H:434:ASP:OD1	1:H:434:ASP:N	2.46	0.47
1:J:435:ARG:NH2	1:L:272:ASP:O	2.46	0.47
1:L:429:HIS:O	1:T:383:LEU:HD11	204.29	0.47
1:L:696:ARG:NE	1:L:698:ASN:OD1	2.42	0.47
1:B:451:THR:HG21	1:M:503:PHE:CZ	132.05	0.47
1:P:529:HIS:ND1	1:P:533:GLU:O	2.47	0.47
1:R:529:HIS:ND1	1:R:533:GLU:O	2.47	0.47
1:W:451:THR:HG21	1:Y:503:PHE:CZ	2.49	0.47
1:W:545:PHE:O	1:W:561:MET:N	2.27	0.47
1:Z:429:HIS:O	1:1:383:LEU:HD11	98.55	0.47
1:2:251:PRO:HG3	1:2:374:MET:HE3	1.96	0.47
1:Z:275:TYR:HD2	1:3:473:MET:HE1	1.78	0.47
1:5:583:ALA:O	1:6:487:ARG:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:529:HIS:ND1	1:6:533:GLU:O	2.47	0.47
1:B:451:THR:HG21	1:J:503:PHE:CZ	2.49	0.47
1:D:434:ASP:N	1:D:434:ASP:OD1	2.45	0.47
1:D:490:ARG:NH1	1:P:586:LEU:HD23	2.28	0.47
1:F:529:HIS:ND1	1:F:533:GLU:O	2.47	0.47
1:G:696:ARG:NE	1:G:698:ASN:OD1	2.42	0.47
1:K:503:PHE:CZ	1:8:451:THR:HG21	2.50	0.47
1:L:434:ASP:N	1:L:434:ASP:OD1	2.45	0.47
1:M:487:ARG:HD2	1:O:583:ALA:O	131.09	0.47
1:Q:451:THR:HG21	1:R:503:PHE:CZ	73.97	0.47
1:R:503:PHE:CZ	1:U:451:THR:HG21	2.50	0.47
1:T:419:GLU:OE2	1:T:643:LYS:N	2.44	0.47
1:X:300:GLN:NE2	1:X:703:TYR:O	2.41	0.47
1:2:434:ASP:N	1:2:434:ASP:OD1	2.46	0.47
1:1:592:ALA:HA	1:2:499:ASN:HD22	1.78	0.47
1:B:487:ARG:HD2	1:C:583:ALA:O	94.35	0.47
1:F:487:ARG:HD2	1:Q:583:ALA:O	2.14	0.47
1:G:272:ASP:O	1:H:435:ARG:NH2	60.17	0.47
1:H:503:PHE:CZ	1:Y:451:THR:HG21	2.49	0.47
1:G:487:ARG:HD2	1:H:583:ALA:O	79.92	0.47
1:B:487:ARG:HD2	1:L:583:ALA:O	2.15	0.47
1:C:583:ALA:O	1:O:487:ARG:HD2	140.95	0.47
1:R:419:GLU:OE2	1:R:643:LYS:N	2.44	0.47
1:R:451:THR:HG21	1:S:503:PHE:CZ	2.49	0.47
1:T:503:PHE:CZ	1:V:451:THR:HG21	118.83	0.47
1:D:499:ASN:HD22	1:T:592:ALA:HA	157.89	0.47
1:U:435:ARG:NH2	1:V:272:ASP:O	60.17	0.47
1:Z:434:ASP:N	1:Z:434:ASP:OD1	2.46	0.47
1:Z:566:GLU:OE2	1:Z:569:LYS:NZ	2.45	0.47
1:1:419:GLU:OE2	1:1:643:LYS:N	2.44	0.47
1:3:251:PRO:HG3	1:3:374:MET:HE3	1.96	0.47
1:5:566:GLU:OE2	1:5:569:LYS:NZ	2.45	0.47
1:5:696:ARG:NE	1:5:698:ASN:OD1	2.42	0.47
1:5:451:THR:HG21	1:6:503:PHE:CZ	2.49	0.47
1:7:434:ASP:OD1	1:7:434:ASP:N	2.46	0.47
1:C:529:HIS:ND1	1:C:533:GLU:O	2.47	0.47
1:D:451:THR:HG21	1:L:503:PHE:CZ	153.28	0.47
1:F:503:PHE:CZ	1:Q:451:THR:HG21	2.49	0.47
1:J:435:ARG:NH2	1:K:272:ASP:O	60.17	0.47
1:K:434:ASP:OD1	1:K:434:ASP:N	2.45	0.47
1:K:490:ARG:NH1	1:8:586:LEU:HD23	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:545:PHE:O	1:N:561:MET:N	2.27	0.47
1:N:451:THR:HG21	1:O:503:PHE:CZ	73.97	0.47
1:C:487:ARG:HD2	1:P:583:ALA:O	82.81	0.47
1:E:503:PHE:CZ	1:V:451:THR:HG21	179.60	0.47
1:V:487:ARG:HD2	1:X:583:ALA:O	2.14	0.47
1:X:583:ALA:O	1:Y:487:ARG:HD2	94.35	0.47
1:X:696:ARG:NE	1:X:698:ASN:OD1	2.42	0.47
1:Z:503:PHE:CZ	1:2:451:THR:HG21	109.96	0.47
1:Z:592:ALA:HA	1:1:499:ASN:ND2	99.40	0.47
1:3:503:PHE:CZ	1:4:451:THR:HG21	2.50	0.47
1:7:529:HIS:ND1	1:7:533:GLU:O	2.47	0.47
1:A:323:VAL:CG1	1:A:675:GLN:HE21	2.28	0.47
1:A:529:HIS:ND1	1:A:533:GLU:O	2.47	0.47
1:F:419:GLU:OE2	1:F:643:LYS:N	2.44	0.47
1:F:435:ARG:NH2	1:H:272:ASP:O	139.23	0.47
1:G:583:ALA:O	1:I:487:ARG:HD2	2.14	0.47
1:I:272:ASP:O	1:K:435:ARG:NH2	98.10	0.47
1:I:487:ARG:HD2	1:K:583:ALA:O	131.10	0.47
1:B:583:ALA:O	1:M:487:ARG:HD2	104.15	0.47
1:N:529:HIS:ND1	1:N:533:GLU:O	2.47	0.47
1:O:435:ARG:NH2	1:P:272:ASP:O	58.98	0.47
1:Q:323:VAL:CG1	1:Q:675:GLN:HE21	2.28	0.47
1:S:435:ARG:NH2	1:U:272:ASP:O	2.46	0.47
1:E:473:MET:HE1	1:X:275:TYR:HD2	169.75	0.47
1:1:592:ALA:HA	1:2:499:ASN:ND2	2.29	0.47
1:4:529:HIS:ND1	1:4:533:GLU:O	2.47	0.47
1:6:419:GLU:OE2	1:6:643:LYS:N	2.44	0.47
1:B:583:ALA:O	1:J:487:ARG:HD2	2.15	0.47
1:D:272:ASP:O	1:P:435:ARG:NH2	2.46	0.47
1:E:434:ASP:OD1	1:E:434:ASP:N	2.46	0.47
1:N:323:VAL:CG1	1:N:675:GLN:HE21	2.28	0.47
1:O:323:VAL:CG1	1:O:675:GLN:HE21	2.28	0.47
1:Q:696:ARG:NE	1:Q:698:ASN:OD1	2.42	0.47
1:U:323:VAL:CG1	1:U:675:GLN:HE21	2.28	0.47
1:S:583:ALA:O	1:U:487:ARG:HD2	2.15	0.47
1:U:583:ALA:O	1:V:487:ARG:HD2	79.93	0.47
1:V:323:VAL:CG1	1:V:675:GLN:HE21	2.28	0.47
1:W:323:VAL:CG1	1:W:675:GLN:HE21	2.28	0.47
1:W:503:PHE:CZ	1:Y:451:THR:HG21	41.55	0.47
1:X:323:VAL:CG1	1:X:675:GLN:HE21	2.28	0.47
1:Z:451:THR:HG21	1:4:503:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:323:VAL:CG1	1:7:675:GLN:HE21	2.28	0.47
1:8:323:VAL:CG1	1:8:675:GLN:HE21	2.28	0.47
1:D:251:PRO:HG3	1:D:374:MET:HE3	1.98	0.47
1:F:586:LEU:HD23	1:H:490:ARG:NH1	147.86	0.47
1:G:473:MET:HE1	1:I:275:TYR:HD2	1.77	0.47
1:L:323:VAL:CG1	1:L:675:GLN:HE21	2.28	0.47
1:L:592:ALA:HA	1:T:499:ASN:ND2	245.92	0.47
1:M:451:THR:HG21	1:N:503:PHE:CZ	102.51	0.47
1:N:583:ALA:O	1:O:487:ARG:HD2	79.93	0.47
1:Q:503:PHE:CZ	1:S:451:THR:HG21	97.38	0.47
1:Q:487:ARG:HD2	1:S:583:ALA:O	86.19	0.47
1:D:499:ASN:ND2	1:T:592:ALA:HA	158.65	0.47
1:T:451:THR:HG21	1:U:503:PHE:CZ	102.51	0.47
1:H:583:ALA:O	1:W:487:ARG:HD2	2.15	0.47
1:Z:323:VAL:CG1	1:Z:675:GLN:HE21	2.28	0.47
1:Z:503:PHE:CZ	1:3:451:THR:HG21	2.49	0.47
1:4:323:VAL:CG1	1:4:675:GLN:HE21	2.28	0.47
1:3:487:ARG:HD2	1:4:583:ALA:O	2.15	0.47
1:5:318:LEU:HB2	1:5:412:PHE:HB3	1.97	0.47
1:A:481:LEU:HD13	1:G:636:LEU:CD1	2.45	0.47
1:D:583:ALA:O	1:L:487:ARG:HD2	143.59	0.47
1:E:323:VAL:CG1	1:E:675:GLN:HE21	2.28	0.47
1:G:545:PHE:O	1:G:561:MET:N	2.27	0.47
1:I:251:PRO:HG3	1:I:374:MET:HE3	1.97	0.47
1:J:323:VAL:CG1	1:J:675:GLN:HE21	2.28	0.47
1:K:318:LEU:HB2	1:K:412:PHE:HB3	1.97	0.47
1:K:323:VAL:CG1	1:K:675:GLN:HE21	2.28	0.47
1:B:503:PHE:CZ	1:L:451:THR:HG21	2.50	0.47
1:P:323:VAL:CG1	1:P:675:GLN:HE21	2.28	0.47
1:R:583:ALA:O	1:S:487:ARG:HD2	2.14	0.47
1:H:451:THR:HG21	1:W:503:PHE:CZ	2.50	0.47
1:Z:487:ARG:HD2	1:2:583:ALA:O	97.41	0.47
1:5:503:PHE:CZ	1:7:451:THR:HG21	2.50	0.47
1:B:503:PHE:CZ	1:C:451:THR:HG21	102.51	0.47
1:C:323:VAL:CG1	1:C:675:GLN:HE21	2.28	0.47
1:D:318:LEU:HB2	1:D:412:PHE:HB3	1.97	0.47
1:F:323:VAL:CG1	1:F:675:GLN:HE21	2.28	0.47
1:G:323:VAL:CG1	1:G:675:GLN:HE21	2.28	0.47
1:H:323:VAL:CG1	1:H:675:GLN:HE21	2.28	0.47
1:J:586:LEU:HD23	1:K:490:ARG:NH1	82.06	0.47
1:I:503:PHE:CZ	1:K:451:THR:HG21	118.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:503:PHE:CZ	1:O:451:THR:HG21	118.81	0.47
1:M:323:VAL:CG1	1:M:675:GLN:HE21	2.28	0.47
1:Q:318:LEU:HB2	1:Q:412:PHE:HB3	1.97	0.47
1:W:318:LEU:HB2	1:W:412:PHE:HB3	1.97	0.47
1:6:488:GLN:OE1	1:6:540:SER:OG	2.33	0.47
1:6:451:THR:HG21	1:7:503:PHE:CZ	2.50	0.47
1:K:272:ASP:O	1:8:435:ARG:NH2	2.46	0.47
1:A:583:ALA:O	1:8:487:ARG:HD2	154.57	0.47
1:D:323:VAL:CG1	1:D:675:GLN:HE21	2.28	0.47
1:E:318:LEU:HB2	1:E:412:PHE:HB3	1.97	0.47
1:E:451:THR:HG21	1:Q:503:PHE:CZ	2.50	0.47
1:E:503:PHE:CZ	1:F:451:THR:HG21	2.50	0.47
1:F:488:GLN:OE1	1:F:540:SER:OG	2.33	0.47
1:E:487:ARG:HD2	1:F:583:ALA:O	2.15	0.47
1:G:503:PHE:CZ	1:H:451:THR:HG21	73.97	0.47
1:J:276:PHE:HB3	1:J:384:ASN:HB3	1.97	0.47
1:L:488:GLN:OE1	1:L:540:SER:OG	2.33	0.47
1:M:251:PRO:HG3	1:M:374:MET:HE3	1.96	0.47
1:M:583:ALA:O	1:N:487:ARG:HD2	94.35	0.47
1:O:318:LEU:HB2	1:O:412:PHE:HB3	1.97	0.47
1:Q:583:ALA:O	1:R:487:ARG:HD2	79.92	0.47
1:U:300:GLN:NE2	1:U:703:TYR:O	2.41	0.47
1:W:473:MET:HE1	1:X:275:TYR:HD2	55.76	0.47
1:Y:488:GLN:OE1	1:Y:540:SER:OG	2.33	0.47
1:2:323:VAL:CG1	1:2:675:GLN:HE21	2.28	0.47
1:7:300:GLN:NE2	1:7:703:TYR:O	2.41	0.47
1:A:276:PHE:HB3	1:A:384:ASN:HB3	1.98	0.47
1:A:318:LEU:HB2	1:A:412:PHE:HB3	1.97	0.47
1:C:488:GLN:OE1	1:C:540:SER:OG	2.33	0.47
1:E:487:ARG:HD2	1:V:583:ALA:O	158.02	0.47
1:F:276:PHE:HB3	1:F:384:ASN:HB3	1.97	0.47
1:H:487:ARG:HD2	1:Y:583:ALA:O	2.14	0.47
1:H:488:GLN:OE1	1:H:540:SER:OG	2.33	0.47
1:H:621:TRP:HA	1:H:640:PHE:H	1.80	0.47
1:I:323:VAL:CG1	1:I:675:GLN:HE21	2.28	0.47
1:I:583:ALA:O	1:J:487:ARG:HD2	94.35	0.47
1:K:621:TRP:HA	1:K:640:PHE:H	1.80	0.47
1:L:276:PHE:HB3	1:L:384:ASN:HB3	1.98	0.47
1:M:276:PHE:HB3	1:M:384:ASN:HB3	1.97	0.47
1:M:318:LEU:HB2	1:M:412:PHE:HB3	1.97	0.47
1:N:276:PHE:HB3	1:N:384:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:488:GLN:OE1	1:N:540:SER:OG	2.33	0.47
1:R:488:GLN:OE1	1:R:540:SER:OG	2.33	0.47
1:S:451:THR:HG21	1:U:503:PHE:CZ	2.50	0.47
1:S:488:GLN:OE1	1:S:540:SER:OG	2.33	0.47
1:S:323:VAL:CG1	1:S:675:GLN:HE21	2.28	0.47
1:U:451:THR:HG21	1:V:503:PHE:CZ	73.97	0.47
1:V:621:TRP:HA	1:V:640:PHE:H	1.80	0.47
1:W:583:ALA:O	1:Y:487:ARG:HD2	2.14	0.47
1:W:487:ARG:HD2	1:Y:583:ALA:O	18.71	0.47
1:Z:583:ALA:O	1:4:487:ARG:HD2	2.14	0.46
1:6:583:ALA:O	1:7:487:ARG:HD2	2.15	0.46
1:A:545:PHE:O	1:A:561:MET:N	2.27	0.46
1:A:592:ALA:HA	1:G:499:ASN:ND2	2.28	0.46
1:G:318:LEU:HB2	1:G:412:PHE:HB3	1.97	0.46
1:F:487:ARG:HD2	1:G:583:ALA:O	86.19	0.46
1:H:566:GLU:OE2	1:H:569:LYS:NZ	2.45	0.46
1:J:251:PRO:HG3	1:J:374:MET:HE3	1.96	0.46
1:J:566:GLU:OE2	1:J:569:LYS:NZ	2.45	0.46
1:N:566:GLU:OE2	1:N:569:LYS:NZ	2.45	0.46
1:P:318:LEU:HB2	1:P:412:PHE:HB3	1.97	0.46
1:N:583:ALA:O	1:P:487:ARG:HD2	2.14	0.46
1:R:323:VAL:CG1	1:R:675:GLN:HE21	2.28	0.46
1:T:276:PHE:HB3	1:T:384:ASN:HB3	1.98	0.46
1:U:318:LEU:HB2	1:U:412:PHE:HB3	1.97	0.46
1:T:583:ALA:O	1:U:487:ARG:HD2	94.35	0.46
1:R:487:ARG:HD2	1:U:583:ALA:O	2.15	0.46
1:V:318:LEU:HB2	1:V:412:PHE:HB3	1.97	0.46
1:V:503:PHE:CZ	1:X:451:THR:HG21	2.50	0.46
1:T:487:ARG:HD2	1:V:583:ALA:O	131.10	0.46
1:X:451:THR:HG21	1:Y:503:PHE:CZ	102.51	0.46
1:Y:621:TRP:HA	1:Y:640:PHE:H	1.80	0.46
1:Y:323:VAL:CG1	1:Y:675:GLN:HE21	2.28	0.46
1:Z:276:PHE:HB3	1:Z:384:ASN:HB3	1.98	0.46
1:Z:318:LEU:HB2	1:Z:412:PHE:HB3	1.97	0.46
1:1:323:VAL:CG1	1:1:675:GLN:HE21	2.28	0.46
1:3:323:VAL:CG1	1:3:675:GLN:HE21	2.28	0.46
1:5:487:ARG:HD2	1:7:583:ALA:O	2.14	0.46
1:7:621:TRP:HA	1:7:640:PHE:H	1.80	0.46
1:A:566:GLU:OE2	1:A:569:LYS:NZ	2.45	0.46
1:A:621:TRP:HA	1:A:640:PHE:H	1.80	0.46
1:B:318:LEU:HB2	1:B:412:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLN:NE2	1:C:276:PHE:HE1	2.14	0.46
1:E:621:TRP:HA	1:E:640:PHE:H	1.80	0.46
1:F:621:TRP:HA	1:F:640:PHE:H	1.80	0.46
1:J:621:TRP:HA	1:J:640:PHE:H	1.80	0.46
1:L:260:GLN:NE2	1:L:276:PHE:HE1	2.14	0.46
1:Q:621:TRP:HA	1:Q:640:PHE:H	1.80	0.46
1:R:276:PHE:HB3	1:R:384:ASN:HB3	1.97	0.46
1:X:566:GLU:OE2	1:X:569:LYS:NZ	2.45	0.46
1:A:251:PRO:HG3	1:A:374:MET:HE3	1.97	0.46
1:A:487:ARG:HD2	1:K:583:ALA:O	147.26	0.46
1:D:275:TYR:HD2	1:T:473:MET:HE1	130.05	0.46
1:E:583:ALA:O	1:Q:487:ARG:HD2	2.14	0.46
1:J:583:ALA:O	1:L:487:ARG:HD2	2.15	0.46
1:N:621:TRP:HA	1:N:640:PHE:H	1.80	0.46
1:O:621:TRP:HA	1:O:640:PHE:H	1.80	0.46
1:P:260:GLN:NE2	1:P:276:PHE:HE1	2.14	0.46
1:S:318:LEU:HB2	1:S:412:PHE:HB3	1.97	0.46
1:T:260:GLN:NE2	1:T:276:PHE:HE1	2.14	0.46
1:W:621:TRP:HA	1:W:640:PHE:H	1.80	0.46
1:Z:260:GLN:NE2	1:Z:276:PHE:HE1	2.14	0.46
1:1:435:ARG:NH2	1:2:272:ASP:O	2.47	0.46
1:4:276:PHE:HB3	1:4:384:ASN:HB3	1.97	0.46
1:4:544:MET:HG2	1:4:562:LEU:HD23	1.98	0.46
1:4:621:TRP:HA	1:4:640:PHE:H	1.80	0.46
1:6:276:PHE:HB3	1:6:384:ASN:HB3	1.97	0.46
1:6:621:TRP:HA	1:6:640:PHE:H	1.80	0.46
1:8:260:GLN:NE2	1:8:276:PHE:HE1	2.14	0.46
1:A:451:THR:HG21	1:8:503:PHE:CZ	175.47	0.46
1:B:251:PRO:HG3	1:B:374:MET:HE3	1.97	0.46
1:B:488:GLN:OE1	1:B:540:SER:OG	2.33	0.46
1:C:503:PHE:CZ	1:M:451:THR:HG21	2.49	0.46
1:H:260:GLN:NE2	1:H:276:PHE:HE1	2.14	0.46
1:J:583:ALA:O	1:K:487:ARG:HD2	79.93	0.46
1:L:419:GLU:OE2	1:L:643:LYS:N	2.44	0.46
1:L:566:GLU:OE2	1:L:569:LYS:NZ	2.45	0.46
1:D:583:ALA:O	1:N:487:ARG:HD2	2.15	0.46
1:R:251:PRO:HG3	1:R:374:MET:HE3	1.97	0.46
1:S:419:GLU:OE2	1:S:643:LYS:N	2.44	0.46
1:T:323:VAL:CG1	1:T:675:GLN:HE21	2.28	0.46
1:U:260:GLN:NE2	1:U:276:PHE:HE1	2.14	0.46
1:V:419:GLU:OE2	1:V:643:LYS:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:318:LEU:HB2	1:X:412:PHE:HB3	1.97	0.46
1:Y:260:GLN:NE2	1:Y:276:PHE:HE1	2.14	0.46
1:1:276:PHE:HB3	1:1:384:ASN:HB3	1.97	0.46
1:1:260:GLN:NE2	1:1:276:PHE:HE1	2.14	0.46
1:1:473:MET:HE1	1:2:275:TYR:HD2	1.80	0.46
1:2:318:LEU:HB2	1:2:412:PHE:HB3	1.97	0.46
1:8:318:LEU:HB2	1:8:412:PHE:HB3	1.97	0.46
1:A:503:PHE:CZ	1:K:451:THR:HG21	151.81	0.46
1:C:487:ARG:HD2	1:M:583:ALA:O	2.15	0.46
1:C:544:MET:HG2	1:C:562:LEU:HD23	1.98	0.46
1:D:451:THR:HG21	1:N:503:PHE:CZ	2.50	0.46
1:E:451:THR:HG21	1:X:503:PHE:CZ	154.21	0.46
1:G:276:PHE:HB3	1:G:384:ASN:HB3	1.98	0.46
1:H:318:LEU:HB2	1:H:412:PHE:HB3	1.97	0.46
1:H:419:GLU:OE2	1:H:643:LYS:N	2.44	0.46
1:I:276:PHE:HB3	1:I:384:ASN:HB3	1.97	0.46
1:J:696:ARG:NE	1:J:698:ASN:OD1	2.42	0.46
1:L:544:MET:HG2	1:L:562:LEU:HD23	1.98	0.46
1:N:544:MET:HG2	1:N:562:LEU:HD23	1.98	0.46
1:R:260:GLN:NE2	1:R:276:PHE:HE1	2.14	0.46
1:R:621:TRP:HA	1:R:640:PHE:H	1.80	0.46
1:S:260:GLN:NE2	1:S:276:PHE:HE1	2.14	0.46
1:U:251:PRO:HG3	1:U:374:MET:HE3	1.98	0.46
1:U:488:GLN:OE1	1:U:540:SER:OG	2.33	0.46
1:V:260:GLN:NE2	1:V:276:PHE:HE1	2.14	0.46
1:V:696:ARG:NE	1:V:698:ASN:OD1	2.42	0.46
1:X:621:TRP:HA	1:X:640:PHE:H	1.80	0.46
1:Y:251:PRO:HG3	1:Y:374:MET:HE3	1.97	0.46
1:4:260:GLN:NE2	1:4:276:PHE:HE1	2.14	0.46
1:6:429:HIS:O	1:7:383:LEU:HD11	2.16	0.46
1:7:566:GLU:OE2	1:7:569:LYS:NZ	2.45	0.46
1:A:318:LEU:HA	1:A:318:LEU:HD13	1.82	0.46
1:A:592:ALA:HA	1:8:499:ASN:ND2	177.34	0.46
1:B:323:VAL:CG1	1:B:675:GLN:HE21	2.28	0.46
1:C:276:PHE:HB3	1:C:384:ASN:HB3	1.98	0.46
1:D:621:TRP:HA	1:D:640:PHE:H	1.80	0.46
1:E:368:PHE:CE2	1:E:370:ALA:HB3	2.51	0.46
1:E:383:LEU:HD11	1:F:429:HIS:O	2.16	0.46
1:E:544:MET:HG2	1:E:562:LEU:HD23	1.98	0.46
1:F:583:ALA:O	1:H:487:ARG:HD2	143.59	0.46
1:I:544:MET:HG2	1:I:562:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:260:GLN:NE2	1:J:276:PHE:HE1	2.14	0.46
1:J:318:LEU:HB2	1:J:412:PHE:HB3	1.97	0.46
1:J:451:THR:HG21	1:L:503:PHE:CZ	2.49	0.46
1:L:368:PHE:CE2	1:L:370:ALA:HB3	2.51	0.46
1:M:368:PHE:CE2	1:M:370:ALA:HB3	2.51	0.46
1:N:260:GLN:NE2	1:N:276:PHE:HE1	2.14	0.46
1:N:451:THR:HG21	1:P:503:PHE:CZ	2.50	0.46
1:P:276:PHE:HB3	1:P:384:ASN:HB3	1.97	0.46
1:C:499:ASN:ND2	1:P:592:ALA:HA	83.37	0.46
1:P:621:TRP:HA	1:P:640:PHE:H	1.80	0.46
1:Q:276:PHE:HB3	1:Q:384:ASN:HB3	1.97	0.46
1:T:621:TRP:HA	1:T:640:PHE:H	1.80	0.46
1:V:276:PHE:HB3	1:V:384:ASN:HB3	1.97	0.46
1:W:276:PHE:HB3	1:W:384:ASN:HB3	1.98	0.46
1:W:583:ALA:O	1:X:487:ARG:HD2	79.93	0.46
1:W:696:ARG:NE	1:W:698:ASN:OD1	2.42	0.46
1:E:583:ALA:O	1:X:487:ARG:HD2	141.87	0.46
1:Z:258:TYR:OH	1:Z:399:GLU:OE1	2.28	0.46
1:2:621:TRP:HA	1:2:640:PHE:H	1.80	0.46
1:7:368:PHE:CE2	1:7:370:ALA:HB3	2.51	0.46
1:K:275:TYR:HD2	1:8:473:MET:HE1	1.78	0.46
1:8:621:TRP:HA	1:8:640:PHE:H	1.80	0.46
1:A:544:MET:HG2	1:A:562:LEU:HD23	1.98	0.46
1:B:368:PHE:CE2	1:B:370:ALA:HB3	2.51	0.46
1:C:368:PHE:CE2	1:C:370:ALA:HB3	2.51	0.46
1:B:499:ASN:HD22	1:C:592:ALA:HA	104.36	0.46
1:D:272:ASP:O	1:T:435:ARG:NH2	131.45	0.46
1:F:368:PHE:CE2	1:F:370:ALA:HB3	2.51	0.46
1:G:499:ASN:HD22	1:H:592:ALA:HA	80.70	0.46
1:G:544:MET:HG2	1:G:562:LEU:HD23	1.98	0.46
1:I:368:PHE:CE2	1:I:370:ALA:HB3	2.51	0.46
1:J:368:PHE:CE2	1:J:370:ALA:HB3	2.51	0.46
1:M:260:GLN:NE2	1:M:276:PHE:HE1	2.14	0.46
1:M:621:TRP:HA	1:M:640:PHE:H	1.80	0.46
1:N:368:PHE:CE2	1:N:370:ALA:HB3	2.51	0.46
1:P:488:GLN:OE1	1:P:540:SER:OG	2.33	0.46
1:N:592:ALA:HA	1:P:499:ASN:ND2	2.31	0.46
1:E:592:ALA:HA	1:Q:499:ASN:HD22	1.81	0.46
1:R:544:MET:HG2	1:R:562:LEU:HD23	1.98	0.46
1:S:251:PRO:HG3	1:S:374:MET:HE3	1.96	0.46
1:W:368:PHE:CE2	1:W:370:ALA:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:451:THR:HG21	1:X:503:PHE:CZ	73.97	0.46
1:Y:419:GLU:OE2	1:Y:643:LYS:N	2.44	0.46
1:Y:544:MET:HG2	1:Y:562:LEU:HD23	1.98	0.46
1:Z:368:PHE:CE2	1:Z:370:ALA:HB3	2.51	0.46
1:Z:544:MET:HG2	1:Z:562:LEU:HD23	1.98	0.46
1:1:621:TRP:HA	1:1:640:PHE:H	1.80	0.46
1:2:260:GLN:NE2	1:2:276:PHE:HE1	2.14	0.46
1:3:260:GLN:NE2	1:3:276:PHE:HE1	2.14	0.46
1:5:592:ALA:HA	1:6:499:ASN:HD22	1.81	0.46
1:6:368:PHE:CE2	1:6:370:ALA:HB3	2.51	0.46
1:6:323:VAL:CG1	1:6:675:GLN:HE21	2.28	0.46
1:5:499:ASN:HD22	1:7:592:ALA:HA	1.81	0.46
1:7:309:PHE:HE2	1:7:731:THR:HG21	1.81	0.46
1:8:276:PHE:HB3	1:8:384:ASN:HB3	1.97	0.46
1:A:368:PHE:CE2	1:A:370:ALA:HB3	2.51	0.46
1:A:499:ASN:ND2	1:K:592:ALA:HA	160.71	0.46
1:B:499:ASN:HD22	1:L:592:ALA:HA	1.81	0.46
1:C:499:ASN:HD22	1:P:592:ALA:HA	83.28	0.46
1:E:276:PHE:HB3	1:E:384:ASN:HB3	1.98	0.46
1:E:499:ASN:ND2	1:F:592:ALA:HA	2.31	0.46
1:E:309:PHE:HE2	1:E:731:THR:HG21	1.81	0.46
1:G:488:GLN:OE1	1:G:540:SER:OG	2.33	0.46
1:I:318:LEU:HB2	1:I:412:PHE:HB3	1.97	0.46
1:I:499:ASN:HD22	1:K:592:ALA:HA	132.18	0.46
1:L:621:TRP:HA	1:L:640:PHE:H	1.80	0.46
1:M:696:ARG:NE	1:M:698:ASN:OD1	2.42	0.46
1:Q:368:PHE:CE2	1:Q:370:ALA:HB3	2.51	0.46
1:R:368:PHE:CE2	1:R:370:ALA:HB3	2.51	0.46
1:S:368:PHE:CE2	1:S:370:ALA:HB3	2.51	0.46
1:T:368:PHE:CE2	1:T:370:ALA:HB3	2.51	0.46
1:T:383:LEU:HD11	1:V:429:HIS:O	97.74	0.46
1:U:276:PHE:HB3	1:U:384:ASN:HB3	1.97	0.46
1:R:383:LEU:HD11	1:U:429:HIS:O	2.16	0.46
1:U:309:PHE:HE2	1:U:731:THR:HG21	1.81	0.46
1:V:383:LEU:HD11	1:X:429:HIS:O	2.16	0.46
1:V:566:GLU:OE2	1:V:569:LYS:NZ	2.45	0.46
1:X:251:PRO:HG3	1:X:374:MET:HE3	2.00	0.46
1:E:429:HIS:O	1:X:383:LEU:HD11	158.91	0.46
1:W:429:HIS:O	1:X:383:LEU:HD11	60.78	0.46
1:3:275:TYR:HD2	1:4:473:MET:HE1	1.79	0.46
1:3:368:PHE:CE2	1:3:370:ALA:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:621:TRP:HA	1:3:640:PHE:H	1.80	0.46
1:4:368:PHE:CE2	1:4:370:ALA:HB3	2.51	0.46
1:4:566:GLU:OE2	1:4:569:LYS:NZ	2.45	0.46
1:5:323:VAL:CG1	1:5:675:GLN:HE21	2.28	0.46
1:5:429:HIS:O	1:6:383:LEU:HD11	2.16	0.46
1:6:592:ALA:HA	1:7:499:ASN:ND2	2.31	0.46
1:7:544:MET:HG2	1:7:562:LEU:HD23	1.98	0.46
1:7:581:VAL:CG1	1:7:595:VAL:HB	2.46	0.46
1:8:544:MET:HG2	1:8:562:LEU:HD23	1.98	0.46
1:8:566:GLU:OE2	1:8:569:LYS:NZ	2.45	0.46
1:A:260:GLN:NE2	1:A:276:PHE:HE1	2.14	0.46
1:A:382:THR:HG21	1:A:394:SER:H	1.81	0.46
1:A:488:GLN:OE1	1:A:540:SER:OG	2.33	0.46
1:C:275:TYR:HD2	1:P:473:MET:HE1	54.21	0.46
1:C:318:LEU:HB2	1:C:412:PHE:HB3	1.97	0.46
1:D:592:ALA:HA	1:N:499:ASN:ND2	2.31	0.46
1:E:260:GLN:NE2	1:E:276:PHE:HE1	2.14	0.46
1:E:592:ALA:HA	1:X:499:ASN:ND2	158.70	0.46
1:F:544:MET:HG2	1:F:562:LEU:HD23	1.98	0.46
1:G:260:GLN:NE2	1:G:276:PHE:HE1	2.14	0.46
1:G:621:TRP:HA	1:G:640:PHE:H	1.80	0.46
1:H:368:PHE:CE2	1:H:370:ALA:HB3	2.51	0.46
1:H:276:PHE:HB3	1:H:384:ASN:HB3	1.97	0.46
1:H:309:PHE:HE2	1:H:731:THR:HG21	1.81	0.46
1:I:260:GLN:NE2	1:I:276:PHE:HE1	2.14	0.46
1:K:276:PHE:HB3	1:K:384:ASN:HB3	1.97	0.46
1:A:499:ASN:HD22	1:K:592:ALA:HA	160.13	0.46
1:M:499:ASN:ND2	1:O:592:ALA:HA	132.08	0.46
1:O:260:GLN:NE2	1:O:276:PHE:HE1	2.14	0.46
1:O:276:PHE:HB3	1:O:384:ASN:HB3	1.97	0.46
1:O:368:PHE:CE2	1:O:370:ALA:HB3	2.51	0.46
1:O:382:THR:HG21	1:O:394:SER:H	1.81	0.46
1:C:503:PHE:CZ	1:P:451:THR:HG21	72.62	0.46
1:P:544:MET:HG2	1:P:562:LEU:HD23	1.98	0.46
1:Q:488:GLN:OE1	1:Q:540:SER:OG	2.33	0.46
1:Q:581:VAL:CG1	1:Q:595:VAL:HB	2.46	0.46
1:F:499:ASN:HD22	1:Q:592:ALA:HA	1.81	0.46
1:R:401:PHE:N	1:R:401:PHE:CD1	2.84	0.46
1:S:309:PHE:HE2	1:S:731:THR:HG21	1.81	0.46
1:T:401:PHE:N	1:T:401:PHE:CD1	2.84	0.46
1:E:383:LEU:HD11	1:V:429:HIS:O	124.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:488:GLN:OE1	1:V:540:SER:OG	2.33	0.46
1:W:383:LEU:HD11	1:Y:429:HIS:O	44.37	0.46
1:W:488:GLN:OE1	1:W:540:SER:OG	2.33	0.46
1:X:429:HIS:O	1:Y:383:LEU:HD11	34.69	0.46
1:Y:566:GLU:OE2	1:Y:569:LYS:NZ	2.45	0.46
1:3:276:PHE:HB3	1:3:384:ASN:HB3	1.97	0.46
1:Z:499:ASN:ND2	1:3:592:ALA:HA	2.31	0.46
1:Z:592:ALA:HA	1:4:499:ASN:ND2	2.31	0.46
1:5:621:TRP:HA	1:5:640:PHE:H	1.80	0.46
1:A:581:VAL:CG1	1:A:595:VAL:HB	2.46	0.46
1:B:260:GLN:NE2	1:B:276:PHE:HE1	2.14	0.46
1:B:429:HIS:O	1:J:383:LEU:HD11	2.16	0.46
1:D:260:GLN:NE2	1:D:276:PHE:HE1	2.14	0.46
1:D:276:PHE:HB3	1:D:384:ASN:HB3	1.98	0.46
1:E:581:VAL:CG1	1:E:595:VAL:HB	2.46	0.46
1:F:696:ARG:NE	1:F:698:ASN:OD1	2.42	0.46
1:G:251:PRO:HG3	1:G:374:MET:HE3	1.98	0.46
1:H:544:MET:HG2	1:H:562:LEU:HD23	1.98	0.46
1:H:592:ALA:HA	1:W:499:ASN:HD22	1.81	0.46
1:I:621:TRP:HA	1:I:640:PHE:H	1.80	0.46
1:K:260:GLN:NE2	1:K:276:PHE:HE1	2.14	0.46
1:L:581:VAL:CG1	1:L:595:VAL:HB	2.46	0.46
1:N:581:VAL:CG1	1:N:595:VAL:HB	2.46	0.46
1:P:368:PHE:CE2	1:P:370:ALA:HB3	2.51	0.46
1:N:429:HIS:O	1:P:383:LEU:HD11	2.16	0.46
1:Q:499:ASN:HD22	1:S:592:ALA:HA	95.88	0.46
1:R:309:PHE:HE2	1:R:731:THR:HG21	1.81	0.46
1:R:429:HIS:O	1:S:383:LEU:HD11	2.16	0.46
1:S:276:PHE:HB3	1:S:384:ASN:HB3	1.97	0.46
1:Q:499:ASN:ND2	1:S:592:ALA:HA	95.91	0.46
1:U:544:MET:HG2	1:U:562:LEU:HD23	1.98	0.46
1:U:621:TRP:HA	1:U:640:PHE:H	1.80	0.46
1:V:251:PRO:HG3	1:V:374:MET:HE3	2.03	0.46
1:W:382:THR:HG21	1:W:394:SER:H	1.81	0.46
1:W:581:VAL:CG1	1:W:595:VAL:HB	2.46	0.46
1:X:368:PHE:CE2	1:X:370:ALA:HB3	2.51	0.46
1:X:276:PHE:HB3	1:X:384:ASN:HB3	1.97	0.46
1:X:526:MET:HE2	1:X:575:ALA:HA	1.98	0.46
1:W:429:HIS:O	1:Y:383:LEU:HD11	2.16	0.46
1:Y:696:ARG:NE	1:Y:698:ASN:OD1	2.42	0.46
1:Z:581:VAL:CG1	1:Z:595:VAL:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:621:TRP:HA	1:Z:640:PHE:H	1.80	0.46
1:2:276:PHE:HB3	1:2:384:ASN:HB3	1.98	0.45
1:2:368:PHE:CE2	1:2:370:ALA:HB3	2.51	0.45
1:Z:383:LEU:HD11	1:3:429:HIS:O	2.16	0.45
1:4:309:PHE:HE2	1:4:731:THR:HG21	1.81	0.45
1:5:276:PHE:HB3	1:5:384:ASN:HB3	1.97	0.45
1:5:382:THR:HG21	1:5:394:SER:H	1.81	0.45
1:A:429:HIS:O	1:8:383:LEU:HD11	149.25	0.45
1:A:592:ALA:HA	1:8:499:ASN:HD22	176.58	0.45
1:B:382:THR:HG21	1:B:394:SER:H	1.82	0.45
1:B:429:HIS:O	1:M:383:LEU:HD11	116.16	0.45
1:B:621:TRP:HA	1:B:640:PHE:H	1.80	0.45
1:D:382:THR:HG21	1:D:394:SER:H	1.81	0.45
1:E:382:THR:HG21	1:E:394:SER:H	1.81	0.45
1:F:309:PHE:HE2	1:F:731:THR:HG21	1.81	0.45
1:H:429:HIS:O	1:W:383:LEU:HD11	2.16	0.45
1:I:592:ALA:HA	1:J:499:ASN:HD22	104.38	0.45
1:J:544:MET:HG2	1:J:562:LEU:HD23	1.98	0.45
1:B:592:ALA:HA	1:M:499:ASN:HD22	126.53	0.45
1:N:401:PHE:N	1:N:401:PHE:CD1	2.84	0.45
1:N:473:MET:HE1	1:O:275:TYR:HD2	55.76	0.45
1:D:592:ALA:HA	1:N:499:ASN:HD22	1.81	0.45
1:M:592:ALA:HA	1:N:499:ASN:ND2	104.62	0.45
1:M:383:LEU:HD11	1:O:429:HIS:O	97.74	0.45
1:O:566:GLU:OE2	1:O:569:LYS:NZ	2.45	0.45
1:O:592:ALA:HA	1:P:499:ASN:ND2	104.63	0.45
1:Q:383:LEU:HD11	1:S:429:HIS:O	97.66	0.45
1:F:383:LEU:HD11	1:Q:429:HIS:O	2.17	0.45
1:Q:429:HIS:O	1:R:383:LEU:HD11	60.77	0.45
1:S:544:MET:HG2	1:S:562:LEU:HD23	1.98	0.45
1:T:309:PHE:HE2	1:T:731:THR:HG21	1.81	0.45
1:T:544:MET:HG2	1:T:562:LEU:HD23	1.98	0.45
1:U:581:VAL:CG1	1:U:595:VAL:HB	2.47	0.45
1:W:260:GLN:NE2	1:W:276:PHE:HE1	2.14	0.45
1:H:592:ALA:HA	1:W:499:ASN:ND2	2.31	0.45
1:W:592:ALA:HA	1:X:499:ASN:ND2	80.58	0.45
1:X:309:PHE:HE2	1:X:731:THR:HG21	1.81	0.45
1:Y:318:LEU:HB2	1:Y:412:PHE:HB3	1.97	0.45
1:Y:276:PHE:HB3	1:Y:384:ASN:HB3	1.97	0.45
1:H:383:LEU:HD11	1:Y:429:HIS:O	2.16	0.45
1:W:592:ALA:HA	1:Y:499:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:499:ASN:ND2	1:2:592:ALA:HA	112.43	0.45
1:1:485:CYS:HB3	1:1:579:TYR:HB2	1.99	0.45
1:1:581:VAL:CG1	1:1:595:VAL:HB	2.46	0.45
1:3:488:GLN:OE1	1:3:540:SER:OG	2.33	0.45
1:4:401:PHE:N	1:4:401:PHE:CD1	2.84	0.45
1:5:485:CYS:HB3	1:5:579:TYR:HB2	1.99	0.45
1:5:592:ALA:HA	1:6:499:ASN:ND2	2.32	0.45
1:7:260:GLN:NE2	1:7:276:PHE:HE1	2.14	0.45
1:7:276:PHE:HB3	1:7:384:ASN:HB3	1.97	0.45
1:A:309:PHE:HE2	1:A:731:THR:HG21	1.81	0.45
1:A:435:ARG:NH2	1:G:272:ASP:O	2.49	0.45
1:B:383:LEU:HD11	1:C:429:HIS:O	34.68	0.45
1:B:485:CYS:HB3	1:B:579:TYR:HB2	1.99	0.45
1:C:382:THR:HG21	1:C:394:SER:H	1.82	0.45
1:C:621:TRP:HA	1:C:640:PHE:H	1.80	0.45
1:B:592:ALA:HA	1:J:499:ASN:HD22	1.82	0.45
1:J:309:PHE:HE2	1:J:731:THR:HG21	1.81	0.45
1:K:382:THR:HG21	1:K:394:SER:H	1.82	0.45
1:K:488:GLN:OE1	1:K:540:SER:OG	2.33	0.45
1:L:251:PRO:HG3	1:L:374:MET:HE3	1.99	0.45
1:L:318:LEU:HB2	1:L:412:PHE:HB3	1.97	0.45
1:M:544:MET:HG2	1:M:562:LEU:HD23	1.98	0.45
1:C:383:LEU:HD11	1:P:429:HIS:O	59.87	0.45
1:Q:382:THR:HG21	1:Q:394:SER:H	1.81	0.45
1:Q:485:CYS:HB3	1:Q:579:TYR:HB2	1.99	0.45
1:R:318:LEU:HB2	1:R:412:PHE:HB3	1.97	0.45
1:Q:592:ALA:HA	1:R:499:ASN:ND2	80.58	0.45
1:S:581:VAL:CG1	1:S:595:VAL:HB	2.47	0.45
1:T:318:LEU:HB2	1:T:412:PHE:HB3	1.97	0.45
1:U:382:THR:HG21	1:U:394:SER:H	1.82	0.45
1:U:419:GLU:OE2	1:U:643:LYS:N	2.44	0.45
1:S:592:ALA:HA	1:U:499:ASN:ND2	2.31	0.45
1:R:499:ASN:HD22	1:U:592:ALA:HA	1.81	0.45
1:V:382:THR:HG21	1:V:394:SER:H	1.81	0.45
1:V:434:ASP:OD1	1:V:434:ASP:N	2.45	0.45
1:U:592:ALA:HA	1:V:499:ASN:ND2	80.58	0.45
1:X:544:MET:HG2	1:X:562:LEU:HD23	1.98	0.45
1:Z:251:PRO:HG3	1:Z:374:MET:HE3	1.99	0.45
1:3:566:GLU:OE2	1:3:569:LYS:NZ	2.45	0.45
1:4:485:CYS:HB3	1:4:579:TYR:HB2	1.99	0.45
1:5:499:ASN:ND2	1:7:592:ALA:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:368:PHE:CE2	1:8:370:ALA:HB3	2.51	0.45
1:A:481:LEU:HD13	1:G:636:LEU:HD11	1.97	0.45
1:C:581:VAL:CG1	1:C:595:VAL:HB	2.46	0.45
1:D:368:PHE:CE2	1:D:370:ALA:HB3	2.51	0.45
1:D:544:MET:HG2	1:D:562:LEU:HD23	1.98	0.45
1:D:592:ALA:HA	1:L:499:ASN:ND2	157.95	0.45
1:F:318:LEU:HB2	1:F:412:PHE:HB3	1.97	0.45
1:F:383:LEU:HD11	1:G:429:HIS:O	97.66	0.45
1:G:368:PHE:CE2	1:G:370:ALA:HB3	2.51	0.45
1:G:499:ASN:ND2	1:H:592:ALA:HA	80.57	0.45
1:I:382:THR:HG21	1:I:394:SER:H	1.82	0.45
1:I:581:VAL:CG1	1:I:595:VAL:HB	2.46	0.45
1:I:429:HIS:O	1:J:383:LEU:HD11	34.67	0.45
1:J:382:THR:HG21	1:J:394:SER:H	1.81	0.45
1:I:592:ALA:HA	1:J:499:ASN:ND2	104.64	0.45
1:K:499:ASN:ND2	1:8:592:ALA:HA	2.31	0.45
1:I:499:ASN:ND2	1:K:592:ALA:HA	132.10	0.45
1:D:592:ALA:HA	1:L:499:ASN:HD22	157.56	0.45
1:M:581:VAL:CG1	1:M:595:VAL:HB	2.46	0.45
1:N:309:PHE:HE2	1:N:731:THR:HG21	1.81	0.45
1:M:429:HIS:O	1:N:383:LEU:HD11	34.69	0.45
1:N:485:CYS:HB3	1:N:579:TYR:HB2	1.99	0.45
1:O:309:PHE:HE2	1:O:731:THR:HG21	1.81	0.45
1:O:318:LEU:HD13	1:O:318:LEU:HA	1.82	0.45
1:N:429:HIS:O	1:O:383:LEU:HD11	60.77	0.45
1:O:429:HIS:O	1:P:383:LEU:HD11	34.69	0.45
1:N:592:ALA:HA	1:P:499:ASN:HD22	1.81	0.45
1:Q:260:GLN:NE2	1:Q:276:PHE:HE1	2.14	0.45
1:R:592:ALA:HA	1:S:499:ASN:HD22	1.81	0.45
1:S:566:GLU:OE2	1:S:569:LYS:NZ	2.45	0.45
1:T:485:CYS:HB3	1:T:579:TYR:HB2	1.99	0.45
1:T:581:VAL:CG1	1:T:595:VAL:HB	2.46	0.45
1:T:592:ALA:HA	1:U:499:ASN:HD22	104.37	0.45
1:U:592:ALA:HA	1:V:499:ASN:HD22	80.70	0.45
1:V:275:TYR:HD2	1:X:473:MET:HE1	1.79	0.45
1:V:499:ASN:ND2	1:X:592:ALA:HA	2.31	0.45
1:V:544:MET:HG2	1:V:562:LEU:HD23	1.98	0.45
1:W:309:PHE:HA	1:W:688:GLU:O	2.17	0.45
1:X:485:CYS:HB3	1:X:579:TYR:HB2	1.99	0.45
1:Y:309:PHE:HE2	1:Y:731:THR:HG21	1.81	0.45
1:Z:429:HIS:O	1:4:383:LEU:HD11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:499:ASN:HD22	1:2:592:ALA:HA	111.70	0.45
1:Z:696:ARG:NE	1:Z:698:ASN:OD1	2.42	0.45
1:1:291:HIS:HD2	1:1:617:GLN:HA	1.82	0.45
1:3:318:LEU:HB2	1:3:412:PHE:HB3	1.97	0.45
1:4:382:THR:HG21	1:4:394:SER:H	1.81	0.45
1:3:383:LEU:HD11	1:4:429:HIS:O	2.16	0.45
1:4:581:VAL:CG1	1:4:595:VAL:HB	2.47	0.45
1:6:581:VAL:CG1	1:6:595:VAL:HB	2.46	0.45
1:B:383:LEU:HD11	1:L:429:HIS:O	2.16	0.45
1:D:419:GLU:OE2	1:D:643:LYS:N	2.44	0.45
1:E:309:PHE:HA	1:E:688:GLU:O	2.17	0.45
1:E:429:HIS:O	1:Q:383:LEU:HD11	2.16	0.45
1:F:382:THR:HG22	1:F:383:LEU:N	2.32	0.45
1:F:499:ASN:HD22	1:G:592:ALA:HA	95.87	0.45
1:F:499:ASN:ND2	1:G:592:ALA:HA	95.90	0.45
1:F:499:ASN:ND2	1:Q:592:ALA:HA	2.32	0.45
1:G:382:THR:HG21	1:G:394:SER:H	1.82	0.45
1:G:485:CYS:HB3	1:G:579:TYR:HB2	1.99	0.45
1:G:581:VAL:CG1	1:G:595:VAL:HB	2.46	0.45
1:I:488:GLN:OE1	1:I:540:SER:OG	2.33	0.45
1:I:485:CYS:HB3	1:I:579:TYR:HB2	1.99	0.45
1:K:544:MET:HG2	1:K:562:LEU:HD23	1.98	0.45
1:M:382:THR:HG21	1:M:394:SER:H	1.81	0.45
1:N:382:THR:HG21	1:N:394:SER:H	1.82	0.45
1:P:485:CYS:HB3	1:P:579:TYR:HB2	1.99	0.45
1:P:581:VAL:CG1	1:P:595:VAL:HB	2.46	0.45
1:O:481:LEU:HD13	1:P:636:LEU:CD1	72.88	0.45
1:R:382:THR:HG22	1:R:383:LEU:N	2.32	0.45
1:R:499:ASN:ND2	1:U:592:ALA:HA	2.31	0.45
1:R:696:ARG:NE	1:R:698:ASN:OD1	2.42	0.45
1:S:621:TRP:HA	1:S:640:PHE:H	1.80	0.45
1:V:368:PHE:CE2	1:V:370:ALA:HB3	2.51	0.45
1:V:499:ASN:HD22	1:X:592:ALA:HA	1.81	0.45
1:V:581:VAL:CG1	1:V:595:VAL:HB	2.47	0.45
1:W:291:HIS:HD2	1:W:617:GLN:HA	1.82	0.45
1:X:473:MET:HE1	1:Y:275:TYR:HD2	58.76	0.45
1:Y:368:PHE:CE2	1:Y:370:ALA:HB3	2.51	0.45
1:X:592:ALA:HA	1:Y:499:ASN:ND2	104.63	0.45
1:1:309:PHE:HA	1:1:688:GLU:O	2.17	0.45
1:1:318:LEU:HB2	1:1:412:PHE:HB3	1.97	0.45
1:2:382:THR:HG22	1:2:383:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:429:HIS:O	1:2:383:LEU:HD11	2.16	0.45
1:5:368:PHE:CE2	1:5:370:ALA:HB3	2.51	0.45
1:8:485:CYS:HB3	1:8:579:TYR:HB2	1.99	0.45
1:8:581:VAL:CG1	1:8:595:VAL:HB	2.46	0.45
1:C:383:LEU:HD11	1:M:429:HIS:O	2.17	0.45
1:D:382:THR:HG22	1:D:383:LEU:N	2.32	0.45
1:E:592:ALA:HA	1:Q:499:ASN:ND2	2.31	0.45
1:F:260:GLN:NE2	1:F:276:PHE:HE1	2.14	0.45
1:H:291:HIS:HD2	1:H:617:GLN:HA	1.82	0.45
1:H:382:THR:HG21	1:H:394:SER:H	1.81	0.45
1:H:581:VAL:CG1	1:H:595:VAL:HB	2.46	0.45
1:I:382:THR:HG22	1:I:383:LEU:N	2.32	0.45
1:I:419:GLU:OE2	1:I:643:LYS:N	2.44	0.45
1:K:485:CYS:HB3	1:K:579:TYR:HB2	1.99	0.45
1:K:581:VAL:CG1	1:K:595:VAL:HB	2.46	0.45
1:K:696:ARG:NE	1:K:698:ASN:OD1	2.42	0.45
1:L:309:PHE:HE2	1:L:731:THR:HG21	1.81	0.45
1:L:485:CYS:HB3	1:L:579:TYR:HB2	1.99	0.45
1:M:309:PHE:HE2	1:M:731:THR:HG21	1.81	0.45
1:O:309:PHE:HA	1:O:688:GLU:O	2.17	0.45
1:O:488:GLN:OE1	1:O:540:SER:OG	2.33	0.45
1:D:499:ASN:ND2	1:P:592:ALA:HA	2.32	0.45
1:S:382:THR:HG21	1:S:394:SER:H	1.82	0.45
1:D:383:LEU:HD11	1:T:429:HIS:O	117.22	0.45
1:T:499:ASN:HD22	1:V:592:ALA:HA	132.19	0.45
1:U:309:PHE:HA	1:U:688:GLU:O	2.17	0.45
1:S:592:ALA:HA	1:U:499:ASN:HD22	1.82	0.45
1:U:426:SER:HB2	1:U:731:THR:O	2.17	0.45
1:W:291:HIS:CD2	1:W:617:GLN:HA	2.52	0.45
1:1:368:PHE:CE2	1:1:370:ALA:HB3	2.51	0.45
1:3:382:THR:HG21	1:3:394:SER:H	1.82	0.45
1:3:581:VAL:CG1	1:3:595:VAL:HB	2.46	0.45
1:4:291:HIS:HD2	1:4:617:GLN:HA	1.82	0.45
1:4:382:THR:HG22	1:4:383:LEU:N	2.32	0.45
1:4:291:HIS:CD2	1:4:617:GLN:HA	2.52	0.45
1:5:382:THR:HG22	1:5:383:LEU:N	2.32	0.45
1:6:318:LEU:HB2	1:6:412:PHE:HB3	1.97	0.45
1:6:382:THR:HG21	1:6:394:SER:H	1.82	0.45
1:7:309:PHE:HA	1:7:688:GLU:O	2.17	0.45
1:5:383:LEU:HD11	1:7:429:HIS:O	2.16	0.45
1:6:592:ALA:HA	1:7:499:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:419:GLU:OE2	1:8:643:LYS:N	2.44	0.45
1:8:426:SER:HB2	1:8:731:THR:O	2.17	0.45
1:K:499:ASN:HD22	1:8:592:ALA:HA	1.81	0.45
1:A:309:PHE:HA	1:A:688:GLU:O	2.17	0.45
1:B:276:PHE:HB3	1:B:384:ASN:HB3	1.98	0.45
1:B:309:PHE:HE2	1:B:731:THR:HG21	1.81	0.45
1:C:382:THR:HG22	1:C:383:LEU:N	2.32	0.45
1:D:581:VAL:CG1	1:D:595:VAL:HB	2.46	0.45
1:E:291:HIS:HD2	1:E:617:GLN:HA	1.82	0.45
1:E:318:LEU:HD13	1:E:318:LEU:HA	1.82	0.45
1:E:401:PHE:N	1:E:401:PHE:CD1	2.84	0.45
1:E:426:SER:HB2	1:E:731:THR:O	2.17	0.45
1:F:382:THR:HG21	1:F:394:SER:H	1.81	0.45
1:F:581:VAL:CG1	1:F:595:VAL:HB	2.46	0.45
1:E:499:ASN:HD22	1:F:592:ALA:HA	1.81	0.45
1:F:309:PHE:HA	1:F:688:GLU:O	2.17	0.45
1:G:382:THR:HG22	1:G:383:LEU:N	2.32	0.45
1:G:309:PHE:HE2	1:G:731:THR:HG21	1.81	0.45
1:I:309:PHE:HE2	1:I:731:THR:HG21	1.81	0.45
1:J:309:PHE:HA	1:J:688:GLU:O	2.17	0.45
1:J:382:THR:HG22	1:J:383:LEU:N	2.32	0.45
1:J:581:VAL:CG1	1:J:595:VAL:HB	2.47	0.45
1:K:291:HIS:HD2	1:K:617:GLN:HA	1.82	0.45
1:J:429:HIS:O	1:L:383:LEU:HD11	2.17	0.45
1:M:309:PHE:HA	1:M:688:GLU:O	2.17	0.45
1:M:382:THR:HG22	1:M:383:LEU:N	2.32	0.45
1:N:291:HIS:HD2	1:N:617:GLN:HA	1.82	0.45
1:O:581:VAL:CG1	1:O:595:VAL:HB	2.46	0.45
1:O:291:HIS:HD2	1:O:617:GLN:HA	1.82	0.45
1:P:382:THR:HG22	1:P:383:LEU:N	2.32	0.45
1:P:426:SER:HB2	1:P:731:THR:O	2.17	0.45
1:Q:382:THR:HG22	1:Q:383:LEU:N	2.32	0.45
1:Q:291:HIS:CD2	1:Q:617:GLN:HA	2.52	0.45
1:R:581:VAL:CG1	1:R:595:VAL:HB	2.46	0.45
1:S:309:PHE:HA	1:S:688:GLU:O	2.17	0.45
1:S:382:THR:HG22	1:S:383:LEU:N	2.32	0.45
1:U:382:THR:HG22	1:U:383:LEU:N	2.32	0.45
1:U:566:GLU:OE2	1:U:569:LYS:NZ	2.45	0.45
1:U:291:HIS:CD2	1:U:617:GLN:HA	2.52	0.45
1:V:382:THR:HG22	1:V:383:LEU:N	2.32	0.45
1:V:485:CYS:HB3	1:V:579:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:499:ASN:ND2	1:V:592:ALA:HA	132.11	0.45
1:V:426:SER:HB2	1:V:731:THR:O	2.17	0.45
1:X:401:PHE:CD1	1:X:401:PHE:N	2.84	0.45
1:X:592:ALA:HA	1:Y:499:ASN:HD22	104.37	0.45
1:Y:382:THR:HG22	1:Y:383:LEU:N	2.32	0.45
1:Y:485:CYS:HB3	1:Y:579:TYR:HB2	1.99	0.45
1:Z:382:THR:HG22	1:Z:383:LEU:N	2.32	0.45
1:Z:488:GLN:OE1	1:Z:540:SER:OG	2.33	0.45
1:Z:485:CYS:HB3	1:Z:579:TYR:HB2	1.99	0.45
1:2:419:GLU:OE2	1:2:643:LYS:N	2.44	0.45
1:3:291:HIS:HD2	1:3:617:GLN:HA	1.82	0.45
1:6:260:GLN:NE2	1:6:276:PHE:HE1	2.14	0.45
1:7:382:THR:HG21	1:7:394:SER:H	1.81	0.45
1:7:401:PHE:CD1	1:7:401:PHE:N	2.84	0.45
1:7:318:LEU:HB2	1:7:412:PHE:HB3	1.97	0.45
1:C:309:PHE:HA	1:C:688:GLU:O	2.17	0.45
1:C:309:PHE:HE2	1:C:731:THR:HG21	1.81	0.45
1:C:485:CYS:HB3	1:C:579:TYR:HB2	1.99	0.45
1:D:488:GLN:OE1	1:D:540:SER:OG	2.33	0.45
1:E:291:HIS:CD2	1:E:617:GLN:HA	2.52	0.45
1:F:426:SER:HB2	1:F:731:THR:O	2.17	0.45
1:H:485:CYS:HB3	1:H:579:TYR:HB2	1.99	0.45
1:I:401:PHE:N	1:I:401:PHE:CD1	2.84	0.45
1:I:309:PHE:HA	1:I:688:GLU:O	2.17	0.45
1:J:291:HIS:CD2	1:J:617:GLN:HA	2.52	0.45
1:J:426:SER:HB2	1:J:731:THR:O	2.17	0.45
1:J:592:ALA:HA	1:K:499:ASN:HD22	80.70	0.45
1:L:382:THR:HG21	1:L:394:SER:H	1.82	0.45
1:M:488:GLN:OE1	1:M:540:SER:OG	2.33	0.45
1:M:291:HIS:CD2	1:M:617:GLN:HA	2.52	0.45
1:N:382:THR:HG22	1:N:383:LEU:N	2.32	0.45
1:N:291:HIS:CD2	1:N:617:GLN:HA	2.52	0.45
1:P:382:THR:HG21	1:P:394:SER:H	1.81	0.45
1:P:291:HIS:CD2	1:P:617:GLN:HA	2.52	0.45
1:Q:401:PHE:CD1	1:Q:401:PHE:N	2.84	0.45
1:S:291:HIS:CD2	1:S:617:GLN:HA	2.52	0.45
1:T:291:HIS:HD2	1:T:617:GLN:HA	1.82	0.45
1:T:309:PHE:HA	1:T:688:GLU:O	2.17	0.45
1:V:309:PHE:HE2	1:V:731:THR:HG21	1.81	0.45
1:W:251:PRO:HG3	1:W:374:MET:HE3	1.99	0.45
1:W:426:SER:HB2	1:W:731:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:260:GLN:NE2	1:X:276:PHE:HE1	2.14	0.45
1:X:419:GLU:OE2	1:X:643:LYS:N	2.44	0.45
1:W:592:ALA:HA	1:X:499:ASN:HD22	80.70	0.45
1:Y:581:VAL:CG1	1:Y:595:VAL:HB	2.46	0.45
1:Y:309:PHE:HA	1:Y:688:GLU:O	2.17	0.45
1:Z:382:THR:HG21	1:Z:394:SER:H	1.82	0.45
1:1:544:MET:HG2	1:1:562:LEU:HD23	1.98	0.45
1:Z:383:LEU:HD11	1:2:429:HIS:O	77.35	0.45
1:2:291:HIS:CD2	1:2:617:GLN:HA	2.52	0.45
1:3:499:ASN:ND2	1:4:592:ALA:HA	2.31	0.45
1:4:309:PHE:HA	1:4:688:GLU:O	2.17	0.45
1:5:544:MET:HG2	1:5:562:LEU:HD23	1.98	0.45
1:7:382:THR:HG22	1:7:383:LEU:N	2.32	0.45
1:A:485:CYS:HB3	1:A:579:TYR:HB2	1.99	0.45
1:A:291:HIS:CD2	1:A:617:GLN:HA	2.52	0.45
1:B:382:THR:HG22	1:B:383:LEU:N	2.32	0.45
1:B:545:PHE:O	1:B:561:MET:N	2.27	0.45
1:C:401:PHE:CD1	1:C:401:PHE:N	2.84	0.45
1:C:451:THR:HG21	1:O:503:PHE:CZ	155.49	0.45
1:D:383:LEU:HD11	1:P:429:HIS:O	2.16	0.45
1:D:485:CYS:HB3	1:D:579:TYR:HB2	1.98	0.45
1:E:382:THR:HG22	1:E:383:LEU:N	2.32	0.45
1:E:485:CYS:HB3	1:E:579:TYR:HB2	1.99	0.45
1:E:592:ALA:HA	1:X:499:ASN:HD22	157.97	0.45
1:F:291:HIS:CD2	1:F:617:GLN:HA	2.52	0.45
1:G:291:HIS:CD2	1:G:617:GLN:HA	2.52	0.45
1:H:499:ASN:ND2	1:Y:592:ALA:HA	2.32	0.45
1:K:309:PHE:HA	1:K:688:GLU:O	2.17	0.45
1:K:368:PHE:CE2	1:K:370:ALA:HB3	2.51	0.45
1:J:610:GLN:HE22	1:K:627:THR:HA	61.35	0.45
1:L:291:HIS:HD2	1:L:617:GLN:HA	1.82	0.45
1:M:485:CYS:HB3	1:M:579:TYR:HB2	1.99	0.45
1:N:309:PHE:HA	1:N:688:GLU:O	2.17	0.45
1:N:592:ALA:HA	1:O:499:ASN:HD22	80.70	0.45
1:N:592:ALA:HA	1:O:499:ASN:ND2	80.58	0.45
1:O:544:MET:HG2	1:O:562:LEU:HD23	1.98	0.45
1:D:499:ASN:HD22	1:P:592:ALA:HA	1.81	0.45
1:S:291:HIS:HD2	1:S:617:GLN:HA	1.82	0.45
1:R:592:ALA:HA	1:S:499:ASN:ND2	2.32	0.45
1:W:382:THR:HG22	1:W:383:LEU:N	2.32	0.45
1:X:309:PHE:HA	1:X:688:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:426:SER:HB2	1:X:731:THR:O	2.17	0.45
1:Y:291:HIS:HD2	1:Y:617:GLN:HA	1.82	0.45
1:1:309:PHE:HE2	1:1:731:THR:HG21	1.82	0.45
1:2:488:GLN:OE1	1:2:540:SER:OG	2.33	0.45
1:2:581:VAL:CG1	1:2:595:VAL:HB	2.46	0.45
1:1:481:LEU:HD13	1:2:636:LEU:HD11	1.99	0.45
1:3:309:PHE:HE2	1:3:731:THR:HG21	1.81	0.45
1:3:499:ASN:HD22	1:4:592:ALA:HA	1.81	0.45
1:5:260:GLN:NE2	1:5:276:PHE:HE1	2.14	0.45
1:5:291:HIS:HD2	1:5:617:GLN:HA	1.82	0.45
1:5:401:PHE:N	1:5:401:PHE:CD1	2.84	0.45
1:6:291:HIS:CD2	1:6:617:GLN:HA	2.52	0.45
1:7:485:CYS:HB3	1:7:579:TYR:HB2	1.99	0.45
1:K:383:LEU:HD11	1:8:429:HIS:O	2.16	0.45
1:A:426:SER:HB2	1:A:731:THR:O	2.17	0.45
1:B:419:GLU:OE2	1:B:643:LYS:N	2.44	0.45
1:B:499:ASN:ND2	1:C:592:ALA:HA	104.62	0.45
1:B:426:SER:HB2	1:B:731:THR:O	2.17	0.45
1:D:275:TYR:HD2	1:P:473:MET:HE1	1.79	0.45
1:D:429:HIS:O	1:L:383:LEU:HD11	127.60	0.45
1:D:291:HIS:CD2	1:D:617:GLN:HA	2.52	0.45
1:D:696:ARG:NE	1:D:698:ASN:OD1	2.42	0.45
1:F:566:GLU:OE2	1:F:569:LYS:NZ	2.45	0.45
1:F:610:GLN:HE22	1:H:627:THR:HA	117.67	0.45
1:F:627:THR:HA	1:G:610:GLN:HE22	85.08	0.45
1:H:382:THR:HG22	1:H:383:LEU:N	2.32	0.45
1:H:401:PHE:CD1	1:H:401:PHE:N	2.84	0.45
1:F:592:ALA:HA	1:H:499:ASN:HD22	157.57	0.45
1:O:485:CYS:HB3	1:O:579:TYR:HB2	1.99	0.45
1:O:291:HIS:CD2	1:O:617:GLN:HA	2.52	0.45
1:Q:291:HIS:HD2	1:Q:617:GLN:HA	1.82	0.45
1:Q:309:PHE:HE2	1:Q:731:THR:HG21	1.81	0.45
1:Q:544:MET:HG2	1:Q:562:LEU:HD23	1.98	0.45
1:Q:309:PHE:HA	1:Q:688:GLU:O	2.17	0.45
1:Q:426:SER:HB2	1:Q:731:THR:O	2.17	0.45
1:R:291:HIS:HD2	1:R:617:GLN:HA	1.82	0.45
1:R:545:PHE:O	1:R:561:MET:N	2.27	0.45
1:R:291:HIS:CD2	1:R:617:GLN:HA	2.52	0.45
1:R:426:SER:HB2	1:R:731:THR:O	2.17	0.45
1:U:368:PHE:CE2	1:U:370:ALA:HB3	2.51	0.45
1:T:429:HIS:O	1:U:383:LEU:HD11	34.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:485:CYS:HB3	1:U:579:TYR:HB2	1.99	0.45
1:T:592:ALA:HA	1:U:499:ASN:ND2	104.63	0.45
1:U:429:HIS:O	1:V:383:LEU:HD11	60.77	0.45
1:V:291:HIS:CD2	1:V:617:GLN:HA	2.52	0.45
1:V:309:PHE:HA	1:V:688:GLU:O	2.17	0.45
1:W:309:PHE:HE2	1:W:731:THR:HG21	1.81	0.45
1:W:485:CYS:HB3	1:W:579:TYR:HB2	1.99	0.45
1:Y:382:THR:HG21	1:Y:394:SER:H	1.81	0.45
1:Y:426:SER:HB2	1:Y:731:THR:O	2.17	0.45
1:1:488:GLN:OE1	1:1:540:SER:OG	2.33	0.45
1:1:426:SER:HB2	1:1:731:THR:O	2.17	0.45
1:2:291:HIS:HD2	1:2:617:GLN:HA	1.82	0.45
1:1:451:THR:HG21	1:2:503:PHE:CZ	2.52	0.45
1:1:481:LEU:HD13	1:2:636:LEU:CD1	2.47	0.45
1:2:309:PHE:HE2	1:2:731:THR:HG21	1.81	0.45
1:5:309:PHE:HA	1:5:688:GLU:O	2.17	0.45
1:5:488:GLN:OE1	1:5:540:SER:OG	2.33	0.45
1:5:309:PHE:HE2	1:5:731:THR:HG21	1.81	0.45
1:6:382:THR:HG22	1:6:383:LEU:N	2.32	0.45
1:8:382:THR:HG21	1:8:394:SER:H	1.82	0.45
1:8:291:HIS:CD2	1:8:617:GLN:HA	2.52	0.45
1:B:291:HIS:CD2	1:B:617:GLN:HA	2.52	0.45
1:D:309:PHE:HA	1:D:688:GLU:O	2.17	0.45
1:D:429:HIS:O	1:N:383:LEU:HD11	2.16	0.45
1:F:291:HIS:HD2	1:F:617:GLN:HA	1.82	0.45
1:A:610:GLN:HE22	1:G:627:THR:HA	1.82	0.45
1:H:426:SER:HB2	1:H:731:THR:O	2.17	0.45
1:I:610:GLN:HE22	1:J:627:THR:HA	43.49	0.45
1:I:291:HIS:CD2	1:I:617:GLN:HA	2.52	0.45
1:K:382:THR:HG22	1:K:383:LEU:N	2.32	0.45
1:A:383:LEU:HD11	1:K:429:HIS:O	92.06	0.45
1:O:382:THR:HG22	1:O:383:LEU:N	2.32	0.45
1:O:426:SER:HB2	1:O:731:THR:O	2.17	0.45
1:R:382:THR:HG22	1:R:383:LEU:H	1.83	0.45
1:Q:592:ALA:HA	1:R:499:ASN:HD22	80.70	0.45
1:R:473:MET:HE1	1:S:275:TYR:HD2	1.83	0.45
1:T:488:GLN:OE1	1:T:540:SER:OG	2.33	0.45
1:T:291:HIS:CD2	1:T:617:GLN:HA	2.52	0.45
1:S:429:HIS:O	1:U:383:LEU:HD11	2.16	0.45
1:V:632:HIS:CE1	3:V:902:DA:C8	3.05	0.45
1:W:401:PHE:CD1	1:W:401:PHE:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:TYR:HD2	1:Y:473:MET:HE1	1.79	0.45
1:W:499:ASN:HD22	1:Y:592:ALA:HA	32.60	0.45
1:Y:632:HIS:CE1	3:Y:902:DA:C8	3.05	0.45
1:Z:291:HIS:HD2	1:Z:617:GLN:HA	1.82	0.45
1:Z:309:PHE:HE2	1:Z:731:THR:HG21	1.81	0.45
1:1:307:TRP:CE2	1:1:692:GLU:HG2	2.53	0.44
1:6:309:PHE:HE2	1:6:731:THR:HG21	1.81	0.44
1:A:696:ARG:NE	1:A:698:ASN:OD1	2.42	0.44
1:C:291:HIS:CD2	1:C:617:GLN:HA	2.52	0.44
1:D:291:HIS:HD2	1:D:617:GLN:HA	1.82	0.44
1:D:309:PHE:HE2	1:D:731:THR:HG21	1.81	0.44
1:D:636:LEU:HD11	1:T:481:LEU:HD13	126.10	0.44
1:D:426:SER:HB2	1:D:731:THR:O	2.17	0.44
1:E:627:THR:HA	1:F:610:GLN:HE22	1.83	0.44
1:G:426:SER:HB2	1:G:731:THR:O	2.17	0.44
1:H:251:PRO:HG3	1:H:374:MET:HE3	1.99	0.44
1:I:426:SER:HB2	1:I:731:THR:O	2.17	0.44
1:K:401:PHE:CD1	1:K:401:PHE:N	2.84	0.44
1:L:451:THR:HG21	1:T:503:PHE:CZ	232.30	0.44
1:B:499:ASN:ND2	1:L:592:ALA:HA	2.31	0.44
1:L:291:HIS:CD2	1:L:617:GLN:HA	2.52	0.44
1:N:251:PRO:HG3	1:N:374:MET:HE3	2.02	0.44
1:N:318:LEU:HB2	1:N:412:PHE:HB3	1.97	0.44
1:P:401:PHE:N	1:P:401:PHE:CD1	2.84	0.44
1:P:309:PHE:HE2	1:P:731:THR:HG21	1.81	0.44
1:Q:610:GLN:HE22	1:R:627:THR:HA	61.35	0.44
1:R:382:THR:HG21	1:R:394:SER:H	1.81	0.44
1:R:610:GLN:HE22	1:S:627:THR:HA	1.82	0.44
1:D:636:LEU:CD1	1:T:481:LEU:HD13	126.96	0.44
1:T:426:SER:HB2	1:T:731:THR:O	2.17	0.44
1:T:427:TYR:N	1:T:732:ARG:HG2	2.31	0.44
1:U:307:TRP:CE2	1:U:692:GLU:HG2	2.53	0.44
1:E:499:ASN:HD22	1:V:592:ALA:HA	180.67	0.44
1:X:382:THR:HG22	1:X:383:LEU:N	2.32	0.44
1:X:382:THR:HG22	1:X:383:LEU:H	1.83	0.44
1:X:382:THR:HG21	1:X:394:SER:H	1.81	0.44
1:Y:291:HIS:CD2	1:Y:617:GLN:HA	2.52	0.44
1:1:401:PHE:CD1	1:1:401:PHE:N	2.84	0.44
1:3:544:MET:HG2	1:3:562:LEU:HD23	1.98	0.44
1:3:426:SER:HB2	1:3:731:THR:O	2.17	0.44
1:4:359:SER:HB2	1:4:361:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:318:LEU:HB2	1:4:412:PHE:HB3	1.97	0.44
1:5:434:ASP:OD1	1:5:434:ASP:N	2.46	0.44
1:5:581:VAL:CG1	1:5:595:VAL:HB	2.47	0.44
1:6:401:PHE:N	1:6:401:PHE:CD1	2.84	0.44
1:6:610:GLN:HE22	1:7:627:THR:HA	1.83	0.44
1:7:426:SER:HB2	1:7:731:THR:O	2.17	0.44
1:8:309:PHE:HE2	1:8:731:THR:HG21	1.81	0.44
1:A:382:THR:HG22	1:A:383:LEU:N	2.32	0.44
1:B:544:MET:HG2	1:B:562:LEU:HD23	1.98	0.44
1:C:291:HIS:HD2	1:C:617:GLN:HA	1.82	0.44
1:F:382:THR:HG22	1:F:383:LEU:H	1.83	0.44
1:F:258:TYR:OH	1:F:399:GLU:OE1	2.28	0.44
1:G:307:TRP:CE2	1:G:692:GLU:HG2	2.53	0.44
1:G:309:PHE:HA	1:G:688:GLU:O	2.17	0.44
1:I:307:TRP:CE2	1:I:692:GLU:HG2	2.53	0.44
1:J:258:TYR:OH	1:J:399:GLU:OE1	2.28	0.44
1:J:488:GLN:OE1	1:J:540:SER:OG	2.33	0.44
1:K:382:THR:HG22	1:K:383:LEU:H	1.83	0.44
1:K:307:TRP:CE2	1:K:692:GLU:HG2	2.53	0.44
1:L:426:SER:HB2	1:L:731:THR:O	2.17	0.44
1:N:359:SER:HB2	1:N:361:HIS:CD2	2.53	0.44
1:P:309:PHE:HA	1:P:688:GLU:O	2.17	0.44
1:Q:251:PRO:HG3	1:Q:374:MET:HE3	1.98	0.44
1:R:309:PHE:HA	1:R:688:GLU:O	2.17	0.44
1:R:427:TYR:N	1:R:732:ARG:HG2	2.31	0.44
1:S:426:SER:HB2	1:S:731:THR:O	2.17	0.44
1:T:307:TRP:CE2	1:T:692:GLU:HG2	2.53	0.44
1:D:503:PHE:CZ	1:T:451:THR:HG21	148.37	0.44
1:T:627:THR:HA	1:V:610:GLN:HE22	100.58	0.44
1:E:627:THR:HA	1:V:610:GLN:HE22	112.92	0.44
1:V:307:TRP:CE2	1:V:692:GLU:HG2	2.53	0.44
1:W:307:TRP:CE2	1:W:692:GLU:HG2	2.53	0.44
1:X:291:HIS:CD2	1:X:617:GLN:HA	2.52	0.44
1:X:581:VAL:CG1	1:X:595:VAL:HB	2.46	0.44
1:Y:382:THR:HG22	1:Y:383:LEU:H	1.83	0.44
1:W:592:ALA:HA	1:Y:499:ASN:HD22	1.81	0.44
1:W:610:GLN:HE22	1:Y:627:THR:HA	1.83	0.44
1:Z:427:TYR:N	1:Z:732:ARG:HG2	2.31	0.44
1:1:291:HIS:CD2	1:1:617:GLN:HA	2.52	0.44
1:2:382:THR:HG21	1:2:394:SER:H	1.81	0.44
1:5:627:THR:HA	1:7:610:GLN:HE22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:382:THR:HG22	1:6:383:LEU:H	1.83	0.44
1:B:581:VAL:CG1	1:B:595:VAL:HB	2.46	0.44
1:C:307:TRP:CE2	1:C:692:GLU:HG2	2.53	0.44
1:C:426:SER:HB2	1:C:731:THR:O	2.17	0.44
1:D:307:TRP:CE2	1:D:692:GLU:HG2	2.53	0.44
1:D:382:THR:HG22	1:D:383:LEU:H	1.83	0.44
1:D:401:PHE:N	1:D:401:PHE:CD1	2.84	0.44
1:E:488:GLN:OE1	1:E:540:SER:OG	2.33	0.44
1:E:307:TRP:CE2	1:E:692:GLU:HG2	2.53	0.44
1:F:401:PHE:N	1:F:401:PHE:CD1	2.84	0.44
1:G:382:THR:HG22	1:G:383:LEU:H	1.83	0.44
1:G:401:PHE:N	1:G:401:PHE:CD1	2.84	0.44
1:H:382:THR:HG22	1:H:383:LEU:H	1.83	0.44
1:H:291:HIS:CD2	1:H:617:GLN:HA	2.52	0.44
1:I:382:THR:HG22	1:I:383:LEU:H	1.83	0.44
1:I:310:ARG:NE	1:I:688:GLU:OE1	2.45	0.44
1:J:291:HIS:HD2	1:J:617:GLN:HA	1.82	0.44
1:J:632:HIS:CE1	3:J:902:DA:C8	3.05	0.44
1:K:309:PHE:HE2	1:K:731:THR:HG21	1.81	0.44
1:K:426:SER:HB2	1:K:731:THR:O	2.17	0.44
1:L:382:THR:HG22	1:L:383:LEU:H	1.83	0.44
1:M:307:TRP:CE2	1:M:692:GLU:HG2	2.53	0.44
1:O:451:THR:HG21	1:P:503:PHE:CZ	102.51	0.44
1:T:610:GLN:HE22	1:U:627:THR:HA	43.49	0.44
1:W:359:SER:HB2	1:W:361:HIS:CD2	2.53	0.44
1:W:544:MET:HG2	1:W:562:LEU:HD23	1.98	0.44
1:W:627:THR:HA	1:Y:610:GLN:HE22	28.19	0.44
1:X:310:ARG:NE	1:X:688:GLU:OE1	2.45	0.44
1:Z:382:THR:HG22	1:Z:383:LEU:H	1.83	0.44
1:Z:451:THR:HG21	1:1:503:PHE:CZ	94.01	0.44
1:1:359:SER:HB2	1:1:361:HIS:CD2	2.53	0.44
1:2:485:CYS:HB3	1:2:579:TYR:HB2	1.99	0.44
1:3:291:HIS:CD2	1:3:617:GLN:HA	2.52	0.44
1:3:627:THR:HA	1:4:610:GLN:HE22	1.83	0.44
1:5:251:PRO:HG3	1:5:374:MET:HE3	1.98	0.44
1:5:382:THR:HG22	1:5:383:LEU:H	1.83	0.44
1:6:566:GLU:OE2	1:6:569:LYS:NZ	2.45	0.44
1:6:426:SER:HB2	1:6:731:THR:O	2.17	0.44
1:8:632:HIS:CE1	3:8:902:DA:C8	3.05	0.44
1:8:696:ARG:NE	1:8:698:ASN:OD1	2.42	0.44
1:A:359:SER:HB2	1:A:361:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:HIS:CE1	3:A:902:DA:C8	3.05	0.44
1:B:309:PHE:HA	1:B:688:GLU:O	2.17	0.44
1:C:382:THR:HG22	1:C:383:LEU:H	1.83	0.44
1:C:499:ASN:ND2	1:M:592:ALA:HA	2.32	0.44
1:E:427:TYR:N	1:E:732:ARG:HG2	2.31	0.44
1:F:251:PRO:HG3	1:F:374:MET:HE3	1.98	0.44
1:F:632:HIS:CE1	3:F:902:DA:C8	3.05	0.44
1:J:359:SER:HB2	1:J:361:HIS:CD2	2.53	0.44
1:J:485:CYS:HB3	1:J:579:TYR:HB2	1.99	0.44
1:J:310:ARG:NE	1:J:688:GLU:OE1	2.45	0.44
1:K:251:PRO:HG3	1:K:374:MET:HE3	1.98	0.44
1:J:429:HIS:O	1:K:383:LEU:HD11	60.78	0.44
1:L:473:MET:HE1	1:T:275:TYR:HD2	218.34	0.44
1:J:592:ALA:HA	1:L:499:ASN:ND2	2.32	0.44
1:M:359:SER:HB2	1:M:361:HIS:CD2	2.53	0.44
1:O:632:HIS:CE1	3:O:902:DA:C8	3.05	0.44
1:P:359:SER:HB2	1:P:361:HIS:CD2	2.53	0.44
1:P:632:HIS:CE1	3:P:902:DA:C8	3.05	0.44
1:Q:359:SER:HB2	1:Q:361:HIS:CD2	2.53	0.44
1:R:359:SER:HB2	1:R:361:HIS:CD2	2.53	0.44
1:R:627:THR:HA	1:U:610:GLN:HE22	1.83	0.44
1:T:318:LEU:HD13	1:T:318:LEU:HA	1.82	0.44
1:T:382:THR:HG22	1:T:383:LEU:N	2.32	0.44
1:T:382:THR:HG21	1:T:394:SER:H	1.82	0.44
1:T:473:MET:HE1	1:U:275:TYR:HD2	58.73	0.44
1:T:545:PHE:O	1:T:561:MET:N	2.27	0.44
1:U:382:THR:HG22	1:U:383:LEU:H	1.83	0.44
1:E:499:ASN:ND2	1:V:592:ALA:HA	181.48	0.44
1:W:318:LEU:HD13	1:W:318:LEU:HA	1.82	0.44
1:W:499:ASN:ND2	1:Y:592:ALA:HA	32.98	0.44
1:Y:359:SER:HB2	1:Y:361:HIS:CD2	2.53	0.44
1:Z:359:SER:HB2	1:Z:361:HIS:CD2	2.53	0.44
1:Z:473:MET:HE1	1:1:275:TYR:HD2	105.21	0.44
1:2:382:THR:HG22	1:2:383:LEU:H	1.83	0.44
1:2:696:ARG:NE	1:2:698:ASN:OD1	2.42	0.44
1:2:426:SER:HB2	1:2:731:THR:O	2.17	0.44
1:6:544:MET:HG2	1:6:562:LEU:HD23	1.98	0.44
1:6:485:CYS:HB3	1:6:579:TYR:HB2	1.99	0.44
1:8:251:PRO:HG3	1:8:374:MET:HE3	1.99	0.44
1:8:309:PHE:HA	1:8:688:GLU:O	2.17	0.44
1:8:382:THR:HG22	1:8:383:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:HIS:HD2	1:A:617:GLN:HA	1.82	0.44
1:A:307:TRP:CE2	1:A:692:GLU:HG2	2.53	0.44
1:E:610:GLN:HE22	1:Q:627:THR:HA	1.83	0.44
1:F:485:CYS:HB3	1:F:579:TYR:HB2	1.99	0.44
1:F:307:TRP:CE2	1:F:692:GLU:HG2	2.53	0.44
1:G:359:SER:HB2	1:G:361:HIS:CD2	2.53	0.44
1:H:318:LEU:HD13	1:H:318:LEU:HA	1.82	0.44
1:H:359:SER:HB2	1:H:361:HIS:CD2	2.53	0.44
1:F:429:HIS:O	1:H:383:LEU:HD11	127.60	0.44
1:F:592:ALA:HA	1:H:499:ASN:ND2	157.95	0.44
1:I:291:HIS:HD2	1:I:617:GLN:HA	1.82	0.44
1:I:383:LEU:HD11	1:K:429:HIS:O	97.74	0.44
1:J:307:TRP:CE2	1:J:692:GLU:HG2	2.53	0.44
1:K:359:SER:HB2	1:K:361:HIS:CD2	2.53	0.44
1:L:359:SER:HB2	1:L:361:HIS:CD2	2.53	0.44
1:L:382:THR:HG22	1:L:383:LEU:N	2.32	0.44
1:M:632:HIS:CE1	3:M:902:DA:C8	3.05	0.44
1:N:312:LYS:HD2	1:N:312:LYS:HA	1.84	0.44
1:N:696:ARG:NE	1:N:698:ASN:OD1	2.42	0.44
1:N:610:GLN:HE22	1:O:627:THR:HA	61.35	0.44
1:P:291:HIS:HD2	1:P:617:GLN:HA	1.82	0.44
1:Q:382:THR:HG22	1:Q:383:LEU:H	1.83	0.44
1:Q:427:TYR:N	1:Q:732:ARG:HG2	2.31	0.44
1:R:632:HIS:CE1	3:R:902:DA:C8	3.05	0.44
1:S:382:THR:HG22	1:S:383:LEU:H	1.83	0.44
1:T:359:SER:HB2	1:T:361:HIS:CD2	2.53	0.44
1:U:291:HIS:HD2	1:U:617:GLN:HA	1.82	0.44
1:U:610:GLN:HE22	1:V:627:THR:HA	61.35	0.44
1:V:627:THR:HA	1:X:610:GLN:HE22	1.83	0.44
1:X:610:GLN:HE22	1:Y:627:THR:HA	43.51	0.44
1:Z:307:TRP:CE2	1:Z:692:GLU:HG2	2.53	0.44
1:Z:291:HIS:CD2	1:Z:617:GLN:HA	2.52	0.44
1:1:382:THR:HG22	1:1:383:LEU:N	2.32	0.44
1:1:382:THR:HG21	1:1:394:SER:H	1.82	0.44
1:5:426:SER:HB2	1:5:731:THR:O	2.17	0.44
1:6:473:MET:HE1	1:7:275:TYR:HB3	2.00	0.44
1:7:291:HIS:CD2	1:7:617:GLN:HA	2.52	0.44
1:C:419:GLU:OE2	1:C:643:LYS:N	2.44	0.44
1:D:312:LYS:HA	1:D:312:LYS:HD2	1.84	0.44
1:D:359:SER:HB2	1:D:361:HIS:CD2	2.53	0.44
1:G:383:LEU:HD11	1:H:429:HIS:O	60.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:610:GLN:HE22	1:W:627:THR:HA	1.83	0.44
1:J:592:ALA:HA	1:K:499:ASN:ND2	80.57	0.44
1:K:291:HIS:CD2	1:K:617:GLN:HA	2.52	0.44
1:J:610:GLN:HE22	1:L:627:THR:HA	1.82	0.44
1:M:426:SER:HB2	1:M:731:THR:O	2.17	0.44
1:O:307:TRP:CE2	1:O:692:GLU:HG2	2.53	0.44
1:P:382:THR:HG22	1:P:383:LEU:H	1.83	0.44
1:S:359:SER:HB2	1:S:361:HIS:CD2	2.53	0.44
1:Q:627:THR:HA	1:S:610:GLN:HE22	85.08	0.44
1:S:610:GLN:HE22	1:U:627:THR:HA	1.83	0.44
1:V:291:HIS:HD2	1:V:617:GLN:HA	1.82	0.44
1:W:427:TYR:N	1:W:732:ARG:HG2	2.31	0.44
1:1:566:GLU:OE2	1:1:569:LYS:NZ	2.45	0.44
1:3:382:THR:HG22	1:3:383:LEU:N	2.32	0.44
1:3:485:CYS:HB3	1:3:579:TYR:HB2	1.99	0.44
1:5:427:TYR:N	1:5:732:ARG:HG2	2.31	0.44
1:5:473:MET:HE1	1:6:275:TYR:HD2	1.81	0.44
1:7:419:GLU:OE2	1:7:643:LYS:N	2.44	0.44
1:7:488:GLN:OE1	1:7:540:SER:OG	2.33	0.44
1:7:526:MET:HE2	1:7:575:ALA:HA	1.99	0.44
1:7:291:HIS:HD2	1:7:617:GLN:HA	1.82	0.44
1:A:429:HIS:O	1:G:383:LEU:HD11	2.17	0.44
1:A:610:GLN:HE22	1:8:627:THR:HA	132.25	0.44
1:B:359:SER:HB2	1:B:361:HIS:CD2	2.53	0.44
1:F:310:ARG:NE	1:F:688:GLU:OE1	2.45	0.44
1:G:291:HIS:HD2	1:G:617:GLN:HA	1.82	0.44
1:G:632:HIS:CE1	3:G:902:DA:C8	3.05	0.44
1:I:359:SER:HB2	1:I:361:HIS:CD2	2.53	0.44
1:I:632:HIS:CE1	3:I:902:DA:C8	3.05	0.44
1:K:312:LYS:HA	1:K:312:LYS:HD2	1.84	0.44
1:I:627:THR:HA	1:K:610:GLN:HE22	100.58	0.44
1:L:307:TRP:CE2	1:L:692:GLU:HG2	2.53	0.44
1:N:610:GLN:HE22	1:P:627:THR:HA	1.83	0.44
1:Q:419:GLU:OE2	1:Q:643:LYS:N	2.44	0.44
1:S:485:CYS:HB3	1:S:579:TYR:HB2	1.99	0.44
1:S:307:TRP:CE2	1:S:692:GLU:HG2	2.53	0.44
1:U:359:SER:HB2	1:U:361:HIS:CD2	2.53	0.44
1:V:359:SER:HB2	1:V:361:HIS:CD2	2.53	0.44
1:W:632:HIS:CE1	3:W:902:DA:C8	3.05	0.44
1:X:291:HIS:HD2	1:X:617:GLN:HA	1.82	0.44
1:X:359:SER:HB2	1:X:361:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:610:GLN:HE22	1:2:627:THR:HA	1.83	0.44
1:2:309:PHE:HA	1:2:688:GLU:O	2.17	0.44
1:3:307:TRP:CE2	1:3:692:GLU:HG2	2.53	0.44
1:6:309:PHE:HA	1:6:688:GLU:O	2.17	0.44
1:8:359:SER:HB2	1:8:361:HIS:CD2	2.53	0.44
1:B:291:HIS:HD2	1:B:617:GLN:HA	1.82	0.44
1:B:307:TRP:CE2	1:B:692:GLU:HG2	2.53	0.44
1:C:627:THR:HA	1:M:610:GLN:HE22	1.82	0.44
1:E:632:HIS:CE1	3:E:902:DA:C8	3.05	0.44
1:G:627:THR:HA	1:H:610:GLN:HE22	61.35	0.44
1:H:627:THR:HA	1:Y:610:GLN:HE22	1.83	0.44
1:K:419:GLU:OE2	1:K:643:LYS:N	2.44	0.44
1:L:309:PHE:HA	1:L:688:GLU:O	2.17	0.44
1:M:382:THR:HG22	1:M:383:LEU:H	1.83	0.44
1:P:251:PRO:HG3	1:P:374:MET:HE3	2.01	0.44
1:R:312:LYS:HA	1:R:312:LYS:HD2	1.84	0.44
1:D:627:THR:HA	1:T:610:GLN:HE22	113.15	0.44
1:W:382:THR:HG22	1:W:383:LEU:H	1.83	0.44
1:H:499:ASN:HD22	1:Y:592:ALA:HA	1.81	0.44
1:Z:309:PHE:HA	1:Z:688:GLU:O	2.17	0.44
1:3:632:HIS:CE1	3:3:902:DA:C8	3.05	0.44
1:4:312:LYS:HD2	1:4:312:LYS:HA	1.84	0.44
1:4:426:SER:HB2	1:4:731:THR:O	2.17	0.44
1:8:291:HIS:HD2	1:8:617:GLN:HA	1.82	0.44
1:8:382:THR:HG22	1:8:383:LEU:N	2.32	0.44
1:A:328:GLN:HE22	1:A:333:LYS:HG3	1.84	0.44
1:B:401:PHE:CD1	1:B:401:PHE:N	2.84	0.44
1:D:632:HIS:CE1	3:D:902:DA:C8	3.05	0.44
1:H:309:PHE:HA	1:H:688:GLU:O	2.17	0.44
1:I:696:ARG:NE	1:I:698:ASN:OD1	2.42	0.44
1:J:545:PHE:O	1:J:561:MET:N	2.27	0.44
1:M:592:ALA:HA	1:N:499:ASN:HD22	104.37	0.44
1:M:427:TYR:N	1:M:732:ARG:HG2	2.31	0.44
1:N:426:SER:HB2	1:N:731:THR:O	2.17	0.44
1:O:359:SER:HB2	1:O:361:HIS:CD2	2.53	0.44
1:F:275:TYR:HD2	1:Q:473:MET:HE1	1.81	0.44
1:R:485:CYS:HB3	1:R:579:TYR:HB2	1.99	0.44
1:S:632:HIS:CE1	3:S:902:DA:C8	3.05	0.44
1:T:632:HIS:CE1	3:T:902:DA:C8	3.05	0.44
1:X:307:TRP:CE2	1:X:692:GLU:HG2	2.53	0.44
1:Y:328:GLN:HE22	1:Y:333:LYS:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:427:TYR:N	1:2:732:ARG:HG2	2.31	0.43
1:3:359:SER:HB2	1:3:361:HIS:CD2	2.53	0.43
1:3:309:PHE:HA	1:3:688:GLU:O	2.17	0.43
1:5:291:HIS:CD2	1:5:617:GLN:HA	2.52	0.43
1:A:382:THR:HG22	1:A:383:LEU:H	1.83	0.43
1:A:401:PHE:CD1	1:A:401:PHE:N	2.84	0.43
1:B:592:ALA:HA	1:J:499:ASN:ND2	2.32	0.43
1:C:328:GLN:HE22	1:C:333:LYS:HG3	1.83	0.43
1:H:632:HIS:CE1	3:H:902:DA:C8	3.05	0.43
1:I:328:GLN:HE22	1:I:333:LYS:HG3	1.84	0.43
1:L:289:ARG:NE	1:L:617:GLN:O	2.46	0.43
1:N:289:ARG:NE	1:N:617:GLN:O	2.46	0.43
1:O:382:THR:HG22	1:O:383:LEU:H	1.83	0.43
1:P:566:GLU:OE2	1:P:569:LYS:NZ	2.45	0.43
1:O:481:LEU:HD13	1:P:636:LEU:HD11	72.35	0.43
1:R:318:LEU:HD13	1:R:318:LEU:HA	1.82	0.43
1:S:318:LEU:HA	1:S:318:LEU:HD13	1.82	0.43
1:S:328:GLN:HE22	1:S:333:LYS:HG3	1.83	0.43
1:S:401:PHE:CD1	1:S:401:PHE:N	2.84	0.43
1:T:251:PRO:HG3	1:T:374:MET:HE3	1.99	0.43
1:U:328:GLN:HE22	1:U:333:LYS:HG3	1.83	0.43
1:V:382:THR:HG22	1:V:383:LEU:H	1.83	0.43
1:Z:592:ALA:HA	1:4:499:ASN:HD22	1.81	0.43
1:1:382:THR:HG22	1:1:383:LEU:H	1.83	0.43
1:1:632:HIS:CE1	3:1:902:DA:C8	3.05	0.43
1:2:328:GLN:HE22	1:2:333:LYS:HG3	1.83	0.43
1:2:401:PHE:CD1	1:2:401:PHE:N	2.84	0.43
1:Z:636:LEU:HD11	1:3:481:LEU:HD13	2.01	0.43
1:3:310:ARG:NE	1:3:688:GLU:OE1	2.45	0.43
1:4:696:ARG:NE	1:4:698:ASN:OD1	2.42	0.43
1:5:610:GLN:HE22	1:6:627:THR:HA	1.82	0.43
1:6:310:ARG:NE	1:6:688:GLU:OE1	2.45	0.43
1:8:312:LYS:HA	1:8:312:LYS:HD2	1.84	0.43
1:8:434:ASP:N	1:8:434:ASP:OD1	2.45	0.43
1:D:328:GLN:HE22	1:D:333:LYS:HG3	1.83	0.43
1:E:328:GLN:HE22	1:E:333:LYS:HG3	1.83	0.43
1:E:382:THR:HG22	1:E:383:LEU:H	1.83	0.43
1:F:312:LYS:HD2	1:F:312:LYS:HA	1.84	0.43
1:G:451:THR:HG21	1:I:503:PHE:CZ	2.52	0.43
1:H:328:GLN:HE22	1:H:333:LYS:HG3	1.83	0.43
1:K:328:GLN:HE22	1:K:333:LYS:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:632:HIS:CE1	3:K:902:DA:C8	3.05	0.43
1:L:318:LEU:HA	1:L:318:LEU:HD13	1.82	0.43
1:M:291:HIS:HD2	1:M:617:GLN:HA	1.82	0.43
1:B:592:ALA:HA	1:M:499:ASN:ND2	127.29	0.43
1:N:328:GLN:HE22	1:N:333:LYS:HG3	1.83	0.43
1:P:307:TRP:CE2	1:P:692:GLU:HG2	2.53	0.43
1:F:627:THR:HA	1:Q:610:GLN:HE22	1.82	0.43
1:Q:632:HIS:CE1	3:Q:902:DA:C8	3.05	0.43
1:R:328:GLN:HE22	1:R:333:LYS:HG3	1.84	0.43
1:T:328:GLN:HE22	1:T:333:LYS:HG3	1.83	0.43
1:X:632:HIS:CE1	3:X:902:DA:C8	3.05	0.43
1:Y:307:TRP:CE2	1:Y:692:GLU:HG2	2.53	0.43
1:Z:499:ASN:HD22	1:3:592:ALA:HA	1.81	0.43
1:Z:632:HIS:CE1	3:Z:902:DA:C8	3.05	0.43
1:Z:426:SER:HB2	1:Z:731:THR:O	2.17	0.43
1:1:328:GLN:HE22	1:1:333:LYS:HG3	1.84	0.43
1:2:544:MET:HG2	1:2:562:LEU:HD23	1.98	0.43
1:5:632:HIS:CE1	3:5:902:DA:C8	3.05	0.43
1:8:307:TRP:CE2	1:8:692:GLU:HG2	2.53	0.43
1:A:312:LYS:HA	1:A:312:LYS:HD2	1.84	0.43
1:A:627:THR:HA	1:K:610:GLN:HE22	96.51	0.43
1:B:382:THR:HG22	1:B:383:LEU:H	1.83	0.43
1:D:427:TYR:N	1:D:732:ARG:HG2	2.31	0.43
1:J:318:LEU:HA	1:J:318:LEU:HD13	1.82	0.43
1:J:382:THR:HG22	1:J:383:LEU:H	1.83	0.43
1:L:328:GLN:HE22	1:L:333:LYS:HG3	1.83	0.43
1:M:636:LEU:HD11	1:O:481:LEU:HD13	106.12	0.43
1:O:312:LYS:HA	1:O:312:LYS:HD2	1.84	0.43
1:M:499:ASN:HD22	1:O:592:ALA:HA	132.16	0.43
1:P:310:ARG:NE	1:P:688:GLU:OE1	2.45	0.43
1:Q:307:TRP:CE2	1:Q:692:GLU:HG2	2.53	0.43
1:R:307:TRP:CE2	1:R:692:GLU:HG2	2.53	0.43
1:S:312:LYS:HD2	1:S:312:LYS:HA	1.84	0.43
1:R:481:LEU:HD13	1:S:636:LEU:CD1	2.49	0.43
1:T:382:THR:HG22	1:T:383:LEU:H	1.83	0.43
1:T:289:ARG:NE	1:T:617:GLN:O	2.46	0.43
1:V:328:GLN:HE22	1:V:333:LYS:HG3	1.84	0.43
1:W:328:GLN:HE22	1:W:333:LYS:HG3	1.83	0.43
1:2:289:ARG:NE	1:2:617:GLN:O	2.46	0.43
1:2:307:TRP:CE2	1:2:692:GLU:HG2	2.53	0.43
1:7:328:GLN:HE22	1:7:333:LYS:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:251:PRO:HG3	1:7:374:MET:HE3	2.01	0.43
1:C:359:SER:HB2	1:C:361:HIS:CD2	2.53	0.43
1:C:527:ALA:HB3	1:C:574:VAL:HA	2.01	0.43
1:D:481:LEU:HD13	1:L:636:LEU:HD11	127.97	0.43
1:D:610:GLN:HE22	1:N:627:THR:HA	1.83	0.43
1:D:289:ARG:NE	1:D:617:GLN:O	2.46	0.43
1:E:312:LYS:HA	1:E:312:LYS:HD2	1.84	0.43
1:E:359:SER:HB2	1:E:361:HIS:CD2	2.53	0.43
1:G:310:ARG:NE	1:G:688:GLU:OE1	2.45	0.43
1:H:312:LYS:HD2	1:H:312:LYS:HA	1.84	0.43
1:F:481:LEU:HD13	1:H:636:LEU:CD1	127.52	0.43
1:A:636:LEU:CD1	1:K:481:LEU:HD13	122.13	0.43
1:N:527:ALA:HB3	1:N:574:VAL:HA	2.01	0.43
1:P:312:LYS:HD2	1:P:312:LYS:HA	1.84	0.43
1:X:328:GLN:HE22	1:X:333:LYS:HG3	1.84	0.43
1:X:527:ALA:HB3	1:X:574:VAL:HA	2.01	0.43
1:Z:289:ARG:NE	1:Z:617:GLN:O	2.46	0.43
1:4:251:PRO:HG3	1:4:374:MET:HE3	2.01	0.43
1:4:382:THR:HG22	1:4:383:LEU:H	1.83	0.43
1:4:527:ALA:HB3	1:4:574:VAL:HA	2.01	0.43
1:6:307:TRP:CE2	1:6:692:GLU:HG2	2.53	0.43
1:6:359:SER:HB2	1:6:361:HIS:CD2	2.53	0.43
1:7:359:SER:HB2	1:7:361:HIS:CD2	2.53	0.43
1:A:258:TYR:OH	1:A:399:GLU:OE1	2.28	0.43
1:A:451:THR:HG21	1:G:503:PHE:CZ	2.53	0.43
1:B:527:ALA:HB3	1:B:574:VAL:HA	2.01	0.43
1:B:632:HIS:CE1	3:B:902:DA:C8	3.05	0.43
1:F:359:SER:HB2	1:F:361:HIS:CD2	2.53	0.43
1:H:307:TRP:CE2	1:H:692:GLU:HG2	2.53	0.43
1:K:527:ALA:HB3	1:K:574:VAL:HA	2.01	0.43
1:J:481:LEU:HD13	1:K:636:LEU:CD1	64.06	0.43
1:L:527:ALA:HB3	1:L:574:VAL:HA	2.01	0.43
1:L:632:HIS:CE1	3:L:902:DA:C8	3.05	0.43
1:B:481:LEU:HD13	1:M:636:LEU:HD11	102.10	0.43
1:N:382:THR:HG22	1:N:383:LEU:H	1.83	0.43
1:O:328:GLN:HE22	1:O:333:LYS:HG3	1.83	0.43
1:O:258:TYR:OH	1:O:399:GLU:OE1	2.28	0.43
1:O:310:ARG:NE	1:O:688:GLU:OE1	2.45	0.43
1:N:481:LEU:HD13	1:P:636:LEU:CD1	2.49	0.43
1:R:636:LEU:CD1	1:U:481:LEU:HD13	2.49	0.43
1:U:481:LEU:HD13	1:V:636:LEU:CD1	64.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:427:TYR:N	1:X:732:ARG:HG2	2.31	0.43
1:Y:312:LYS:HA	1:Y:312:LYS:HD2	1.85	0.43
1:H:636:LEU:CD1	1:Y:481:LEU:HD13	2.49	0.43
1:Z:328:GLN:HE22	1:Z:333:LYS:HG3	1.83	0.43
1:Z:636:LEU:HD11	1:2:481:LEU:HD13	85.58	0.43
1:Z:628:ASP:OD1	1:3:425:SER:OG	2.37	0.43
1:3:636:LEU:CD1	1:4:481:LEU:HD13	2.49	0.43
1:4:328:GLN:HE22	1:4:333:LYS:HG3	1.83	0.43
1:4:284:TYR:HB3	1:4:650:LEU:HD13	2.01	0.43
1:5:526:MET:HE2	1:5:575:ALA:HA	1.99	0.43
1:6:291:HIS:HD2	1:6:617:GLN:HA	1.82	0.43
1:8:284:TYR:HB3	1:8:650:LEU:HD13	2.01	0.43
1:K:636:LEU:HD11	1:8:481:LEU:HD13	2.01	0.43
1:A:481:LEU:HD13	1:8:636:LEU:CD1	144.06	0.43
1:A:527:ALA:HB3	1:A:574:VAL:HA	2.01	0.43
1:C:632:HIS:CE1	3:C:902:DA:C8	3.05	0.43
1:D:481:LEU:HD13	1:N:636:LEU:CD1	2.49	0.43
1:G:709:LYS:HZ1	1:H:532:ASP:CG	2.22	0.43
1:H:527:ALA:HB3	1:H:574:VAL:HA	2.01	0.43
1:I:312:LYS:HA	1:I:312:LYS:HD2	1.84	0.43
1:J:328:GLN:HE22	1:J:333:LYS:HG3	1.83	0.43
1:C:499:ASN:HD22	1:M:592:ALA:HA	1.82	0.43
1:N:284:TYR:HB3	1:N:650:LEU:HD13	2.01	0.43
1:N:481:LEU:HD13	1:O:636:LEU:CD1	64.06	0.43
1:P:284:TYR:HB3	1:P:650:LEU:HD13	2.01	0.43
1:P:527:ALA:HB3	1:P:574:VAL:HA	2.01	0.43
1:O:610:GLN:HE22	1:P:627:THR:HA	43.51	0.43
1:T:636:LEU:CD1	1:V:481:LEU:HD13	105.41	0.43
1:S:481:LEU:HD13	1:U:636:LEU:CD1	2.49	0.43
1:T:481:LEU:HD13	1:U:636:LEU:CD1	72.87	0.43
1:1:312:LYS:HA	1:1:312:LYS:HD2	1.84	0.43
1:1:289:ARG:NE	1:1:617:GLN:O	2.46	0.43
1:2:359:SER:HB2	1:2:361:HIS:CD2	2.53	0.43
1:3:527:ALA:HB3	1:3:574:VAL:HA	2.00	0.43
1:3:636:LEU:HD11	1:4:481:LEU:HD13	2.01	0.43
1:4:632:HIS:CE1	3:4:902:DA:C8	3.05	0.43
1:7:307:TRP:CE2	1:7:692:GLU:HG2	2.53	0.43
1:7:382:THR:HG22	1:7:383:LEU:H	1.83	0.43
1:6:481:LEU:HD13	1:7:636:LEU:HD11	2.01	0.43
1:F:427:TYR:N	1:F:732:ARG:HG2	2.31	0.43
1:G:527:ALA:HB3	1:G:574:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:636:LEU:CD1	1:H:481:LEU:HD13	64.05	0.43
1:G:275:TYR:HD2	1:H:473:MET:HE1	55.75	0.43
1:H:709:LYS:HZ1	1:K:532:ASP:CG	112.60	0.43
1:I:628:ASP:OD1	1:K:425:SER:OG	104.33	0.43
1:J:592:ALA:HA	1:L:499:ASN:HD22	1.82	0.43
1:J:427:TYR:N	1:J:732:ARG:HG2	2.31	0.43
1:K:627:THR:HA	1:8:610:GLN:HE22	1.83	0.43
1:H:532:ASP:CG	1:K:709:LYS:HZ1	137.90	0.43
1:K:427:TYR:N	1:K:732:ARG:HG2	2.31	0.43
1:L:401:PHE:CD1	1:L:401:PHE:N	2.84	0.43
1:P:318:LEU:HA	1:P:318:LEU:HD13	1.82	0.43
1:D:627:THR:HA	1:P:610:GLN:HE22	1.83	0.43
1:Q:284:TYR:HB3	1:Q:650:LEU:HD13	2.01	0.43
1:R:527:ALA:HB3	1:R:574:VAL:HA	2.01	0.43
1:Q:481:LEU:HD13	1:R:636:LEU:CD1	64.05	0.43
1:U:284:TYR:HB3	1:U:650:LEU:HD13	2.01	0.43
1:V:527:ALA:HB3	1:V:574:VAL:HA	2.01	0.43
1:W:284:TYR:HB3	1:W:650:LEU:HD13	2.01	0.43
1:Y:527:ALA:HB3	1:Y:574:VAL:HA	2.01	0.43
1:1:318:LEU:HD13	1:1:318:LEU:HA	1.82	0.43
1:Z:636:LEU:CD1	1:2:481:LEU:HD13	86.18	0.43
1:3:382:THR:HG22	1:3:383:LEU:H	1.83	0.43
1:5:359:SER:HB2	1:5:361:HIS:CD2	2.53	0.43
1:B:481:LEU:HD13	1:J:636:LEU:HD11	2.01	0.43
1:B:636:LEU:CD1	1:L:481:LEU:HD13	2.49	0.43
1:C:284:TYR:HB3	1:C:650:LEU:HD13	2.01	0.43
1:C:318:LEU:HA	1:C:318:LEU:HD13	1.82	0.43
1:E:481:LEU:HD13	1:Q:636:LEU:HD11	2.01	0.43
1:E:636:LEU:HD11	1:F:481:LEU:HD13	2.01	0.43
1:F:328:GLN:HE22	1:F:333:LYS:HG3	1.83	0.43
1:I:284:TYR:HB3	1:I:650:LEU:HD13	2.01	0.43
1:I:636:LEU:CD1	1:K:481:LEU:HD13	105.40	0.43
1:J:401:PHE:CD1	1:J:401:PHE:N	2.84	0.43
1:L:284:TYR:HB3	1:L:650:LEU:HD13	2.01	0.43
1:N:632:HIS:CE1	3:N:902:DA:C8	3.05	0.43
1:N:307:TRP:CE2	1:N:692:GLU:HG2	2.53	0.43
1:Q:527:ALA:HB3	1:Q:574:VAL:HA	2.01	0.43
1:S:289:ARG:NE	1:S:617:GLN:O	2.46	0.43
1:U:401:PHE:CD1	1:U:401:PHE:N	2.84	0.43
1:V:284:TYR:HB3	1:V:650:LEU:HD13	2.01	0.43
1:W:481:LEU:HD13	1:Y:636:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:632:HIS:CE1	3:2:902:DA:C8	3.05	0.43
1:Z:610:GLN:HE22	1:4:627:THR:HA	1.83	0.43
1:5:636:LEU:HD11	1:7:481:LEU:HD13	2.01	0.43
1:B:636:LEU:CD1	1:C:481:LEU:HD13	72.88	0.43
1:B:636:LEU:HD11	1:C:481:LEU:HD13	72.35	0.43
1:F:481:LEU:HD13	1:H:636:LEU:HD11	127.97	0.43
1:J:312:LYS:HD2	1:J:312:LYS:HA	1.84	0.43
1:K:545:PHE:O	1:K:561:MET:N	2.27	0.43
1:O:527:ALA:HB3	1:O:574:VAL:HA	2.01	0.43
1:N:481:LEU:HD13	1:O:636:LEU:HD11	64.93	0.43
1:D:636:LEU:HD11	1:P:481:LEU:HD13	2.01	0.43
1:R:275:TYR:HD2	1:U:473:MET:HE1	1.82	0.43
1:R:284:TYR:HB3	1:R:650:LEU:HD13	2.01	0.43
1:S:527:ALA:HB3	1:S:574:VAL:HA	2.01	0.43
1:U:532:ASP:CG	1:V:709:LYS:HZ1	2.22	0.43
1:W:239:ARG:NH1	1:W:688:GLU:HG3	2.34	0.43
1:W:527:ALA:HB3	1:W:574:VAL:HA	2.01	0.43
1:X:488:GLN:OE1	1:X:540:SER:OG	2.33	0.43
1:V:532:ASP:CG	1:Y:709:LYS:HZ1	141.96	0.43
1:Z:401:PHE:CD1	1:Z:401:PHE:N	2.84	0.43
1:Z:284:TYR:HB3	1:Z:650:LEU:HD13	2.01	0.43
1:1:284:TYR:HB3	1:1:650:LEU:HD13	2.01	0.43
1:3:328:GLN:HE22	1:3:333:LYS:HG3	1.83	0.43
1:5:328:GLN:HE22	1:5:333:LYS:HG3	1.84	0.43
1:5:307:TRP:CE2	1:5:692:GLU:HG2	2.53	0.43
1:6:632:HIS:CE1	3:6:902:DA:C8	3.05	0.43
1:7:312:LYS:HA	1:7:312:LYS:HD2	1.85	0.43
1:7:432:SER:HA	1:7:570:THR:HB	2.01	0.43
1:B:239:ARG:NH1	1:B:688:GLU:HG3	2.34	0.43
1:C:561:MET:HB3	1:C:728:PRO:HD3	2.01	0.43
1:C:570:THR:O	1:O:513:LEU:HD21	152.48	0.43
1:D:481:LEU:HD13	1:L:636:LEU:CD1	127.52	0.43
1:E:481:LEU:HD13	1:Q:636:LEU:CD1	2.49	0.43
1:F:318:LEU:HD13	1:F:318:LEU:HA	1.82	0.43
1:G:239:ARG:NH1	1:G:688:GLU:HG3	2.34	0.43
1:H:289:ARG:NE	1:H:617:GLN:O	2.46	0.43
1:J:481:LEU:HD13	1:K:636:LEU:HD11	64.93	0.43
1:K:239:ARG:NH1	1:K:688:GLU:HG3	2.34	0.43
1:B:636:LEU:HD11	1:L:481:LEU:HD13	2.01	0.43
1:M:401:PHE:CD1	1:M:401:PHE:N	2.84	0.43
1:M:527:ALA:HB3	1:M:574:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:401:PHE:CD1	1:O:401:PHE:N	2.84	0.43
1:Q:239:ARG:NH1	1:Q:688:GLU:HG3	2.34	0.43
1:T:312:LYS:HA	1:T:312:LYS:HD2	1.84	0.43
1:T:275:TYR:HD2	1:V:473:MET:HE1	89.22	0.43
1:W:636:LEU:CD1	1:Y:481:LEU:HD13	24.13	0.43
1:X:239:ARG:NH1	1:X:688:GLU:HG3	2.34	0.43
1:Y:284:TYR:HB3	1:Y:650:LEU:HD13	2.01	0.43
1:2:284:TYR:HB3	1:2:650:LEU:HD13	2.01	0.42
1:2:432:SER:HA	1:2:570:THR:HB	2.01	0.42
1:Z:636:LEU:CD1	1:3:481:LEU:HD13	2.49	0.42
1:3:628:ASP:OD1	1:4:425:SER:OG	2.37	0.42
1:5:240:VAL:HG13	1:5:687:TRP:HB2	2.01	0.42
1:5:481:LEU:HD13	1:6:636:LEU:HD11	2.01	0.42
1:5:636:LEU:CD1	1:7:481:LEU:HD13	2.49	0.42
1:8:328:GLN:HE22	1:8:333:LYS:HG3	1.84	0.42
1:A:636:LEU:CD1	1:I:481:LEU:HD13	2.49	0.42
1:B:481:LEU:HD13	1:M:636:LEU:CD1	102.78	0.42
1:B:432:SER:HA	1:B:570:THR:HB	2.01	0.42
1:B:610:GLN:HE22	1:M:627:THR:HA	95.09	0.42
1:C:636:LEU:CD1	1:P:481:LEU:HD13	66.94	0.42
1:D:284:TYR:HB3	1:D:650:LEU:HD13	2.01	0.42
1:E:432:SER:HA	1:E:570:THR:HB	2.01	0.42
1:F:636:LEU:HD11	1:Q:481:LEU:HD13	2.01	0.42
1:F:240:VAL:HG13	1:F:687:TRP:HB2	2.01	0.42
1:H:481:LEU:HD13	1:W:636:LEU:CD1	2.49	0.42
1:H:239:ARG:NH1	1:H:688:GLU:HG3	2.34	0.42
1:J:527:ALA:HB3	1:J:574:VAL:HA	2.01	0.42
1:J:284:TYR:HB3	1:J:650:LEU:HD13	2.01	0.42
1:K:318:LEU:HD13	1:K:318:LEU:HA	1.82	0.42
1:L:239:ARG:NH1	1:L:688:GLU:HG3	2.34	0.42
1:L:481:LEU:HD13	1:T:636:LEU:CD1	201.85	0.42
1:D:610:GLN:HE22	1:L:627:THR:HA	117.67	0.42
1:L:561:MET:HB3	1:L:728:PRO:HD3	2.01	0.42
1:M:610:GLN:HE22	1:N:627:THR:HA	43.51	0.42
1:M:481:LEU:HD13	1:N:636:LEU:CD1	72.88	0.42
1:M:636:LEU:CD1	1:O:481:LEU:HD13	105.40	0.42
1:N:425:SER:OG	1:O:628:ASP:OD1	63.12	0.42
1:C:627:THR:HA	1:P:610:GLN:HE22	63.52	0.42
1:P:240:VAL:HG13	1:P:687:TRP:HB2	2.01	0.42
1:P:709:LYS:HZ1	1:S:532:ASP:CG	112.35	0.42
1:Q:328:GLN:HE22	1:Q:333:LYS:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:240:VAL:HG13	1:Q:687:TRP:HB2	2.01	0.42
1:R:481:LEU:HD13	1:S:636:LEU:HD11	2.01	0.42
1:S:240:VAL:HG13	1:S:687:TRP:HB2	2.02	0.42
1:T:284:TYR:HB3	1:T:650:LEU:HD13	2.01	0.42
1:U:527:ALA:HB3	1:U:574:VAL:HA	2.01	0.42
1:T:481:LEU:HD13	1:U:636:LEU:HD11	72.34	0.42
1:U:240:VAL:HG13	1:U:687:TRP:HB2	2.01	0.42
1:E:636:LEU:CD1	1:V:481:LEU:HD13	139.83	0.42
1:T:636:LEU:HD11	1:V:481:LEU:HD13	106.12	0.42
1:V:240:VAL:HG13	1:V:687:TRP:HB2	2.02	0.42
1:V:239:ARG:NH1	1:V:688:GLU:HG3	2.34	0.42
1:X:432:SER:HA	1:X:570:THR:HB	2.01	0.42
1:Z:610:GLN:HE22	1:1:627:THR:HA	86.81	0.42
1:Z:561:MET:HB3	1:Z:728:PRO:HD3	2.01	0.42
1:Z:481:LEU:HD13	1:1:636:LEU:CD1	85.23	0.42
1:Z:627:THR:HA	1:2:610:GLN:HE22	69.38	0.42
1:3:284:TYR:HB3	1:3:650:LEU:HD13	2.01	0.42
1:3:240:VAL:HG13	1:3:687:TRP:HB2	2.02	0.42
1:4:307:TRP:CE2	1:4:692:GLU:HG2	2.53	0.42
1:6:240:VAL:HG13	1:6:687:TRP:HB2	2.02	0.42
1:8:240:VAL:HG13	1:8:687:TRP:HB2	2.02	0.42
1:C:610:GLN:HE22	1:O:627:THR:HA	138.73	0.42
1:C:239:ARG:NH1	1:C:688:GLU:HG3	2.34	0.42
1:D:239:ARG:NH1	1:D:688:GLU:HG3	2.34	0.42
1:D:432:SER:HA	1:D:570:THR:HB	2.02	0.42
1:F:284:TYR:HB3	1:F:650:LEU:HD13	2.01	0.42
1:G:636:LEU:HD11	1:H:481:LEU:HD13	64.92	0.42
1:H:561:MET:HB3	1:H:728:PRO:HD3	2.01	0.42
1:H:240:VAL:HG13	1:H:687:TRP:HB2	2.01	0.42
1:A:513:LEU:HD21	1:I:570:THR:O	2.19	0.42
1:I:239:ARG:NH1	1:I:688:GLU:HG3	2.34	0.42
1:B:481:LEU:HD13	1:J:636:LEU:CD1	2.49	0.42
1:I:636:LEU:HD11	1:K:481:LEU:HD13	106.12	0.42
1:B:627:THR:HA	1:L:610:GLN:HE22	1.83	0.42
1:J:481:LEU:HD13	1:L:636:LEU:CD1	2.49	0.42
1:C:532:ASP:CG	1:L:709:LYS:HZ1	2.21	0.42
1:M:561:MET:HB3	1:M:728:PRO:HD3	2.01	0.42
1:M:627:THR:HA	1:O:610:GLN:HE22	100.59	0.42
1:N:240:VAL:HG13	1:N:687:TRP:HB2	2.01	0.42
1:O:239:ARG:NH1	1:O:688:GLU:HG3	2.34	0.42
1:O:240:VAL:HG13	1:O:687:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:328:GLN:HE22	1:P:333:LYS:HG3	1.84	0.42
1:N:481:LEU:HD13	1:P:636:LEU:HD11	2.01	0.42
1:P:351:TYR:OH	1:P:645:PRO:O	2.26	0.42
1:P:239:ARG:NH1	1:P:688:GLU:HG3	2.34	0.42
1:Q:636:LEU:CD1	1:S:481:LEU:HD13	82.48	0.42
1:R:636:LEU:HD11	1:U:481:LEU:HD13	2.01	0.42
1:R:240:VAL:HG13	1:R:687:TRP:HB2	2.01	0.42
1:S:239:ARG:NH1	1:S:688:GLU:HG3	2.34	0.42
1:S:310:ARG:NE	1:S:688:GLU:OE1	2.45	0.42
1:L:610:GLN:HE22	1:T:627:THR:HA	190.67	0.42
1:T:240:VAL:HG13	1:T:687:TRP:HB2	2.01	0.42
1:U:561:MET:HB3	1:U:728:PRO:HD3	2.02	0.42
1:V:561:MET:HB3	1:V:728:PRO:HD3	2.01	0.42
1:X:561:MET:HB3	1:X:728:PRO:HD3	2.01	0.42
1:E:481:LEU:HD13	1:X:636:LEU:CD1	136.20	0.42
1:Y:239:ARG:NH1	1:Y:688:GLU:HG3	2.34	0.42
1:Y:709:LYS:HZ1	1:Z:532:ASP:CG	2.22	0.42
1:Z:481:LEU:HD13	1:4:636:LEU:CD1	2.49	0.42
1:1:527:ALA:HB3	1:1:574:VAL:HA	2.01	0.42
1:2:239:ARG:NH1	1:2:688:GLU:HG3	2.34	0.42
1:Z:627:THR:HA	1:3:610:GLN:HE22	1.83	0.42
1:4:426:SER:HB2	1:4:731:THR:HG22	2.02	0.42
1:5:426:SER:HB2	1:5:731:THR:HG22	2.02	0.42
1:6:251:PRO:HG3	1:6:374:MET:HE3	2.00	0.42
1:7:527:ALA:HB3	1:7:574:VAL:HA	2.01	0.42
1:A:239:ARG:NH1	1:A:688:GLU:HG3	2.34	0.42
1:A:419:GLU:OE2	1:A:643:LYS:N	2.44	0.42
1:A:481:LEU:HD13	1:8:636:LEU:HD11	143.25	0.42
1:A:636:LEU:HD11	1:K:481:LEU:HD13	121.37	0.42
1:A:240:VAL:HG13	1:A:687:TRP:HB2	2.02	0.42
1:A:561:MET:HB3	1:A:728:PRO:HD3	2.01	0.42
1:B:328:GLN:HE22	1:B:333:LYS:HG3	1.83	0.42
1:C:481:LEU:HD13	1:O:636:LEU:CD1	135.14	0.42
1:D:481:LEU:HD13	1:N:636:LEU:HD11	2.01	0.42
1:E:240:VAL:HG13	1:E:687:TRP:HB2	2.01	0.42
1:G:312:LYS:HA	1:G:312:LYS:HD2	1.84	0.42
1:H:284:TYR:HB3	1:H:650:LEU:HD13	2.01	0.42
1:G:570:THR:O	1:I:513:LEU:HD21	2.19	0.42
1:I:527:ALA:HB3	1:I:574:VAL:HA	2.01	0.42
1:I:561:MET:HB3	1:I:728:PRO:HD3	2.01	0.42
1:J:561:MET:HB3	1:J:728:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:284:TYR:HB3	1:K:650:LEU:HD13	2.01	0.42
1:N:426:SER:HB2	1:N:731:THR:HG22	2.02	0.42
1:N:561:MET:HB3	1:N:728:PRO:HD3	2.01	0.42
1:O:284:TYR:HB3	1:O:650:LEU:HD13	2.01	0.42
1:Q:426:SER:HB2	1:Q:731:THR:HG22	2.02	0.42
1:F:636:LEU:CD1	1:Q:481:LEU:HD13	2.48	0.42
1:M:532:ASP:CG	1:R:709:LYS:HZ1	145.23	0.42
1:S:561:MET:HB3	1:S:728:PRO:HD3	2.02	0.42
1:T:527:ALA:HB3	1:T:574:VAL:HA	2.01	0.42
1:T:700:GLU:HB2	1:T:702:GLN:HE21	1.85	0.42
1:U:426:SER:HB2	1:U:731:THR:HG22	2.02	0.42
1:U:432:SER:HA	1:U:570:THR:HB	2.01	0.42
1:U:700:GLU:HB2	1:U:702:GLN:HE21	1.85	0.42
1:V:636:LEU:CD1	1:X:481:LEU:HD13	2.49	0.42
1:W:240:VAL:HG13	1:W:687:TRP:HB2	2.01	0.42
1:W:481:LEU:HD13	1:X:636:LEU:CD1	64.05	0.42
1:X:481:LEU:HD13	1:Y:636:LEU:CD1	72.88	0.42
1:Y:561:MET:HB3	1:Y:728:PRO:HD3	2.01	0.42
1:3:351:TYR:OH	1:3:645:PRO:O	2.26	0.42
1:4:432:SER:HA	1:4:570:THR:HB	2.01	0.42
1:6:481:LEU:HD13	1:7:636:LEU:CD1	2.49	0.42
1:8:561:MET:HB3	1:8:728:PRO:HD3	2.01	0.42
1:8:700:GLU:HB2	1:8:702:GLN:HE21	1.85	0.42
1:A:426:SER:HB2	1:A:731:THR:HG22	2.02	0.42
1:E:527:ALA:HB3	1:E:574:VAL:HA	2.01	0.42
1:E:636:LEU:CD1	1:F:481:LEU:HD13	2.49	0.42
1:G:284:TYR:HB3	1:G:650:LEU:HD13	2.01	0.42
1:B:610:GLN:HE22	1:J:627:THR:HA	1.82	0.42
1:I:481:LEU:HD13	1:J:636:LEU:CD1	72.87	0.42
1:B:425:SER:OG	1:M:628:ASP:OD1	90.57	0.42
1:N:439:PRO:O	1:N:470:PRO:HG3	2.20	0.42
1:N:432:SER:HA	1:N:570:THR:HB	2.02	0.42
1:C:636:LEU:HD11	1:P:481:LEU:HD13	66.69	0.42
1:P:700:GLU:HB2	1:P:702:GLN:HE21	1.85	0.42
1:R:439:PRO:O	1:R:470:PRO:HG3	2.20	0.42
1:Q:481:LEU:HD13	1:R:636:LEU:HD11	64.93	0.42
1:R:700:GLU:HB2	1:R:702:GLN:HE21	1.85	0.42
1:S:439:PRO:O	1:S:470:PRO:HG3	2.20	0.42
1:S:426:SER:HB2	1:S:731:THR:HG22	2.02	0.42
1:U:239:ARG:NH1	1:U:688:GLU:HG3	2.34	0.42
1:U:310:ARG:NE	1:U:688:GLU:OE1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:636:LEU:HD11	1:V:481:LEU:HD13	139.03	0.42
1:V:700:GLU:HB2	1:V:702:GLN:HE21	1.85	0.42
1:V:426:SER:HB2	1:V:731:THR:HG22	2.02	0.42
1:W:346:PHE:CE1	1:W:401:PHE:HD2	2.38	0.42
1:W:432:SER:HA	1:W:570:THR:HB	2.01	0.42
1:X:240:VAL:HG13	1:X:687:TRP:HB2	2.01	0.42
1:X:439:PRO:O	1:X:470:PRO:HG3	2.20	0.42
1:Y:426:SER:HB2	1:Y:731:THR:HG22	2.02	0.42
1:Y:439:PRO:O	1:Y:470:PRO:HG3	2.20	0.42
1:W:636:LEU:HD11	1:Y:481:LEU:HD13	23.17	0.42
1:Z:570:THR:O	1:1:513:LEU:HD21	95.21	0.42
1:1:239:ARG:NH1	1:1:688:GLU:HG3	2.34	0.42
1:1:545:PHE:O	1:1:561:MET:N	2.27	0.42
1:2:700:GLU:HB2	1:2:702:GLN:HE21	1.85	0.42
1:3:401:PHE:CD1	1:3:401:PHE:N	2.84	0.42
1:3:561:MET:HB3	1:3:728:PRO:HD3	2.02	0.42
1:3:700:GLU:HB2	1:3:702:GLN:HE21	1.85	0.42
1:6:346:PHE:CE1	1:6:401:PHE:HD2	2.38	0.42
1:6:432:SER:HA	1:6:570:THR:HB	2.01	0.42
1:7:426:SER:HB2	1:7:731:THR:HG22	2.02	0.42
1:7:439:PRO:O	1:7:470:PRO:HG3	2.20	0.42
1:7:240:VAL:HG13	1:7:687:TRP:HB2	2.02	0.42
1:7:709:LYS:HZ1	1:8:532:ASP:CG	2.23	0.42
1:8:432:SER:HA	1:8:570:THR:HB	2.01	0.42
1:8:527:ALA:HB3	1:8:574:VAL:HA	2.01	0.42
1:8:239:ARG:NH1	1:8:688:GLU:HG3	2.34	0.42
1:8:692:GLU:HG3	1:8:734:LEU:HD13	2.02	0.42
1:B:426:SER:HB2	1:B:731:THR:HG22	2.02	0.42
1:B:627:THR:HA	1:C:610:GLN:HE22	43.51	0.42
1:D:318:LEU:HD13	1:D:318:LEU:HA	1.82	0.42
1:D:426:SER:HB2	1:D:731:THR:HG22	2.02	0.42
1:D:700:GLU:HB2	1:D:702:GLN:HE21	1.85	0.42
1:E:346:PHE:CE1	1:E:401:PHE:HD2	2.38	0.42
1:E:426:SER:HB2	1:E:731:THR:HG22	2.02	0.42
1:F:239:ARG:NH1	1:F:688:GLU:HG3	2.34	0.42
1:G:700:GLU:HB2	1:G:702:GLN:HE21	1.85	0.42
1:H:426:SER:HB2	1:H:731:THR:HG22	2.02	0.42
1:I:700:GLU:HB2	1:I:702:GLN:HE21	1.85	0.42
1:I:481:LEU:HD13	1:J:636:LEU:HD11	72.33	0.42
1:K:426:SER:HB2	1:K:731:THR:HG22	2.02	0.42
1:L:570:THR:O	1:T:513:LEU:HD21	209.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:328:GLN:HE22	1:M:333:LYS:HG3	1.83	0.42
1:C:636:LEU:CD1	1:M:481:LEU:HD13	2.49	0.42
1:O:700:GLU:HB2	1:O:702:GLN:HE21	1.85	0.42
1:P:561:MET:HB3	1:P:728:PRO:HD3	2.01	0.42
1:Q:432:SER:HA	1:Q:570:THR:HB	2.01	0.42
1:R:561:MET:HB3	1:R:728:PRO:HD3	2.02	0.42
1:T:561:MET:HB3	1:T:728:PRO:HD3	2.01	0.42
1:T:692:GLU:HG3	1:T:734:LEU:HD13	2.02	0.42
1:U:439:PRO:O	1:U:470:PRO:HG3	2.20	0.42
1:V:432:SER:HA	1:V:570:THR:HB	2.02	0.42
1:W:700:GLU:HB2	1:W:702:GLN:HE21	1.85	0.42
1:X:284:TYR:HB3	1:X:650:LEU:HD13	2.01	0.42
1:W:481:LEU:HD13	1:Y:636:LEU:HD11	2.01	0.42
1:1:700:GLU:HB2	1:1:702:GLN:HE21	1.85	0.42
1:1:561:MET:HB3	1:1:728:PRO:HD3	2.01	0.42
1:1:692:GLU:HG3	1:1:734:LEU:HD13	2.02	0.42
1:3:346:PHE:CE1	1:3:401:PHE:HD2	2.38	0.42
1:4:439:PRO:O	1:4:470:PRO:HG3	2.20	0.42
1:Z:425:SER:OG	1:4:628:ASP:OD1	2.37	0.42
1:4:240:VAL:HG13	1:4:687:TRP:HB2	2.02	0.42
1:5:481:LEU:HD13	1:6:636:LEU:CD1	2.49	0.42
1:6:239:ARG:NH1	1:6:688:GLU:HG3	2.34	0.42
1:6:692:GLU:HG3	1:6:734:LEU:HD13	2.02	0.42
1:K:636:LEU:CD1	1:8:481:LEU:HD13	2.49	0.42
1:A:425:SER:OG	1:8:628:ASP:OD1	128.01	0.42
1:A:692:GLU:HG3	1:A:734:LEU:HD13	2.02	0.42
1:B:439:PRO:O	1:B:470:PRO:HG3	2.20	0.42
1:B:557:TYR:HE1	1:B:562:LEU:HD11	1.85	0.42
1:C:346:PHE:CE1	1:C:401:PHE:HD2	2.38	0.42
1:C:439:PRO:O	1:C:470:PRO:HG3	2.20	0.42
1:C:700:GLU:HB2	1:C:702:GLN:HE21	1.85	0.42
1:C:692:GLU:HG3	1:C:734:LEU:HD13	2.02	0.42
1:E:439:PRO:O	1:E:470:PRO:HG3	2.20	0.42
1:E:557:TYR:HE1	1:E:562:LEU:HD11	1.85	0.42
1:F:346:PHE:CE1	1:F:401:PHE:HD2	2.38	0.42
1:F:432:SER:HA	1:F:570:THR:HB	2.01	0.42
1:F:527:ALA:HB3	1:F:574:VAL:HA	2.01	0.42
1:F:632:HIS:O	1:F:634:SER:N	2.52	0.42
1:F:692:GLU:HG3	1:F:734:LEU:HD13	2.02	0.42
1:A:532:ASP:CG	1:F:709:LYS:HZ1	2.21	0.42
1:G:346:PHE:CE1	1:G:401:PHE:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:PHE:CE1	1:H:401:PHE:HD2	2.38	0.42
1:H:439:PRO:O	1:H:470:PRO:HG3	2.20	0.42
1:H:432:SER:HA	1:H:570:THR:HB	2.01	0.42
1:H:700:GLU:HB2	1:H:702:GLN:HE21	1.85	0.42
1:I:346:PHE:CE1	1:I:401:PHE:HD2	2.38	0.42
1:I:426:SER:HB2	1:I:731:THR:HG22	2.02	0.42
1:A:503:PHE:CZ	1:I:451:THR:HG21	2.54	0.42
1:B:709:LYS:HZ1	1:I:532:ASP:CG	2.23	0.42
1:I:240:VAL:HG13	1:I:687:TRP:HB2	2.02	0.42
1:J:439:PRO:O	1:J:470:PRO:HG3	2.20	0.42
1:J:240:VAL:HG13	1:J:687:TRP:HB2	2.01	0.42
1:K:346:PHE:CE1	1:K:401:PHE:HD2	2.38	0.42
1:K:439:PRO:O	1:K:470:PRO:HG3	2.20	0.42
1:K:561:MET:HB3	1:K:728:PRO:HD3	2.02	0.42
1:K:700:GLU:HB2	1:K:702:GLN:HE21	1.85	0.42
1:L:432:SER:HA	1:L:570:THR:HB	2.02	0.42
1:L:692:GLU:HG3	1:L:734:LEU:HD13	2.02	0.42
1:M:439:PRO:O	1:M:470:PRO:HG3	2.20	0.42
1:M:425:SER:OG	1:N:628:ASP:OD1	39.45	0.42
1:O:561:MET:HB3	1:O:728:PRO:HD3	2.02	0.42
1:P:426:SER:HB2	1:P:731:THR:HG22	2.02	0.42
1:P:692:GLU:HG3	1:P:734:LEU:HD13	2.02	0.42
1:Q:346:PHE:CE1	1:Q:401:PHE:HD2	2.38	0.42
1:Q:439:PRO:O	1:Q:470:PRO:HG3	2.20	0.42
1:R:426:SER:HB2	1:R:731:THR:HG22	2.02	0.42
1:S:632:HIS:O	1:S:634:SER:N	2.52	0.42
1:S:700:GLU:HB2	1:S:702:GLN:HE21	1.85	0.42
1:T:239:ARG:NH1	1:T:688:GLU:HG3	2.34	0.42
1:U:557:TYR:HE1	1:U:562:LEU:HD11	1.85	0.42
1:U:481:LEU:HD13	1:V:636:LEU:HD11	64.93	0.42
1:W:258:TYR:OH	1:W:399:GLU:OE1	2.28	0.42
1:W:426:SER:HB2	1:W:731:THR:HG22	2.02	0.42
1:W:439:PRO:O	1:W:470:PRO:HG3	2.20	0.42
1:Y:632:HIS:O	1:Y:634:SER:N	2.52	0.42
1:Y:240:VAL:HG13	1:Y:687:TRP:HB2	2.01	0.42
1:Z:239:ARG:NH1	1:Z:688:GLU:HG3	2.34	0.42
1:Z:432:SER:HA	1:Z:570:THR:HB	2.01	0.42
1:Z:628:ASP:OD1	1:2:425:SER:OG	63.12	0.42
1:2:557:TYR:HE1	1:2:562:LEU:HD11	1.85	0.42
1:4:239:ARG:NH1	1:4:688:GLU:HG3	2.34	0.42
1:5:346:PHE:CE1	1:5:401:PHE:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:419:GLU:OE2	1:5:643:LYS:N	2.44	0.42
1:6:426:SER:HB2	1:6:731:THR:HG22	2.02	0.42
1:7:239:ARG:NH1	1:7:688:GLU:HG3	2.34	0.42
1:7:346:PHE:CE1	1:7:401:PHE:HD2	2.38	0.42
1:7:284:TYR:HB3	1:7:650:LEU:HD13	2.01	0.42
1:8:488:GLN:OE1	1:8:540:SER:OG	2.33	0.42
1:A:284:TYR:HB3	1:A:650:LEU:HD13	2.01	0.42
1:B:346:PHE:CE1	1:B:401:PHE:HD2	2.38	0.42
1:C:557:TYR:HE1	1:C:562:LEU:HD11	1.85	0.42
1:D:346:PHE:CE1	1:D:401:PHE:HD2	2.38	0.42
1:D:439:PRO:O	1:D:470:PRO:HG3	2.20	0.42
1:D:561:MET:HB3	1:D:728:PRO:HD3	2.01	0.42
1:E:284:TYR:HB3	1:E:650:LEU:HD13	2.01	0.42
1:E:239:ARG:NH1	1:E:688:GLU:HG3	2.34	0.42
1:F:636:LEU:CD1	1:G:481:LEU:HD13	82.48	0.42
1:G:426:SER:HB2	1:G:731:THR:HG22	2.02	0.42
1:G:432:SER:HA	1:G:570:THR:HB	2.01	0.42
1:G:240:VAL:HG13	1:G:687:TRP:HB2	2.01	0.42
1:H:632:HIS:O	1:H:634:SER:N	2.52	0.42
1:J:432:SER:HA	1:J:570:THR:HB	2.01	0.42
1:K:432:SER:HA	1:K:570:THR:HB	2.02	0.42
1:L:439:PRO:O	1:L:470:PRO:HG3	2.20	0.42
1:L:700:GLU:HB2	1:L:702:GLN:HE21	1.85	0.42
1:M:700:GLU:HB2	1:M:702:GLN:HE21	1.85	0.42
1:N:239:ARG:NH1	1:N:688:GLU:HG3	2.34	0.42
1:O:346:PHE:CE1	1:O:401:PHE:HD2	2.38	0.42
1:O:692:GLU:HG3	1:O:734:LEU:HD13	2.02	0.42
1:P:346:PHE:CE1	1:P:401:PHE:HD2	2.38	0.42
1:P:432:SER:HA	1:P:570:THR:HB	2.02	0.42
1:R:632:HIS:O	1:R:634:SER:N	2.52	0.42
1:S:284:TYR:HB3	1:S:650:LEU:HD13	2.01	0.42
1:S:557:TYR:HE1	1:S:562:LEU:HD11	1.85	0.42
1:S:427:TYR:N	1:S:732:ARG:HG2	2.31	0.42
1:S:481:LEU:HD13	1:U:636:LEU:HD11	2.01	0.42
1:U:427:TYR:N	1:U:732:ARG:HG2	2.31	0.42
1:V:636:LEU:HD11	1:X:481:LEU:HD13	2.01	0.42
1:W:557:TYR:HE1	1:W:562:LEU:HD11	1.85	0.42
1:H:481:LEU:HD13	1:W:636:LEU:HD11	2.01	0.42
1:X:258:TYR:OH	1:X:399:GLU:OE1	2.28	0.42
1:Y:401:PHE:N	1:Y:401:PHE:CD1	2.84	0.42
1:Z:632:HIS:O	1:Z:634:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:700:GLU:HB2	1:Z:702:GLN:HE21	1.85	0.42
1:2:527:ALA:HB3	1:2:574:VAL:HA	2.01	0.42
1:2:561:MET:HB3	1:2:728:PRO:HD3	2.02	0.42
1:6:328:GLN:HE22	1:6:333:LYS:HG3	1.83	0.42
1:7:289:ARG:NE	1:7:617:GLN:O	2.46	0.42
1:7:632:HIS:CE1	3:7:902:DA:C8	3.05	0.42
1:7:692:GLU:HG3	1:7:734:LEU:HD13	2.02	0.42
1:8:346:PHE:CE1	1:8:401:PHE:HD2	2.38	0.42
1:8:401:PHE:N	1:8:401:PHE:CD1	2.84	0.42
1:C:240:VAL:HG13	1:C:687:TRP:HB2	2.01	0.42
1:C:426:SER:HB2	1:C:731:THR:HG22	2.02	0.42
1:D:527:ALA:HB3	1:D:574:VAL:HA	2.01	0.42
1:D:240:VAL:HG13	1:D:687:TRP:HB2	2.01	0.42
1:E:700:GLU:HB2	1:E:702:GLN:HE21	1.85	0.42
1:F:426:SER:HB2	1:F:731:THR:HG22	2.02	0.42
1:F:561:MET:HB3	1:F:728:PRO:HD3	2.02	0.42
1:G:561:MET:HB3	1:G:728:PRO:HD3	2.01	0.42
1:G:532:ASP:CG	1:H:709:LYS:HZ1	2.23	0.42
1:I:557:TYR:HE1	1:I:562:LEU:HD11	1.85	0.42
1:G:481:LEU:HD13	1:I:636:LEU:CD1	2.49	0.42
1:J:632:HIS:O	1:J:634:SER:N	2.52	0.42
1:K:240:VAL:HG13	1:K:687:TRP:HB2	2.02	0.42
1:L:346:PHE:CE1	1:L:401:PHE:HD2	2.38	0.42
1:M:557:TYR:HE1	1:M:562:LEU:HD11	1.85	0.42
1:M:692:GLU:HG3	1:M:734:LEU:HD13	2.02	0.42
1:Q:532:ASP:CG	1:X:709:LYS:HZ1	132.29	0.42
1:Q:557:TYR:HE1	1:Q:562:LEU:HD11	1.85	0.42
1:Q:700:GLU:HB2	1:Q:702:GLN:HE21	1.85	0.42
1:R:346:PHE:CE1	1:R:401:PHE:HD2	2.38	0.42
1:U:346:PHE:CE1	1:U:401:PHE:HD2	2.38	0.42
1:V:439:PRO:O	1:V:470:PRO:HG3	2.20	0.42
1:V:557:TYR:HE1	1:V:562:LEU:HD11	1.85	0.42
1:W:692:GLU:HG3	1:W:734:LEU:HD13	2.02	0.42
1:Y:557:TYR:HE1	1:Y:562:LEU:HD11	1.85	0.42
1:2:240:VAL:HG13	1:2:687:TRP:HB2	2.01	0.42
1:3:239:ARG:NH1	1:3:688:GLU:HG3	2.34	0.42
1:4:289:ARG:NE	1:4:617:GLN:O	2.46	0.42
1:4:692:GLU:HG3	1:4:734:LEU:HD13	2.02	0.42
1:5:312:LYS:HD2	1:5:312:LYS:HA	1.84	0.42
1:5:318:LEU:HA	1:5:318:LEU:HD13	1.82	0.42
1:5:527:ALA:HB3	1:5:574:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:318:LEU:HD13	1:6:318:LEU:HA	1.82	0.42
1:6:527:ALA:HB3	1:6:574:VAL:HA	2.01	0.42
1:B:284:TYR:HB3	1:B:650:LEU:HD13	2.01	0.42
1:B:561:MET:HB3	1:B:728:PRO:HD3	2.02	0.42
1:C:432:SER:HA	1:C:570:THR:HB	2.02	0.42
1:C:613:ASP:OD1	1:C:614:VAL:N	2.53	0.42
1:D:557:TYR:HE1	1:D:562:LEU:HD11	1.85	0.42
1:D:636:LEU:CD1	1:P:481:LEU:HD13	2.49	0.42
1:E:561:MET:HB3	1:E:728:PRO:HD3	2.02	0.42
1:E:610:GLN:HE22	1:X:627:THR:HA	139.40	0.42
1:E:692:GLU:HG3	1:E:734:LEU:HD13	2.02	0.42
1:F:636:LEU:HD11	1:G:481:LEU:HD13	83.27	0.42
1:H:613:ASP:OD1	1:H:614:VAL:N	2.53	0.42
1:H:427:TYR:N	1:H:732:ARG:HG2	2.31	0.42
1:I:439:PRO:O	1:I:470:PRO:HG3	2.20	0.42
1:J:239:ARG:NH1	1:J:688:GLU:HG3	2.34	0.42
1:J:346:PHE:CE1	1:J:401:PHE:HD2	2.38	0.42
1:J:692:GLU:HG3	1:J:734:LEU:HD13	2.02	0.42
1:K:557:TYR:HE1	1:K:562:LEU:HD11	1.85	0.42
1:K:613:ASP:OD1	1:K:614:VAL:N	2.53	0.42
1:K:632:HIS:O	1:K:634:SER:N	2.52	0.42
1:L:613:ASP:OD1	1:L:614:VAL:N	2.53	0.42
1:L:427:TYR:N	1:L:732:ARG:HG2	2.31	0.42
1:M:284:TYR:HB3	1:M:650:LEU:HD13	2.01	0.42
1:N:532:ASP:CG	1:O:709:LYS:HZ1	2.22	0.42
1:P:427:TYR:N	1:P:732:ARG:HG2	2.31	0.42
1:Q:312:LYS:HD2	1:Q:312:LYS:HA	1.84	0.42
1:Q:636:LEU:HD11	1:S:481:LEU:HD13	83.27	0.42
1:Q:692:GLU:HG3	1:Q:734:LEU:HD13	2.02	0.42
1:S:346:PHE:CE1	1:S:401:PHE:HD2	2.38	0.42
1:U:632:HIS:CE1	3:U:902:DA:C8	3.05	0.42
1:W:610:GLN:HE22	1:X:627:THR:HA	61.35	0.42
1:W:532:ASP:CG	1:X:709:LYS:HZ1	2.22	0.42
1:Y:346:PHE:CE1	1:Y:401:PHE:HD2	2.38	0.42
1:H:636:LEU:HD11	1:Y:481:LEU:HD13	2.01	0.42
1:X:481:LEU:HD13	1:Y:636:LEU:HD11	72.35	0.42
1:Z:439:PRO:O	1:Z:470:PRO:HG3	2.20	0.42
1:Z:557:TYR:HE1	1:Z:562:LEU:HD11	1.85	0.42
1:Z:692:GLU:HG3	1:Z:734:LEU:HD13	2.02	0.42
1:1:251:PRO:HG3	1:1:374:MET:HE3	2.00	0.42
1:2:346:PHE:CE1	1:2:401:PHE:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:613:ASP:OD1	1:3:614:VAL:N	2.53	0.42
1:A:532:ASP:CG	1:3:709:LYS:HZ1	170.28	0.42
1:2:532:ASP:CG	1:4:709:LYS:HZ1	2.24	0.42
1:5:557:TYR:HE1	1:5:562:LEU:HD11	1.85	0.42
1:5:613:ASP:OD1	1:5:614:VAL:N	2.53	0.42
1:6:700:GLU:HB2	1:6:702:GLN:HE21	1.85	0.42
1:6:427:TYR:N	1:6:732:ARG:HG2	2.31	0.42
1:A:432:SER:HA	1:A:570:THR:HB	2.01	0.42
1:C:312:LYS:HD2	1:C:312:LYS:HA	1.84	0.42
1:B:664:PHE:CD1	1:C:376:PRO:HA	2.55	0.42
1:E:289:ARG:NE	1:E:617:GLN:O	2.46	0.42
1:F:557:TYR:HE1	1:F:562:LEU:HD11	1.85	0.42
1:G:632:HIS:O	1:G:634:SER:N	2.52	0.42
1:G:692:GLU:HG3	1:G:734:LEU:HD13	2.02	0.42
1:H:557:TYR:HE1	1:H:562:LEU:HD11	1.85	0.42
1:J:557:TYR:HE1	1:J:562:LEU:HD11	1.85	0.42
1:J:709:LYS:HZ1	1:K:532:ASP:CG	2.22	0.42
1:L:426:SER:HB2	1:L:731:THR:HG22	2.02	0.42
1:L:632:HIS:O	1:L:634:SER:N	2.52	0.42
1:M:376:PRO:HA	1:S:664:PHE:CD1	127.54	0.42
1:M:426:SER:HB2	1:M:731:THR:HG22	2.02	0.42
1:M:240:VAL:HG13	1:M:687:TRP:HB2	2.01	0.42
1:M:239:ARG:NH1	1:M:688:GLU:HG3	2.34	0.42
1:N:692:GLU:HG3	1:N:734:LEU:HD13	2.02	0.42
1:O:557:TYR:HE1	1:O:562:LEU:HD11	1.85	0.42
1:O:613:ASP:OD1	1:O:614:VAL:N	2.53	0.42
1:P:557:TYR:HE1	1:P:562:LEU:HD11	1.85	0.42
1:Q:299:TRP:HE1	1:Q:729:ILE:HG22	1.85	0.42
1:Q:613:ASP:OD1	1:Q:614:VAL:N	2.53	0.42
1:R:613:ASP:OD1	1:R:614:VAL:N	2.53	0.42
1:S:432:SER:HA	1:S:570:THR:HB	2.01	0.42
1:T:346:PHE:CE1	1:T:401:PHE:HD2	2.38	0.42
1:V:346:PHE:CE1	1:V:401:PHE:HD2	2.38	0.42
1:V:401:PHE:CD1	1:V:401:PHE:N	2.84	0.42
1:X:346:PHE:CE1	1:X:401:PHE:HD2	2.38	0.42
1:X:426:SER:HB2	1:X:731:THR:HG22	2.02	0.42
1:X:692:GLU:HG3	1:X:734:LEU:HD13	2.02	0.42
1:Y:700:GLU:HB2	1:Y:702:GLN:HE21	1.85	0.42
1:Z:346:PHE:CE1	1:Z:401:PHE:HD2	2.38	0.42
1:Z:527:ALA:HB3	1:Z:574:VAL:HA	2.01	0.42
1:1:426:SER:HB2	1:1:731:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:545:PHE:O	1:2:561:MET:N	2.27	0.41
1:2:692:GLU:HG3	1:2:734:LEU:HD13	2.02	0.41
1:6:439:PRO:O	1:6:470:PRO:HG3	2.20	0.41
1:6:557:TYR:HE1	1:6:562:LEU:HD11	1.85	0.41
1:T:376:PRO:HA	1:6:664:PHE:CD1	179.24	0.41
1:6:696:ARG:NE	1:6:698:ASN:OD1	2.42	0.41
1:7:561:MET:HB3	1:7:728:PRO:HD3	2.02	0.41
1:8:426:SER:HB2	1:8:731:THR:HG22	2.02	0.41
1:G:557:TYR:HE1	1:G:562:LEU:HD11	1.85	0.41
1:H:664:PHE:CD1	1:Z:376:PRO:HA	2.55	0.41
1:L:312:LYS:HA	1:L:312:LYS:HD2	1.84	0.41
1:B:664:PHE:CD1	1:L:376:PRO:HA	74.09	0.41
1:L:557:TYR:HE1	1:L:562:LEU:HD11	1.85	0.41
1:M:432:SER:HA	1:M:570:THR:HB	2.02	0.41
1:M:613:ASP:OD1	1:M:614:VAL:N	2.53	0.41
1:O:439:PRO:O	1:O:470:PRO:HG3	2.20	0.41
1:Q:318:LEU:HA	1:Q:318:LEU:HD13	1.82	0.41
1:Q:258:TYR:OH	1:Q:399:GLU:OE1	2.28	0.41
1:S:613:ASP:OD1	1:S:614:VAL:N	2.53	0.41
1:T:426:SER:HB2	1:T:731:THR:HG22	2.02	0.41
1:T:613:ASP:OD1	1:T:614:VAL:N	2.53	0.41
1:U:613:ASP:OD1	1:U:614:VAL:N	2.53	0.41
1:V:613:ASP:OD1	1:V:614:VAL:N	2.53	0.41
1:W:368:PHE:HA	1:W:369:PRO:HD3	1.97	0.41
1:X:545:PHE:O	1:X:561:MET:N	2.27	0.41
1:W:481:LEU:HD13	1:X:636:LEU:HD11	64.93	0.41
1:X:700:GLU:HB2	1:X:702:GLN:HE21	1.85	0.41
1:Y:432:SER:HA	1:Y:570:THR:HB	2.02	0.41
1:3:439:PRO:O	1:3:470:PRO:HG3	2.20	0.41
1:3:513:LEU:HD21	1:4:570:THR:O	2.21	0.41
1:4:561:MET:HB3	1:4:728:PRO:HD3	2.02	0.41
1:5:299:TRP:HE1	1:5:729:ILE:HG22	1.85	0.41
1:7:700:GLU:HB2	1:7:702:GLN:HE21	1.85	0.41
1:A:298:ASP:OD1	1:A:301:ARG:NH1	2.54	0.41
1:A:439:PRO:O	1:A:470:PRO:HG3	2.20	0.41
1:A:613:ASP:OD1	1:A:614:VAL:N	2.53	0.41
1:D:692:GLU:HG3	1:D:734:LEU:HD13	2.02	0.41
1:E:368:PHE:HA	1:E:369:PRO:HD3	1.97	0.41
1:F:613:ASP:OD1	1:F:614:VAL:N	2.53	0.41
1:F:700:GLU:HB2	1:F:702:GLN:HE21	1.85	0.41
1:G:568:ILE:HD12	1:G:572:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:TRP:HE1	1:G:729:ILE:HG22	1.86	0.41
1:I:299:TRP:HE1	1:I:729:ILE:HG22	1.85	0.41
1:I:568:ILE:HD12	1:I:572:ASN:HD22	1.86	0.41
1:J:613:ASP:OD1	1:J:614:VAL:N	2.53	0.41
1:J:481:LEU:HD13	1:L:636:LEU:HD11	2.01	0.41
1:C:636:LEU:HD11	1:M:481:LEU:HD13	2.01	0.41
1:D:532:ASP:CG	1:M:709:LYS:HZ1	2.22	0.41
1:N:298:ASP:OD1	1:N:301:ARG:NH1	2.54	0.41
1:M:481:LEU:HD13	1:N:636:LEU:HD11	72.35	0.41
1:P:613:ASP:OD1	1:P:614:VAL:N	2.53	0.41
1:P:632:HIS:O	1:P:634:SER:N	2.52	0.41
1:S:709:LYS:HZ1	1:T:532:ASP:CG	2.22	0.41
1:U:289:ARG:NE	1:U:617:GLN:O	2.46	0.41
1:U:692:GLU:HG3	1:U:734:LEU:HD13	2.02	0.41
1:1:427:TYR:N	1:1:732:ARG:HG2	2.31	0.41
1:4:298:ASP:OD1	1:4:301:ARG:NH1	2.53	0.41
1:5:439:PRO:O	1:5:470:PRO:HG3	2.20	0.41
1:5:239:ARG:NH1	1:5:688:GLU:HG3	2.34	0.41
1:8:427:TYR:N	1:8:732:ARG:HG2	2.31	0.41
1:A:557:TYR:HE1	1:A:562:LEU:HD11	1.85	0.41
1:A:700:GLU:HB2	1:A:702:GLN:HE21	1.85	0.41
1:B:613:ASP:OD1	1:B:614:VAL:N	2.53	0.41
1:B:240:VAL:HG13	1:B:687:TRP:HB2	2.02	0.41
1:B:299:TRP:HE1	1:B:729:ILE:HG22	1.85	0.41
1:C:568:ILE:HD12	1:C:572:ASN:HD22	1.86	0.41
1:C:628:ASP:OD1	1:M:425:SER:OG	2.37	0.41
1:C:299:TRP:HE1	1:C:729:ILE:HG22	1.85	0.41
1:D:298:ASP:OD1	1:D:301:ARG:NH1	2.54	0.41
1:D:613:ASP:OD1	1:D:614:VAL:N	2.53	0.41
1:E:481:LEU:HD13	1:X:636:LEU:HD11	135.91	0.41
1:F:439:PRO:O	1:F:470:PRO:HG3	2.20	0.41
1:G:613:ASP:OD1	1:G:614:VAL:N	2.53	0.41
1:F:376:PRO:HA	1:G:664:PHE:CD1	2.56	0.41
1:J:298:ASP:OD1	1:J:301:ARG:NH1	2.54	0.41
1:K:298:ASP:OD1	1:K:301:ARG:NH1	2.54	0.41
1:I:275:TYR:HD2	1:K:473:MET:HE1	89.22	0.41
1:M:298:ASP:OD1	1:M:301:ARG:NH1	2.54	0.41
1:M:346:PHE:CE1	1:M:401:PHE:HD2	2.38	0.41
1:M:299:TRP:HE1	1:M:729:ILE:HG22	1.85	0.41
1:N:557:TYR:HE1	1:N:562:LEU:HD11	1.85	0.41
1:N:613:ASP:OD1	1:N:614:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:310:ARG:NE	1:N:688:GLU:OE1	2.45	0.41
1:P:376:PRO:HA	1:Q:664:PHE:CD1	2.56	0.41
1:Q:561:MET:HB3	1:Q:728:PRO:HD3	2.02	0.41
1:R:239:ARG:NH1	1:R:688:GLU:HG3	2.34	0.41
1:S:692:GLU:HG3	1:S:734:LEU:HD13	2.02	0.41
1:T:432:SER:HA	1:T:570:THR:HB	2.01	0.41
1:U:299:TRP:HE1	1:U:729:ILE:HG22	1.85	0.41
1:W:561:MET:HB3	1:W:728:PRO:HD3	2.02	0.41
1:X:298:ASP:OD1	1:X:301:ARG:NH1	2.54	0.41
1:Y:613:ASP:OD1	1:Y:614:VAL:N	2.53	0.41
1:X:425:SER:OG	1:Y:628:ASP:OD1	39.45	0.41
1:Z:426:SER:HB2	1:Z:731:THR:HG22	2.02	0.41
1:Z:613:ASP:OD1	1:Z:614:VAL:N	2.53	0.41
1:Z:351:TYR:OH	1:Z:645:PRO:O	2.26	0.41
1:Z:299:TRP:HE1	1:Z:729:ILE:HG22	1.85	0.41
1:Z:481:LEU:HD13	1:1:636:LEU:HD11	84.45	0.41
1:2:568:ILE:HD12	1:2:572:ASN:HD22	1.86	0.41
1:Z:513:LEU:HD21	1:2:570:THR:O	80.18	0.41
1:2:613:ASP:OD1	1:2:614:VAL:N	2.53	0.41
1:3:299:TRP:HE1	1:3:729:ILE:HG22	1.85	0.41
1:5:513:LEU:HD21	1:7:570:THR:O	2.21	0.41
1:5:692:GLU:HG3	1:5:734:LEU:HD13	2.02	0.41
1:5:664:PHE:CD1	1:8:376:PRO:HA	2.56	0.41
1:8:568:ILE:HD12	1:8:572:ASN:HD22	1.86	0.41
1:A:632:HIS:O	1:A:634:SER:N	2.52	0.41
1:B:298:ASP:OD1	1:B:301:ARG:NH1	2.54	0.41
1:B:709:LYS:HZ1	1:C:532:ASP:CG	98.08	0.41
1:D:570:THR:O	1:L:513:LEU:HD21	130.03	0.41
1:E:513:LEU:HD21	1:V:570:THR:O	130.61	0.41
1:E:570:THR:O	1:Q:513:LEU:HD21	2.21	0.41
1:G:328:GLN:HE22	1:G:333:LYS:HG3	1.84	0.41
1:I:432:SER:HA	1:I:570:THR:HB	2.01	0.41
1:G:481:LEU:HD13	1:I:636:LEU:HD11	2.02	0.41
1:J:700:GLU:HB2	1:J:702:GLN:HE21	1.85	0.41
1:L:481:LEU:HD13	1:T:636:LEU:HD11	201.88	0.41
1:L:568:ILE:HD12	1:L:572:ASN:HD22	1.86	0.41
1:M:568:ILE:HD12	1:M:572:ASN:HD22	1.86	0.41
1:N:570:THR:O	1:O:513:LEU:HD21	64.07	0.41
1:O:432:SER:HA	1:O:570:THR:HB	2.01	0.41
1:P:568:ILE:HD12	1:P:572:ASN:HD22	1.86	0.41
1:R:299:TRP:HE1	1:R:729:ILE:HG22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:298:ASP:OD1	1:S:301:ARG:NH1	2.54	0.41
1:T:557:TYR:HE1	1:T:562:LEU:HD11	1.85	0.41
1:U:298:ASP:OD1	1:U:301:ARG:NH1	2.54	0.41
1:V:299:TRP:HE1	1:V:729:ILE:HG22	1.86	0.41
1:W:312:LYS:HA	1:W:312:LYS:HD2	1.84	0.41
1:W:513:LEU:HD21	1:Y:570:THR:O	32.54	0.41
1:W:613:ASP:OD1	1:W:614:VAL:N	2.53	0.41
1:Y:299:TRP:HE1	1:Y:729:ILE:HG22	1.85	0.41
1:Z:568:ILE:HD12	1:Z:572:ASN:HD22	1.86	0.41
1:1:346:PHE:CE1	1:1:401:PHE:HD2	2.38	0.41
1:2:632:HIS:O	1:2:634:SER:N	2.52	0.41
1:3:432:SER:HA	1:3:570:THR:HB	2.01	0.41
1:3:427:TYR:N	1:3:732:ARG:HG2	2.31	0.41
1:4:632:HIS:O	1:4:634:SER:N	2.52	0.41
1:Z:481:LEU:HD13	1:4:636:LEU:HD11	2.01	0.41
1:5:284:TYR:HB3	1:5:650:LEU:HD13	2.01	0.41
1:5:432:SER:HA	1:5:570:THR:HB	2.01	0.41
1:5:700:GLU:HB2	1:5:702:GLN:HE21	1.85	0.41
1:6:298:ASP:OD1	1:6:301:ARG:NH1	2.54	0.41
1:6:613:ASP:OD1	1:6:614:VAL:N	2.53	0.41
1:6:561:MET:HB3	1:6:728:PRO:HD3	2.01	0.41
1:7:557:TYR:HE1	1:7:562:LEU:HD11	1.85	0.41
1:8:298:ASP:OD1	1:8:301:ARG:NH1	2.54	0.41
1:A:346:PHE:CE1	1:A:401:PHE:HD2	2.38	0.41
1:A:310:ARG:NE	1:A:688:GLU:OE1	2.45	0.41
1:B:700:GLU:HB2	1:B:702:GLN:HE21	1.85	0.41
1:C:298:ASP:OD1	1:C:301:ARG:NH1	2.54	0.41
1:D:568:ILE:HD12	1:D:572:ASN:HD22	1.86	0.41
1:D:628:ASP:OD1	1:T:425:SER:OG	110.33	0.41
1:D:632:HIS:O	1:D:634:SER:N	2.52	0.41
1:F:664:PHE:CD1	1:R:376:PRO:HA	2.55	0.41
1:G:318:LEU:HD13	1:G:318:LEU:HA	1.82	0.41
1:H:298:ASP:OD1	1:H:301:ARG:NH1	2.53	0.41
1:H:299:TRP:HE1	1:H:729:ILE:HG22	1.85	0.41
1:A:664:PHE:CD1	1:J:376:PRO:HA	66.26	0.41
1:J:426:SER:HB2	1:J:731:THR:HG22	2.02	0.41
1:K:692:GLU:HG3	1:K:734:LEU:HD13	2.02	0.41
1:L:298:ASP:OD1	1:L:301:ARG:NH1	2.54	0.41
1:N:346:PHE:CE1	1:N:401:PHE:HD2	2.38	0.41
1:N:632:HIS:O	1:N:634:SER:N	2.52	0.41
1:N:692:GLU:OE2	1:N:694:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:709:LYS:HZ1	1:X:532:ASP:CG	114.94	0.41
1:R:557:TYR:HE1	1:R:562:LEU:HD11	1.85	0.41
1:R:432:SER:HA	1:R:570:THR:HB	2.01	0.41
1:D:664:PHE:CD1	1:S:376:PRO:HA	98.83	0.41
1:S:692:GLU:OE2	1:S:694:SER:HB3	2.21	0.41
1:U:376:PRO:HA	1:2:664:PHE:CD1	193.11	0.41
1:U:692:GLU:OE2	1:U:694:SER:HB3	2.21	0.41
1:V:513:LEU:HD21	1:X:570:THR:O	2.21	0.41
1:X:299:TRP:HE1	1:X:729:ILE:HG22	1.86	0.41
1:Y:289:ARG:NE	1:Y:617:GLN:O	2.46	0.41
1:1:557:TYR:HE1	1:1:562:LEU:HD11	1.85	0.41
1:1:432:SER:HA	1:1:570:THR:HB	2.02	0.41
1:2:376:PRO:HA	1:3:664:PHE:CD1	2.56	0.41
1:1:425:SER:OG	1:2:628:ASP:OD1	2.38	0.41
1:2:692:GLU:OE2	1:2:694:SER:HB3	2.21	0.41
1:3:557:TYR:HE1	1:3:562:LEU:HD11	1.85	0.41
1:4:692:GLU:OE2	1:4:694:SER:HB3	2.21	0.41
1:A:627:THR:HA	1:I:610:GLN:HE22	1.86	0.41
1:A:664:PHE:CD1	1:B:376:PRO:HA	2.55	0.41
1:A:427:TYR:N	1:A:732:ARG:HG2	2.31	0.41
1:E:632:HIS:O	1:E:634:SER:N	2.52	0.41
1:E:299:TRP:HE1	1:E:729:ILE:HG22	1.86	0.41
1:F:298:ASP:OD1	1:F:301:ARG:NH1	2.54	0.41
1:F:368:PHE:HA	1:F:369:PRO:HD3	1.97	0.41
1:G:376:PRO:HA	1:W:664:PHE:CD1	2.56	0.41
1:G:439:PRO:O	1:G:470:PRO:HG3	2.20	0.41
1:G:664:PHE:CD1	1:K:376:PRO:HA	176.05	0.41
1:H:692:GLU:HG3	1:H:734:LEU:HD13	2.02	0.41
1:I:692:GLU:OE2	1:I:694:SER:HB3	2.21	0.41
1:K:299:TRP:HE1	1:K:729:ILE:HG22	1.85	0.41
1:J:664:PHE:CD1	1:L:376:PRO:HA	97.00	0.41
1:L:240:VAL:HG13	1:L:687:TRP:HB2	2.02	0.41
1:L:692:GLU:OE2	1:L:694:SER:HB3	2.21	0.41
1:M:513:LEU:HD21	1:O:570:THR:O	105.10	0.41
1:N:427:TYR:N	1:N:732:ARG:HG2	2.31	0.41
1:O:426:SER:HB2	1:O:731:THR:HG22	2.02	0.41
1:P:298:ASP:OD1	1:P:301:ARG:NH1	2.54	0.41
1:P:439:PRO:O	1:P:470:PRO:HG3	2.20	0.41
1:P:664:PHE:CD1	1:6:376:PRO:HA	181.62	0.41
1:R:298:ASP:OD1	1:R:301:ARG:NH1	2.54	0.41
1:C:664:PHE:CD1	1:S:376:PRO:HA	111.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:299:TRP:HE1	1:T:729:ILE:HG22	1.85	0.41
1:T:298:ASP:OD1	1:T:301:ARG:NH1	2.54	0.41
1:T:439:PRO:O	1:T:470:PRO:HG3	2.20	0.41
1:V:692:GLU:HG3	1:V:734:LEU:HD13	2.02	0.41
1:W:299:TRP:HE1	1:W:729:ILE:HG22	1.85	0.41
1:X:568:ILE:HD12	1:X:572:ASN:HD22	1.86	0.41
1:Y:318:LEU:HD13	1:Y:318:LEU:HA	1.82	0.41
1:1:298:ASP:OD1	1:1:301:ARG:NH1	2.54	0.41
1:Z:425:SER:OG	1:1:628:ASP:OD1	85.93	0.41
1:4:488:GLN:OE1	1:4:540:SER:OG	2.33	0.41
1:5:298:ASP:OD1	1:5:301:ARG:NH1	2.53	0.41
1:5:526:MET:CE	1:5:575:ALA:HA	2.51	0.41
1:7:632:HIS:O	1:7:634:SER:N	2.52	0.41
1:O:376:PRO:HA	1:7:664:PHE:CD1	168.46	0.41
1:8:613:ASP:OD1	1:8:614:VAL:N	2.53	0.41
1:A:709:LYS:HZ1	1:F:532:ASP:CG	2.24	0.41
1:B:310:ARG:NE	1:B:688:GLU:OE1	2.45	0.41
1:C:526:MET:CE	1:C:575:ALA:HA	2.51	0.41
1:C:692:GLU:OE2	1:C:694:SER:HB3	2.21	0.41
1:D:692:GLU:OE2	1:D:694:SER:HB3	2.21	0.41
1:E:692:GLU:OE2	1:E:694:SER:HB3	2.21	0.41
1:G:692:GLU:OE2	1:G:694:SER:HB3	2.21	0.41
1:H:568:ILE:HD12	1:H:572:ASN:HD22	1.86	0.41
1:H:692:GLU:OE2	1:H:694:SER:HB3	2.21	0.41
1:I:613:ASP:OD1	1:I:614:VAL:N	2.53	0.41
1:H:376:PRO:HA	1:I:664:PHE:CD1	2.56	0.41
1:J:376:PRO:HA	1:X:664:PHE:CD1	162.58	0.41
1:L:425:SER:OG	1:T:628:ASP:OD1	188.66	0.41
1:L:526:MET:CE	1:L:575:ALA:HA	2.51	0.41
1:L:299:TRP:HE1	1:L:729:ILE:HG22	1.85	0.41
1:M:709:LYS:HZ1	1:R:532:ASP:CG	145.29	0.41
1:M:664:PHE:CD1	1:N:376:PRO:HA	58.53	0.41
1:M:376:PRO:HA	1:N:664:PHE:CD1	2.56	0.41
1:N:709:LYS:HZ1	1:O:532:ASP:CG	2.24	0.41
1:O:299:TRP:HE1	1:O:729:ILE:HG22	1.86	0.41
1:O:289:ARG:NE	1:O:617:GLN:O	2.46	0.41
1:D:376:PRO:HA	1:O:664:PHE:CD1	119.62	0.41
1:O:427:TYR:N	1:O:732:ARG:HG2	2.31	0.41
1:Q:568:ILE:HD12	1:Q:572:ASN:HD22	1.86	0.41
1:R:568:ILE:HD12	1:R:572:ASN:HD22	1.86	0.41
1:S:570:THR:O	1:U:513:LEU:HD21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:568:ILE:HD12	1:S:572:ASN:HD22	1.86	0.41
1:W:632:HIS:O	1:W:634:SER:N	2.52	0.41
1:W:692:GLU:OE2	1:W:694:SER:HB3	2.21	0.41
1:R:664:PHE:CD1	1:X:376:PRO:HA	68.04	0.41
1:X:376:PRO:HA	1:Y:664:PHE:CD1	2.56	0.41
1:X:570:THR:O	1:Y:513:LEU:HD21	51.19	0.41
1:Z:298:ASP:OD1	1:Z:301:ARG:NH1	2.54	0.41
1:1:439:PRO:O	1:1:470:PRO:HG3	2.20	0.41
1:Z:513:LEU:HD21	1:3:570:THR:O	2.21	0.41
1:3:526:MET:CE	1:3:575:ALA:HA	2.51	0.41
1:4:446:TYR:CE1	1:4:467:GLN:HG3	2.56	0.41
1:4:557:TYR:HE1	1:4:562:LEU:HD11	1.85	0.41
1:6:570:THR:O	1:7:513:LEU:HD21	2.21	0.41
1:7:692:GLU:OE2	1:7:694:SER:HB3	2.21	0.41
1:8:557:TYR:HE1	1:8:562:LEU:HD11	1.85	0.41
1:A:446:TYR:CE1	1:A:467:GLN:HG3	2.56	0.41
1:A:513:LEU:HD21	1:K:570:THR:O	107.66	0.41
1:C:664:PHE:CD1	1:D:376:PRO:HA	2.56	0.41
1:D:473:MET:HE1	1:N:275:TYR:HD2	1.85	0.41
1:E:513:LEU:HD21	1:F:570:THR:O	2.21	0.41
1:E:613:ASP:OD1	1:E:614:VAL:N	2.53	0.41
1:F:376:PRO:HA	1:X:664:PHE:CD1	146.36	0.41
1:F:526:MET:CE	1:F:575:ALA:HA	2.51	0.41
1:F:664:PHE:CD1	1:Z:376:PRO:HA	147.79	0.41
1:F:692:GLU:OE2	1:F:694:SER:HB3	2.21	0.41
1:G:446:TYR:CE1	1:G:467:GLN:HG3	2.56	0.41
1:H:446:TYR:CE1	1:H:467:GLN:HG3	2.56	0.41
1:G:513:LEU:HD21	1:H:570:THR:O	64.06	0.41
1:I:526:MET:CE	1:I:575:ALA:HA	2.51	0.41
1:J:446:TYR:CE1	1:J:467:GLN:HG3	2.56	0.41
1:J:526:MET:CE	1:J:575:ALA:HA	2.51	0.41
1:J:692:GLU:OE2	1:J:694:SER:HB3	2.21	0.41
1:I:513:LEU:HD21	1:K:570:THR:O	105.10	0.41
1:N:446:TYR:CE1	1:N:467:GLN:HG3	2.56	0.41
1:D:570:THR:O	1:N:513:LEU:HD21	2.21	0.41
1:N:700:GLU:HB2	1:N:702:GLN:HE21	1.85	0.41
1:N:299:TRP:HE1	1:N:729:ILE:HG22	1.86	0.41
1:O:446:TYR:CE1	1:O:467:GLN:HG3	2.56	0.41
1:O:526:MET:CE	1:O:575:ALA:HA	2.51	0.41
1:P:446:TYR:CE1	1:P:467:GLN:HG3	2.56	0.41
1:P:526:MET:CE	1:P:575:ALA:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:LEU:HD21	1:P:570:THR:O	2.21	0.41
1:Q:298:ASP:OD1	1:Q:301:ARG:NH1	2.54	0.41
1:Q:692:GLU:OE2	1:Q:694:SER:HB3	2.21	0.41
1:Q:709:LYS:HZ1	1:R:532:ASP:CG	2.23	0.41
1:R:258:TYR:OH	1:R:399:GLU:OE1	2.28	0.41
1:R:526:MET:CE	1:R:575:ALA:HA	2.51	0.41
1:S:446:TYR:CE1	1:S:467:GLN:HG3	2.56	0.41
1:T:568:ILE:HD12	1:T:572:ASN:HD22	1.86	0.41
1:U:570:THR:O	1:V:513:LEU:HD21	64.07	0.41
1:U:664:PHE:CD1	1:5:376:PRO:HA	204.58	0.41
1:V:427:TYR:N	1:V:732:ARG:HG2	2.31	0.41
1:W:568:ILE:HD12	1:W:572:ASN:HD22	1.86	0.41
1:Y:298:ASP:OD1	1:Y:301:ARG:NH1	2.54	0.41
1:1:613:ASP:OD1	1:1:614:VAL:N	2.53	0.41
1:2:298:ASP:OD1	1:2:301:ARG:NH1	2.54	0.41
1:2:426:SER:HB2	1:2:731:THR:HG22	2.02	0.41
1:4:346:PHE:CE1	1:4:401:PHE:HD2	2.38	0.41
1:4:526:MET:CE	1:4:575:ALA:HA	2.51	0.41
1:4:299:TRP:HE1	1:4:729:ILE:HG22	1.86	0.41
1:5:446:TYR:CE1	1:5:467:GLN:HG3	2.56	0.41
1:7:446:TYR:CE1	1:7:467:GLN:HG3	2.56	0.41
1:8:439:PRO:O	1:8:470:PRO:HG3	2.20	0.41
1:A:568:ILE:HD12	1:A:572:ASN:HD22	1.86	0.41
1:B:692:GLU:OE2	1:B:694:SER:HB3	2.21	0.41
1:C:425:SER:OG	1:O:628:ASP:OD1	138.99	0.41
1:E:298:ASP:OD1	1:E:301:ARG:NH1	2.54	0.41
1:E:446:TYR:CE1	1:E:467:GLN:HG3	2.56	0.41
1:E:570:THR:O	1:X:513:LEU:HD21	153.09	0.41
1:F:701:ILE:O	1:F:733:TYR:HB3	2.21	0.41
1:G:526:MET:CE	1:G:575:ALA:HA	2.51	0.41
1:I:446:TYR:CE1	1:I:467:GLN:HG3	2.56	0.41
1:I:634:SER:HB2	3:I:902:DA:N7	2.36	0.41
1:J:701:ILE:O	1:J:733:TYR:HB3	2.21	0.41
1:J:299:TRP:HE1	1:J:729:ILE:HG22	1.85	0.41
1:K:692:GLU:OE2	1:K:694:SER:HB3	2.21	0.41
1:L:446:TYR:CE1	1:L:467:GLN:HG3	2.56	0.41
1:I:532:ASP:CG	1:L:709:LYS:HZ1	99.86	0.41
1:M:446:TYR:CE1	1:M:467:GLN:HG3	2.56	0.41
1:M:701:ILE:O	1:M:733:TYR:HB3	2.21	0.41
1:O:568:ILE:HD12	1:O:572:ASN:HD22	1.86	0.41
1:C:513:LEU:HD21	1:P:570:THR:O	66.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:376:PRO:HA	1:S:664:PHE:CD1	2.55	0.41
1:S:734:LEU:HA	1:S:734:LEU:HD23	1.92	0.41
1:T:446:TYR:CE1	1:T:467:GLN:HG3	2.56	0.41
1:V:446:TYR:CE1	1:V:467:GLN:HG3	2.56	0.41
1:V:289:ARG:NE	1:V:617:GLN:O	2.46	0.41
1:K:664:PHE:CD1	1:W:376:PRO:HA	187.57	0.41
1:W:446:TYR:CE1	1:W:467:GLN:HG3	2.56	0.41
1:W:709:LYS:HZ1	1:X:532:ASP:CG	2.23	0.41
1:Y:526:MET:CE	1:Y:575:ALA:HA	2.51	0.41
1:Y:692:GLU:HG3	1:Y:734:LEU:HD13	2.02	0.41
1:A:376:PRO:HA	1:Z:664:PHE:CD1	110.99	0.41
1:Z:240:VAL:HG13	1:Z:687:TRP:HB2	2.02	0.41
1:Z:701:ILE:O	1:Z:733:TYR:HB3	2.21	0.41
1:G:532:ASP:CG	1:Z:709:LYS:HZ1	70.19	0.41
1:1:240:VAL:HG13	1:1:687:TRP:HB2	2.02	0.41
1:6:312:LYS:HA	1:6:312:LYS:HD2	1.84	0.41
1:6:701:ILE:O	1:6:733:TYR:HB3	2.21	0.41
1:A:289:ARG:NE	1:A:617:GLN:O	2.46	0.41
1:A:692:GLU:OE2	1:A:694:SER:HB3	2.21	0.41
1:A:709:LYS:HZ1	1:3:532:ASP:CG	178.94	0.41
1:B:446:TYR:CE1	1:B:467:GLN:HG3	2.56	0.41
1:C:446:TYR:CE1	1:C:467:GLN:HG3	2.56	0.41
1:E:376:PRO:HA	1:H:664:PHE:CD1	147.57	0.41
1:G:298:ASP:OD1	1:G:301:ARG:NH1	2.54	0.41
1:G:634:SER:HB2	3:G:902:DA:N7	2.36	0.41
1:G:610:GLN:HE22	1:I:627:THR:HA	1.85	0.41
1:I:632:HIS:O	1:I:634:SER:N	2.52	0.41
1:K:513:LEU:HD21	1:8:570:THR:O	2.21	0.41
1:J:570:THR:O	1:K:513:LEU:HD21	64.07	0.41
1:K:701:ILE:O	1:K:733:TYR:HB3	2.21	0.41
1:N:526:MET:CE	1:N:575:ALA:HA	2.51	0.41
1:P:701:ILE:O	1:P:733:TYR:HB3	2.21	0.41
1:Q:446:TYR:CE1	1:Q:467:GLN:HG3	2.56	0.41
1:R:446:TYR:CE1	1:R:467:GLN:HG3	2.56	0.41
1:R:634:SER:HB2	3:R:902:DA:N7	2.36	0.41
1:S:299:TRP:HE1	1:S:729:ILE:HG22	1.85	0.41
1:Q:513:LEU:HD21	1:S:570:THR:O	93.64	0.41
1:T:664:PHE:CD1	1:Y:376:PRO:HA	140.93	0.41
1:W:298:ASP:OD1	1:W:301:ARG:NH1	2.54	0.41
1:J:532:ASP:CG	1:W:709:LYS:HZ1	187.01	0.41
1:X:557:TYR:HE1	1:X:562:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:692:GLU:OE2	1:X:694:SER:HB3	2.21	0.41
1:Y:376:PRO:HA	1:4:664:PHE:CD1	2.55	0.41
1:Y:446:TYR:CE1	1:Y:467:GLN:HG3	2.56	0.41
1:Y:427:TYR:N	1:Y:732:ARG:HG2	2.31	0.41
1:Z:446:TYR:CE1	1:Z:467:GLN:HG3	2.56	0.41
1:Z:526:MET:CE	1:Z:575:ALA:HA	2.51	0.41
1:1:299:TRP:HE1	1:1:729:ILE:HG22	1.85	0.41
1:1:692:GLU:OE2	1:1:694:SER:HB3	2.21	0.41
1:2:299:TRP:HE1	1:2:729:ILE:HG22	1.86	0.41
1:2:634:SER:HB2	3:2:902:DA:N7	2.36	0.41
1:3:376:PRO:HA	1:8:664:PHE:CD1	2.55	0.41
1:4:568:ILE:HD12	1:4:572:ASN:HD22	1.86	0.41
1:4:613:ASP:OD1	1:4:614:VAL:N	2.53	0.41
1:6:284:TYR:HB3	1:6:650:LEU:HD13	2.01	0.41
1:6:368:PHE:HA	1:6:369:PRO:HD3	1.97	0.41
1:6:446:TYR:CE1	1:6:467:GLN:HG3	2.56	0.41
1:6:451:THR:HG21	1:7:503:PHE:CE2	2.57	0.41
1:6:568:ILE:HD12	1:6:572:ASN:HD22	1.86	0.41
1:6:526:MET:CE	1:6:575:ALA:HA	2.51	0.41
1:6:692:GLU:OE2	1:6:694:SER:HB3	2.21	0.41
1:7:298:ASP:OD1	1:7:301:ARG:NH1	2.54	0.41
1:K:664:PHE:CD1	1:7:376:PRO:HA	2.56	0.41
1:7:613:ASP:OD1	1:7:614:VAL:N	2.53	0.41
1:A:701:ILE:O	1:A:733:TYR:HB3	2.21	0.41
1:C:632:HIS:O	1:C:634:SER:N	2.52	0.41
1:D:299:TRP:HE1	1:D:729:ILE:HG22	1.86	0.41
1:D:664:PHE:CD1	1:E:376:PRO:HA	2.56	0.41
1:D:634:SER:HB2	3:D:902:DA:N7	2.36	0.41
1:F:446:TYR:CE1	1:F:467:GLN:HG3	2.56	0.41
1:E:503:PHE:CE2	1:F:451:THR:HG21	2.56	0.41
1:G:701:ILE:O	1:G:733:TYR:HB3	2.21	0.41
1:F:570:THR:O	1:H:513:LEU:HD21	130.03	0.41
1:H:701:ILE:O	1:H:733:TYR:HB3	2.21	0.41
1:I:298:ASP:OD1	1:I:301:ARG:NH1	2.53	0.41
1:I:570:THR:O	1:J:513:LEU:HD21	51.18	0.41
1:K:526:MET:CE	1:K:575:ALA:HA	2.51	0.41
1:D:425:SER:OG	1:L:628:ASP:OD1	115.38	0.41
1:J:425:SER:OG	1:L:628:ASP:OD1	2.37	0.41
1:O:632:HIS:O	1:O:634:SER:N	2.52	0.41
1:Q:570:THR:O	1:R:513:LEU:HD21	64.07	0.41
1:N:664:PHE:CD1	1:R:376:PRO:HA	176.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:664:PHE:CD1	1:V:376:PRO:HA	2.56	0.41
1:R:692:GLU:OE2	1:R:694:SER:HB3	2.21	0.41
1:R:701:ILE:O	1:R:733:TYR:HB3	2.21	0.41
1:T:701:ILE:O	1:T:733:TYR:HB3	2.21	0.41
1:T:376:PRO:HA	1:U:664:PHE:CD1	2.56	0.41
1:V:298:ASP:OD1	1:V:301:ARG:NH1	2.54	0.41
1:V:376:PRO:HA	1:W:664:PHE:CD1	58.53	0.41
1:V:628:ASP:OD1	1:X:425:SER:OG	2.37	0.41
1:V:664:PHE:CD1	1:1:376:PRO:HA	166.69	0.41
1:H:570:THR:O	1:W:513:LEU:HD21	2.21	0.41
1:W:570:THR:O	1:X:513:LEU:HD21	64.07	0.41
1:W:570:THR:O	1:Y:513:LEU:HD21	2.21	0.41
1:X:613:ASP:OD1	1:X:614:VAL:N	2.53	0.41
1:Y:634:SER:HB2	3:Y:902:DA:N7	2.36	0.41
1:Z:634:SER:HB2	3:Z:902:DA:N7	2.36	0.41
1:Z:692:GLU:OE2	1:Z:694:SER:HB3	2.21	0.41
1:3:298:ASP:OD1	1:3:301:ARG:NH1	2.54	0.40
1:3:446:TYR:CE1	1:3:467:GLN:HG3	2.56	0.40
1:3:568:ILE:HD12	1:3:572:ASN:HD22	1.86	0.40
1:3:289:ARG:NE	1:3:617:GLN:O	2.46	0.40
1:5:701:ILE:O	1:5:733:TYR:HB3	2.21	0.40
1:B:570:THR:O	1:J:513:LEU:HD21	2.21	0.40
1:B:692:GLU:HG3	1:B:734:LEU:HD13	2.02	0.40
1:D:503:PHE:CE2	1:P:451:THR:HG21	2.56	0.40
1:D:701:ILE:O	1:D:733:TYR:HB3	2.21	0.40
1:F:451:THR:HG21	1:H:503:PHE:CE2	154.42	0.40
1:H:503:PHE:CE2	1:Y:451:THR:HG21	2.56	0.40
1:I:701:ILE:O	1:I:733:TYR:HB3	2.21	0.40
1:J:451:THR:HG21	1:K:503:PHE:CE2	74.56	0.40
1:J:568:ILE:HD12	1:J:572:ASN:HD22	1.86	0.40
1:K:376:PRO:HA	1:L:664:PHE:CD1	2.56	0.40
1:K:446:TYR:CE1	1:K:467:GLN:HG3	2.56	0.40
1:M:570:THR:O	1:N:513:LEU:HD21	51.19	0.40
1:M:634:SER:HB2	3:M:902:DA:N7	2.36	0.40
1:N:568:ILE:HD12	1:N:572:ASN:HD22	1.86	0.40
1:N:701:ILE:O	1:N:733:TYR:HB3	2.21	0.40
1:O:298:ASP:OD1	1:O:301:ARG:NH1	2.54	0.40
1:O:368:PHE:HA	1:O:369:PRO:HD3	1.97	0.40
1:Q:634:SER:HB2	3:Q:902:DA:N7	2.36	0.40
1:Q:701:ILE:O	1:Q:733:TYR:HB3	2.21	0.40
1:R:692:GLU:HG3	1:R:734:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:451:THR:HG21	1:S:503:PHE:CE2	2.56	0.40
1:S:701:ILE:O	1:S:733:TYR:HB3	2.21	0.40
1:T:526:MET:CE	1:T:575:ALA:HA	2.51	0.40
1:T:692:GLU:OE2	1:T:694:SER:HB3	2.21	0.40
1:T:634:SER:HB2	3:T:902:DA:N7	2.36	0.40
1:T:570:THR:O	1:U:513:LEU:HD21	51.18	0.40
1:V:312:LYS:HD2	1:V:312:LYS:HA	1.84	0.40
1:W:526:MET:CE	1:W:575:ALA:HA	2.51	0.40
1:W:634:SER:HB2	3:W:902:DA:N7	2.36	0.40
1:X:701:ILE:O	1:X:733:TYR:HB3	2.21	0.40
1:Y:310:ARG:NE	1:Y:688:GLU:OE1	2.45	0.40
1:1:568:ILE:HD12	1:1:572:ASN:HD22	1.86	0.40
1:1:701:ILE:O	1:1:733:TYR:HB3	2.21	0.40
1:2:526:MET:CE	1:2:575:ALA:HA	2.51	0.40
1:2:701:ILE:O	1:2:733:TYR:HB3	2.21	0.40
1:3:426:SER:HB2	1:3:731:THR:HG22	2.02	0.40
1:4:634:SER:HB2	3:4:902:DA:N7	2.36	0.40
1:5:561:MET:HB3	1:5:728:PRO:HD3	2.01	0.40
1:8:692:GLU:OE2	1:8:694:SER:HB3	2.21	0.40
1:C:634:SER:HB2	3:C:902:DA:N7	2.36	0.40
1:C:701:ILE:O	1:C:733:TYR:HB3	2.21	0.40
1:D:526:MET:CE	1:D:575:ALA:HA	2.51	0.40
1:E:310:ARG:NE	1:E:688:GLU:OE1	2.45	0.40
1:E:709:LYS:HZ1	1:F:532:ASP:CG	68.58	0.40
1:K:634:SER:HB2	3:K:902:DA:N7	2.36	0.40
1:B:503:PHE:CE2	1:L:451:THR:HG21	2.57	0.40
1:B:570:THR:O	1:M:513:LEU:HD21	109.45	0.40
1:C:513:LEU:HD21	1:M:570:THR:O	2.21	0.40
1:M:632:HIS:O	1:M:634:SER:N	2.52	0.40
1:M:692:GLU:OE2	1:M:694:SER:HB3	2.21	0.40
1:D:532:ASP:CG	1:N:709:LYS:HZ1	68.57	0.40
1:O:376:PRO:HA	1:P:664:PHE:CD1	2.55	0.40
1:O:734:LEU:HA	1:O:734:LEU:HD23	1.92	0.40
1:P:692:GLU:OE2	1:P:694:SER:HB3	2.21	0.40
1:R:570:THR:O	1:S:513:LEU:HD21	2.21	0.40
1:S:312:LYS:HD3	1:S:688:GLU:HB2	2.04	0.40
1:T:258:TYR:OH	1:T:399:GLU:OE1	2.28	0.40
1:U:368:PHE:HA	1:U:369:PRO:HD3	1.97	0.40
1:U:568:ILE:HD12	1:U:572:ASN:HD22	1.86	0.40
1:U:634:SER:HB2	3:U:902:DA:N7	2.36	0.40
1:V:526:MET:CE	1:V:575:ALA:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:376:PRO:HA	1:Y:664:PHE:CD1	159.44	0.40
1:Z:312:LYS:HD3	1:Z:688:GLU:HB2	2.04	0.40
1:Z:664:PHE:CD1	1:4:376:PRO:HA	97.00	0.40
1:1:446:TYR:CE1	1:1:467:GLN:HG3	2.56	0.40
1:1:526:MET:CE	1:1:575:ALA:HA	2.51	0.40
1:1:634:SER:HB2	3:1:902:DA:N7	2.36	0.40
1:G:376:PRO:HA	1:1:664:PHE:CD1	181.61	0.40
1:2:310:ARG:NE	1:2:688:GLU:OE1	2.45	0.40
1:5:451:THR:HG22	1:5:451:THR:O	2.22	0.40
1:8:446:TYR:CE1	1:8:467:GLN:HG3	2.56	0.40
1:8:299:TRP:HE1	1:8:729:ILE:HG22	1.86	0.40
1:A:634:SER:HB2	3:A:902:DA:N7	2.36	0.40
1:B:701:ILE:O	1:B:733:TYR:HB3	2.21	0.40
1:B:503:PHE:CE2	1:C:451:THR:HG21	102.58	0.40
1:D:446:TYR:CE1	1:D:467:GLN:HG3	2.56	0.40
1:D:310:ARG:NE	1:D:688:GLU:OE1	2.45	0.40
1:E:451:THR:HG21	1:Q:503:PHE:CE2	2.57	0.40
1:E:526:MET:CE	1:E:575:ALA:HA	2.51	0.40
1:A:376:PRO:HA	1:E:664:PHE:CD1	2.57	0.40
1:E:634:SER:HB2	3:E:902:DA:N7	2.36	0.40
1:F:299:TRP:HE1	1:F:729:ILE:HG22	1.85	0.40
1:F:312:LYS:HD3	1:F:688:GLU:HB2	2.04	0.40
1:F:568:ILE:HD12	1:F:572:ASN:HD22	1.86	0.40
1:F:513:LEU:HD21	1:G:570:THR:O	93.64	0.40
1:H:634:SER:HB2	3:H:902:DA:N7	2.36	0.40
1:H:312:LYS:HD3	1:H:688:GLU:HB2	2.04	0.40
1:I:692:GLU:HG3	1:I:734:LEU:HD13	2.02	0.40
1:M:312:LYS:HD3	1:M:688:GLU:HB2	2.04	0.40
1:N:634:SER:HB2	3:N:902:DA:N7	2.36	0.40
1:O:692:GLU:OE2	1:O:694:SER:HB3	2.21	0.40
1:P:299:TRP:HE1	1:P:729:ILE:HG22	1.86	0.40
1:Q:632:HIS:O	1:Q:634:SER:N	2.52	0.40
1:S:451:THR:HG21	1:U:503:PHE:CE2	2.56	0.40
1:E:664:PHE:CD1	1:U:376:PRO:HA	158.48	0.40
1:U:451:THR:HG21	1:V:503:PHE:CE2	74.56	0.40
1:U:446:TYR:CE1	1:U:467:GLN:HG3	2.56	0.40
1:V:568:ILE:HD12	1:V:572:ASN:HD22	1.86	0.40
1:V:664:PHE:CD1	1:W:376:PRO:HA	2.56	0.40
1:2:446:TYR:CE1	1:2:467:GLN:HG3	2.56	0.40
1:2:426:SER:HA	1:2:732:ARG:HG2	2.04	0.40
1:3:692:GLU:HG3	1:3:734:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:503:PHE:CE2	1:7:451:THR:HG21	2.57	0.40
1:7:532:ASP:CG	1:8:709:LYS:HZ1	2.24	0.40
1:A:426:SER:HA	1:A:732:ARG:HG2	2.04	0.40
1:B:513:LEU:HD21	1:C:570:THR:O	51.18	0.40
1:C:426:SER:HA	1:C:732:ARG:HG2	2.04	0.40
1:G:451:THR:HG22	1:G:451:THR:O	2.22	0.40
1:G:289:ARG:NE	1:G:617:GLN:O	2.46	0.40
1:H:351:TYR:OH	1:H:645:PRO:O	2.26	0.40
1:I:289:ARG:NE	1:I:617:GLN:O	2.46	0.40
1:J:312:LYS:HD3	1:J:688:GLU:HB2	2.04	0.40
1:J:570:THR:O	1:L:513:LEU:HD21	2.21	0.40
1:J:289:ARG:NE	1:J:617:GLN:O	2.46	0.40
1:J:634:SER:HB2	3:J:902:DA:N7	2.36	0.40
1:K:503:PHE:CE2	1:8:451:THR:HG21	2.57	0.40
1:K:628:ASP:OD1	1:8:425:SER:OG	2.37	0.40
1:L:426:SER:HA	1:L:732:ARG:HG2	2.04	0.40
1:L:664:PHE:CD1	1:N:376:PRO:HA	147.58	0.40
1:O:426:SER:HA	1:O:732:ARG:HG2	2.04	0.40
1:O:634:SER:HB2	3:O:902:DA:N7	2.36	0.40
1:P:451:THR:HG22	1:P:451:THR:O	2.22	0.40
1:Q:451:THR:O	1:Q:451:THR:HG22	2.22	0.40
1:Q:526:MET:CE	1:Q:575:ALA:HA	2.51	0.40
1:S:634:SER:HB2	3:S:902:DA:N7	2.36	0.40
1:V:312:LYS:HD3	1:V:688:GLU:HB2	2.03	0.40
1:V:368:PHE:HA	1:V:369:PRO:HD3	1.97	0.40
1:W:451:THR:HG22	1:W:451:THR:O	2.22	0.40
1:H:425:SER:OG	1:W:628:ASP:OD1	2.37	0.40
1:X:318:LEU:HD13	1:X:318:LEU:HA	1.82	0.40
1:Y:312:LYS:HD3	1:Y:688:GLU:HB2	2.04	0.40
1:Z:570:THR:O	1:4:513:LEU:HD21	2.21	0.40
1:1:312:LYS:HD3	1:1:688:GLU:HB2	2.04	0.40
1:2:439:PRO:O	1:2:470:PRO:HG3	2.20	0.40
1:3:318:LEU:HD13	1:3:318:LEU:HA	1.82	0.40
1:A:368:PHE:HA	1:A:369:PRO:HD3	1.97	0.40
1:B:568:ILE:HD12	1:B:572:ASN:HD22	1.86	0.40
1:B:634:SER:HB2	3:B:902:DA:N7	2.36	0.40
1:C:376:PRO:HA	1:M:664:PHE:CD1	97.00	0.40
1:D:513:LEU:HD21	1:T:570:THR:O	124.82	0.40
1:D:628:ASP:OD1	1:P:425:SER:OG	2.37	0.40
1:D:312:LYS:HD3	1:D:688:GLU:HB2	2.04	0.40
1:D:426:SER:HA	1:D:732:ARG:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:LYS:HD3	1:E:688:GLU:HB2	2.04	0.40
1:F:289:ARG:NE	1:F:617:GLN:O	2.46	0.40
1:F:634:SER:HB2	3:F:902:DA:N7	2.36	0.40
1:G:426:SER:HA	1:G:732:ARG:HG2	2.04	0.40
1:H:451:THR:O	1:H:451:THR:HG22	2.22	0.40
1:H:526:MET:CE	1:H:575:ALA:HA	2.51	0.40
1:A:636:LEU:HD11	1:I:481:LEU:HD13	2.02	0.40
1:I:709:LYS:HZ1	1:L:532:ASP:CG	55.13	0.40
1:J:451:THR:HG22	1:J:451:THR:O	2.22	0.40
1:K:451:THR:HG22	1:K:451:THR:O	2.22	0.40
1:J:532:ASP:CG	1:K:709:LYS:HZ1	2.24	0.40
1:B:513:LEU:HD21	1:L:570:THR:O	2.21	0.40
1:M:451:THR:O	1:M:451:THR:HG22	2.22	0.40
1:N:451:THR:HG22	1:N:451:THR:O	2.22	0.40
1:N:451:THR:HG21	1:O:503:PHE:CE2	74.56	0.40
1:V:310:ARG:NE	1:V:688:GLU:OE1	2.45	0.40
1:V:701:ILE:O	1:V:733:TYR:HB3	2.21	0.40
1:X:446:TYR:CE1	1:X:467:GLN:HG3	2.56	0.40
1:Y:568:ILE:HD12	1:Y:572:ASN:HD22	1.86	0.40
1:Y:701:ILE:O	1:Y:733:TYR:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	2	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	3	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	4	518/520 (100%)	507 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	6	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	7	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	8	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	A	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	B	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	C	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	D	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	E	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	F	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	G	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	H	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	I	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	J	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	K	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	L	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	M	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	N	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	O	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	P	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	Q	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	R	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	S	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	T	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	U	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	V	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	W	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	X	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	Y	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	Z	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	a	518/520 (100%)	507 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	c	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	d	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	e	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	f	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	g	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	h	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	i	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	j	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	k	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	l	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	m	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	n	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	o	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	p	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	q	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	r	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	s	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	t	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	u	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	v	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	w	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	x	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	y	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	z	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
All	All	31080/31200 (100%)	30420 (98%)	660 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	1	452/452 (100%)	452 (100%)	0	100	100
1	2	452/452 (100%)	452 (100%)	0	100	100
1	3	452/452 (100%)	452 (100%)	0	100	100
1	4	452/452 (100%)	452 (100%)	0	100	100
1	5	452/452 (100%)	452 (100%)	0	100	100
1	6	452/452 (100%)	452 (100%)	0	100	100
1	7	452/452 (100%)	452 (100%)	0	100	100
1	8	452/452 (100%)	452 (100%)	0	100	100
1	A	452/452 (100%)	452 (100%)	0	100	100
1	B	452/452 (100%)	452 (100%)	0	100	100
1	C	452/452 (100%)	452 (100%)	0	100	100
1	D	452/452 (100%)	452 (100%)	0	100	100
1	E	452/452 (100%)	452 (100%)	0	100	100
1	F	452/452 (100%)	452 (100%)	0	100	100
1	G	452/452 (100%)	452 (100%)	0	100	100
1	H	452/452 (100%)	452 (100%)	0	100	100
1	I	452/452 (100%)	452 (100%)	0	100	100
1	J	452/452 (100%)	452 (100%)	0	100	100
1	K	452/452 (100%)	452 (100%)	0	100	100
1	L	452/452 (100%)	452 (100%)	0	100	100
1	M	452/452 (100%)	452 (100%)	0	100	100
1	N	452/452 (100%)	452 (100%)	0	100	100
1	O	452/452 (100%)	452 (100%)	0	100	100
1	P	452/452 (100%)	452 (100%)	0	100	100
1	Q	452/452 (100%)	452 (100%)	0	100	100
1	R	452/452 (100%)	452 (100%)	0	100	100
1	S	452/452 (100%)	452 (100%)	0	100	100
1	T	452/452 (100%)	452 (100%)	0	100	100
1	U	452/452 (100%)	452 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	452/452 (100%)	452 (100%)	0	100	100
1	W	452/452 (100%)	452 (100%)	0	100	100
1	X	452/452 (100%)	452 (100%)	0	100	100
1	Y	452/452 (100%)	452 (100%)	0	100	100
1	Z	452/452 (100%)	452 (100%)	0	100	100
1	a	452/452 (100%)	452 (100%)	0	100	100
1	b	452/452 (100%)	452 (100%)	0	100	100
1	c	452/452 (100%)	452 (100%)	0	100	100
1	d	452/452 (100%)	452 (100%)	0	100	100
1	e	452/452 (100%)	452 (100%)	0	100	100
1	f	452/452 (100%)	452 (100%)	0	100	100
1	g	452/452 (100%)	452 (100%)	0	100	100
1	h	452/452 (100%)	452 (100%)	0	100	100
1	i	452/452 (100%)	452 (100%)	0	100	100
1	j	452/452 (100%)	452 (100%)	0	100	100
1	k	452/452 (100%)	452 (100%)	0	100	100
1	l	452/452 (100%)	452 (100%)	0	100	100
1	m	452/452 (100%)	452 (100%)	0	100	100
1	n	452/452 (100%)	452 (100%)	0	100	100
1	o	452/452 (100%)	452 (100%)	0	100	100
1	p	452/452 (100%)	452 (100%)	0	100	100
1	q	452/452 (100%)	452 (100%)	0	100	100
1	r	452/452 (100%)	452 (100%)	0	100	100
1	s	452/452 (100%)	452 (100%)	0	100	100
1	t	452/452 (100%)	452 (100%)	0	100	100
1	u	452/452 (100%)	452 (100%)	0	100	100
1	v	452/452 (100%)	452 (100%)	0	100	100
1	w	452/452 (100%)	452 (100%)	0	100	100
1	x	452/452 (100%)	452 (100%)	0	100	100
1	y	452/452 (100%)	452 (100%)	0	100	100
1	z	452/452 (100%)	452 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	27120/27120 (100%)	27120 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (539) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	362	GLN
1	A	431	GLN
1	A	467	GLN
1	A	587	GLN
1	A	610	GLN
1	A	653	ASN
1	A	675	GLN
1	A	737	ASN
1	B	328	GLN
1	B	362	GLN
1	B	431	GLN
1	B	467	GLN
1	B	587	GLN
1	B	610	GLN
1	B	653	ASN
1	B	675	GLN
1	B	737	ASN
1	C	328	GLN
1	C	362	GLN
1	C	431	GLN
1	C	467	GLN
1	C	587	GLN
1	C	610	GLN
1	C	653	ASN
1	C	675	GLN
1	C	737	ASN
1	D	328	GLN
1	D	362	GLN
1	D	431	GLN
1	D	467	GLN
1	D	587	GLN
1	D	610	GLN
1	D	653	ASN
1	D	675	GLN

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Mol	Chain	Res	Type
1	D	737	ASN
1	E	328	GLN
1	E	362	GLN
1	E	431	GLN
1	E	467	GLN
1	E	587	GLN
1	E	610	GLN
1	E	653	ASN
1	E	675	GLN
1	E	737	ASN
1	F	328	GLN
1	F	362	GLN
1	F	431	GLN
1	F	467	GLN
1	F	587	GLN
1	F	610	GLN
1	F	653	ASN
1	F	675	GLN
1	F	737	ASN
1	G	328	GLN
1	G	362	GLN
1	G	431	GLN
1	G	467	GLN
1	G	587	GLN
1	G	610	GLN
1	G	653	ASN
1	G	675	GLN
1	G	737	ASN
1	H	328	GLN
1	H	362	GLN
1	H	431	GLN
1	H	467	GLN
1	H	587	GLN
1	H	610	GLN
1	H	653	ASN
1	H	675	GLN
1	H	737	ASN
1	I	328	GLN
1	I	362	GLN
1	I	431	GLN
1	I	467	GLN
1	I	587	GLN

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Mol	Chain	Res	Type
1	I	610	GLN
1	I	653	ASN
1	I	675	GLN
1	I	737	ASN
1	J	328	GLN
1	J	362	GLN
1	J	431	GLN
1	J	467	GLN
1	J	587	GLN
1	J	610	GLN
1	J	653	ASN
1	J	675	GLN
1	J	737	ASN
1	K	328	GLN
1	K	362	GLN
1	K	431	GLN
1	K	467	GLN
1	K	587	GLN
1	K	610	GLN
1	K	653	ASN
1	K	675	GLN
1	K	737	ASN
1	L	328	GLN
1	L	362	GLN
1	L	431	GLN
1	L	467	GLN
1	L	587	GLN
1	L	610	GLN
1	L	653	ASN
1	L	675	GLN
1	L	737	ASN
1	M	328	GLN
1	M	362	GLN
1	M	431	GLN
1	M	467	GLN
1	M	587	GLN
1	M	610	GLN
1	M	653	ASN
1	M	675	GLN
1	M	737	ASN
1	N	328	GLN
1	N	362	GLN

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Mol	Chain	Res	Type
1	N	431	GLN
1	N	467	GLN
1	N	587	GLN
1	N	610	GLN
1	N	653	ASN
1	N	675	GLN
1	N	737	ASN
1	O	328	GLN
1	O	362	GLN
1	O	431	GLN
1	O	467	GLN
1	O	587	GLN
1	O	610	GLN
1	O	653	ASN
1	O	675	GLN
1	O	737	ASN
1	P	328	GLN
1	P	362	GLN
1	P	431	GLN
1	P	467	GLN
1	P	587	GLN
1	P	610	GLN
1	P	653	ASN
1	P	675	GLN
1	P	737	ASN
1	Q	328	GLN
1	Q	362	GLN
1	Q	431	GLN
1	Q	467	GLN
1	Q	587	GLN
1	Q	610	GLN
1	Q	653	ASN
1	Q	675	GLN
1	Q	737	ASN
1	R	328	GLN
1	R	362	GLN
1	R	431	GLN
1	R	467	GLN
1	R	587	GLN
1	R	610	GLN
1	R	653	ASN
1	R	675	GLN

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Mol	Chain	Res	Type
1	R	737	ASN
1	S	328	GLN
1	S	362	GLN
1	S	431	GLN
1	S	587	GLN
1	S	610	GLN
1	S	653	ASN
1	S	675	GLN
1	S	737	ASN
1	T	328	GLN
1	T	362	GLN
1	T	431	GLN
1	T	467	GLN
1	T	587	GLN
1	T	610	GLN
1	T	653	ASN
1	T	675	GLN
1	T	737	ASN
1	U	328	GLN
1	U	362	GLN
1	U	431	GLN
1	U	467	GLN
1	U	587	GLN
1	U	610	GLN
1	U	653	ASN
1	U	675	GLN
1	U	737	ASN
1	V	328	GLN
1	V	362	GLN
1	V	431	GLN
1	V	467	GLN
1	V	587	GLN
1	V	610	GLN
1	V	653	ASN
1	V	675	GLN
1	V	737	ASN
1	W	328	GLN
1	W	362	GLN
1	W	431	GLN
1	W	467	GLN
1	W	587	GLN
1	W	610	GLN

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Mol	Chain	Res	Type
1	W	653	ASN
1	W	675	GLN
1	W	737	ASN
1	X	328	GLN
1	X	362	GLN
1	X	431	GLN
1	X	467	GLN
1	X	587	GLN
1	X	610	GLN
1	X	653	ASN
1	X	675	GLN
1	X	737	ASN
1	Y	328	GLN
1	Y	362	GLN
1	Y	431	GLN
1	Y	467	GLN
1	Y	587	GLN
1	Y	610	GLN
1	Y	653	ASN
1	Y	675	GLN
1	Y	737	ASN
1	Z	328	GLN
1	Z	362	GLN
1	Z	431	GLN
1	Z	467	GLN
1	Z	587	GLN
1	Z	610	GLN
1	Z	653	ASN
1	Z	675	GLN
1	Z	737	ASN
1	a	328	GLN
1	a	362	GLN
1	a	431	GLN
1	a	467	GLN
1	a	587	GLN
1	a	610	GLN
1	a	653	ASN
1	a	675	GLN
1	a	737	ASN
1	b	328	GLN
1	b	362	GLN
1	b	431	GLN

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Mol	Chain	Res	Type
1	b	467	GLN
1	b	587	GLN
1	b	610	GLN
1	b	653	ASN
1	b	675	GLN
1	b	737	ASN
1	c	328	GLN
1	c	362	GLN
1	c	431	GLN
1	c	467	GLN
1	c	587	GLN
1	c	610	GLN
1	c	653	ASN
1	c	675	GLN
1	c	737	ASN
1	d	328	GLN
1	d	362	GLN
1	d	431	GLN
1	d	467	GLN
1	d	587	GLN
1	d	610	GLN
1	d	653	ASN
1	d	675	GLN
1	d	737	ASN
1	e	328	GLN
1	e	362	GLN
1	e	431	GLN
1	e	467	GLN
1	e	587	GLN
1	e	610	GLN
1	e	653	ASN
1	e	675	GLN
1	e	737	ASN
1	f	328	GLN
1	f	362	GLN
1	f	431	GLN
1	f	467	GLN
1	f	587	GLN
1	f	610	GLN
1	f	653	ASN
1	f	675	GLN
1	f	737	ASN

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Mol	Chain	Res	Type
1	g	328	GLN
1	g	362	GLN
1	g	431	GLN
1	g	467	GLN
1	g	587	GLN
1	g	610	GLN
1	g	653	ASN
1	g	675	GLN
1	g	737	ASN
1	h	328	GLN
1	h	362	GLN
1	h	431	GLN
1	h	467	GLN
1	h	587	GLN
1	h	610	GLN
1	h	653	ASN
1	h	675	GLN
1	h	737	ASN
1	i	328	GLN
1	i	362	GLN
1	i	431	GLN
1	i	467	GLN
1	i	587	GLN
1	i	610	GLN
1	i	653	ASN
1	i	675	GLN
1	i	737	ASN
1	j	328	GLN
1	j	362	GLN
1	j	431	GLN
1	j	467	GLN
1	j	587	GLN
1	j	610	GLN
1	j	653	ASN
1	j	675	GLN
1	j	737	ASN
1	k	328	GLN
1	k	362	GLN
1	k	431	GLN
1	k	467	GLN
1	k	587	GLN
1	k	610	GLN

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Mol	Chain	Res	Type
1	k	653	ASN
1	k	675	GLN
1	k	737	ASN
1	l	328	GLN
1	l	362	GLN
1	l	431	GLN
1	l	467	GLN
1	l	587	GLN
1	l	610	GLN
1	l	653	ASN
1	l	675	GLN
1	l	737	ASN
1	m	328	GLN
1	m	362	GLN
1	m	431	GLN
1	m	467	GLN
1	m	587	GLN
1	m	610	GLN
1	m	653	ASN
1	m	675	GLN
1	m	737	ASN
1	n	328	GLN
1	n	362	GLN
1	n	431	GLN
1	n	467	GLN
1	n	587	GLN
1	n	610	GLN
1	n	653	ASN
1	n	675	GLN
1	n	737	ASN
1	o	328	GLN
1	o	362	GLN
1	o	431	GLN
1	o	467	GLN
1	o	587	GLN
1	o	610	GLN
1	o	653	ASN
1	o	675	GLN
1	o	737	ASN
1	p	328	GLN
1	p	362	GLN
1	p	431	GLN

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Mol	Chain	Res	Type
1	p	467	GLN
1	p	587	GLN
1	p	610	GLN
1	p	653	ASN
1	p	675	GLN
1	p	737	ASN
1	q	328	GLN
1	q	362	GLN
1	q	431	GLN
1	q	467	GLN
1	q	587	GLN
1	q	610	GLN
1	q	653	ASN
1	q	675	GLN
1	q	737	ASN
1	r	328	GLN
1	r	362	GLN
1	r	431	GLN
1	r	467	GLN
1	r	587	GLN
1	r	610	GLN
1	r	653	ASN
1	r	675	GLN
1	r	737	ASN
1	s	328	GLN
1	s	362	GLN
1	s	431	GLN
1	s	467	GLN
1	s	587	GLN
1	s	610	GLN
1	s	653	ASN
1	s	675	GLN
1	s	737	ASN
1	t	328	GLN
1	t	362	GLN
1	t	431	GLN
1	t	467	GLN
1	t	587	GLN
1	t	610	GLN
1	t	653	ASN
1	t	675	GLN
1	t	737	ASN

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Mol	Chain	Res	Type
1	u	328	GLN
1	u	362	GLN
1	u	431	GLN
1	u	467	GLN
1	u	587	GLN
1	u	610	GLN
1	u	653	ASN
1	u	675	GLN
1	u	737	ASN
1	v	328	GLN
1	v	362	GLN
1	v	431	GLN
1	v	467	GLN
1	v	587	GLN
1	v	610	GLN
1	v	653	ASN
1	v	675	GLN
1	v	737	ASN
1	w	328	GLN
1	w	362	GLN
1	w	431	GLN
1	w	467	GLN
1	w	587	GLN
1	w	610	GLN
1	w	653	ASN
1	w	675	GLN
1	w	737	ASN
1	x	328	GLN
1	x	362	GLN
1	x	431	GLN
1	x	467	GLN
1	x	587	GLN
1	x	610	GLN
1	x	653	ASN
1	x	675	GLN
1	x	737	ASN
1	y	328	GLN
1	y	362	GLN
1	y	431	GLN
1	y	467	GLN
1	y	587	GLN
1	y	610	GLN

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Mol	Chain	Res	Type
1	y	653	ASN
1	y	675	GLN
1	y	737	ASN
1	z	328	GLN
1	z	362	GLN
1	z	431	GLN
1	z	467	GLN
1	z	587	GLN
1	z	610	GLN
1	z	653	ASN
1	z	675	GLN
1	z	737	ASN
1	1	328	GLN
1	1	362	GLN
1	1	431	GLN
1	1	467	GLN
1	1	587	GLN
1	1	610	GLN
1	1	653	ASN
1	1	675	GLN
1	1	737	ASN
1	2	328	GLN
1	2	362	GLN
1	2	431	GLN
1	2	467	GLN
1	2	587	GLN
1	2	610	GLN
1	2	653	ASN
1	2	675	GLN
1	2	737	ASN
1	3	328	GLN
1	3	362	GLN
1	3	431	GLN
1	3	467	GLN
1	3	587	GLN
1	3	610	GLN
1	3	653	ASN
1	3	675	GLN
1	3	737	ASN
1	4	328	GLN
1	4	362	GLN
1	4	431	GLN

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Mol	Chain	Res	Type
1	4	467	GLN
1	4	587	GLN
1	4	610	GLN
1	4	653	ASN
1	4	675	GLN
1	4	737	ASN
1	5	328	GLN
1	5	362	GLN
1	5	431	GLN
1	5	467	GLN
1	5	587	GLN
1	5	610	GLN
1	5	653	ASN
1	5	675	GLN
1	5	737	ASN
1	6	328	GLN
1	6	362	GLN
1	6	431	GLN
1	6	467	GLN
1	6	587	GLN
1	6	610	GLN
1	6	653	ASN
1	6	675	GLN
1	6	737	ASN
1	7	328	GLN
1	7	362	GLN
1	7	431	GLN
1	7	467	GLN
1	7	587	GLN
1	7	610	GLN
1	7	653	ASN
1	7	675	GLN
1	7	737	ASN
1	8	328	GLN
1	8	362	GLN
1	8	431	GLN
1	8	467	GLN
1	8	587	GLN
1	8	610	GLN
1	8	653	ASN
1	8	675	GLN
1	8	737	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

120 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.