



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Dec 4, 2019 – 01:47 PM EST

PDB ID : 6V1Z  
EMDB ID: : EMD-21020  
Title : genome-containing AAVrh.39 particles  
Authors : Mietzsch, M.; Agbandje-McKenna, M.  
Deposited on : 2019-11-21  
Resolution : 3.58 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](mailto: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.

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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

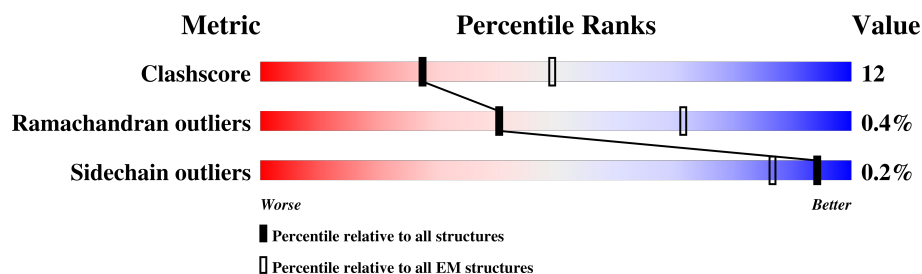
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.58 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  $\geq 3$ , 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	521	63%	37%
1	2	521	62%	37%
1	3	521	62%	38%
1	4	521	62%	38%
1	5	521	63%	37%
1	6	521	62%	38%
1	7	521	62%	38%
1	8	521	62%	38%
1	A	521	61%	38%

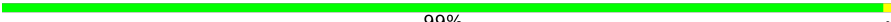














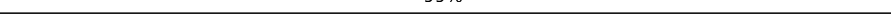
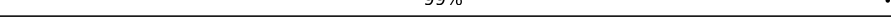
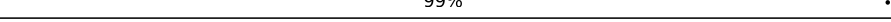
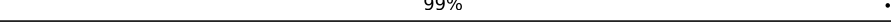
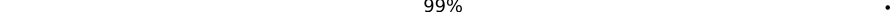
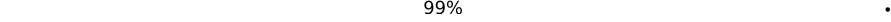
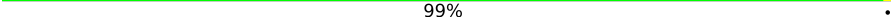
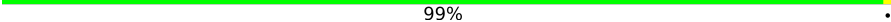

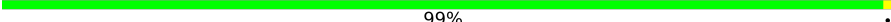
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Mol	Chain	Length	Quality of chain	
1	B	521	 61%	38%
1	C	521	 62%	38%
1	D	521	 62%	38%
1	E	521	 61%	39%
1	F	521	 62%	38%
1	G	521	 61%	39%
1	H	521	 61%	39%
1	I	521	 61%	38%
1	J	521	 62%	37%
1	K	521	 62%	38%
1	L	521	 61%	39%
1	M	521	 61%	39%
1	N	521	 61%	39%
1	O	521	 61%	39%
1	P	521	 62%	38%
1	Q	521	 61%	39%
1	R	521	 61%	38%
1	S	521	 61%	39%
1	T	521	 62%	38%
1	U	521	 61%	39%
1	V	521	 61%	38%
1	W	521	 61%	39%
1	X	521	 62%	38%
1	Y	521	 61%	39%
1	Z	521	 62%	38%

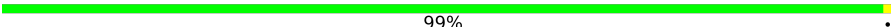
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Mol	Chain	Length	Quality of chain
1	a	521	 99% .
1	b	521	 99% .
1	c	521	 99% .
1	d	521	 99% .
1	e	521	 99% .
1	f	521	 99% .
1	g	521	 99% .
1	h	521	 99% .
1	i	521	 99% .
1	j	521	 99% .
1	k	521	 99% .
1	l	521	 99% .
1	m	521	 99% .
1	n	521	 99% .
1	o	521	 99% .
1	p	521	 99% .
1	q	521	 99% .
1	r	521	 99% .
1	s	521	 99% .
1	t	521	 99% .
1	u	521	 99% .
1	v	521	 99% .
1	w	521	 99% .
1	x	521	 99% .
1	y	521	 99% .

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Mol	Chain	Length	Quality of chain
1	z	521	 99%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 250920 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	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	B	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	C	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	D	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	E	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	F	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	G	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	H	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	I	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	J	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	K	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	L	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	M	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	N	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	O	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	P	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	Q	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	S	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	T	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	U	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	V	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	W	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	X	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	Y	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	Z	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	a	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	b	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	c	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	d	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	e	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	f	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	g	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	h	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	i	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	j	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	k	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	l	521	Total 4145	C 2617	N 717	O 797	S 14	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	n	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	o	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	p	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	q	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	r	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	s	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	t	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	u	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	v	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	w	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	x	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	y	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	z	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	1	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	2	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	3	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	4	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	5	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	6	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	7	521	Total 4145	C 2617	N 717	O 797	S 14	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ASN	SER	conflict	UNP B4Y886
A	417	GLN	THR	conflict	UNP B4Y886
B	315	ASN	SER	conflict	UNP B4Y886
B	417	GLN	THR	conflict	UNP B4Y886
C	315	ASN	SER	conflict	UNP B4Y886
C	417	GLN	THR	conflict	UNP B4Y886
D	315	ASN	SER	conflict	UNP B4Y886
D	417	GLN	THR	conflict	UNP B4Y886
E	315	ASN	SER	conflict	UNP B4Y886
E	417	GLN	THR	conflict	UNP B4Y886
F	315	ASN	SER	conflict	UNP B4Y886
F	417	GLN	THR	conflict	UNP B4Y886
G	315	ASN	SER	conflict	UNP B4Y886
G	417	GLN	THR	conflict	UNP B4Y886
H	315	ASN	SER	conflict	UNP B4Y886
H	417	GLN	THR	conflict	UNP B4Y886
I	315	ASN	SER	conflict	UNP B4Y886
I	417	GLN	THR	conflict	UNP B4Y886
J	315	ASN	SER	conflict	UNP B4Y886
J	417	GLN	THR	conflict	UNP B4Y886
K	315	ASN	SER	conflict	UNP B4Y886
K	417	GLN	THR	conflict	UNP B4Y886
L	315	ASN	SER	conflict	UNP B4Y886
L	417	GLN	THR	conflict	UNP B4Y886
M	315	ASN	SER	conflict	UNP B4Y886
M	417	GLN	THR	conflict	UNP B4Y886
N	315	ASN	SER	conflict	UNP B4Y886
N	417	GLN	THR	conflict	UNP B4Y886
O	315	ASN	SER	conflict	UNP B4Y886
O	417	GLN	THR	conflict	UNP B4Y886
P	315	ASN	SER	conflict	UNP B4Y886
P	417	GLN	THR	conflict	UNP B4Y886
Q	315	ASN	SER	conflict	UNP B4Y886
Q	417	GLN	THR	conflict	UNP B4Y886
R	315	ASN	SER	conflict	UNP B4Y886
R	417	GLN	THR	conflict	UNP B4Y886

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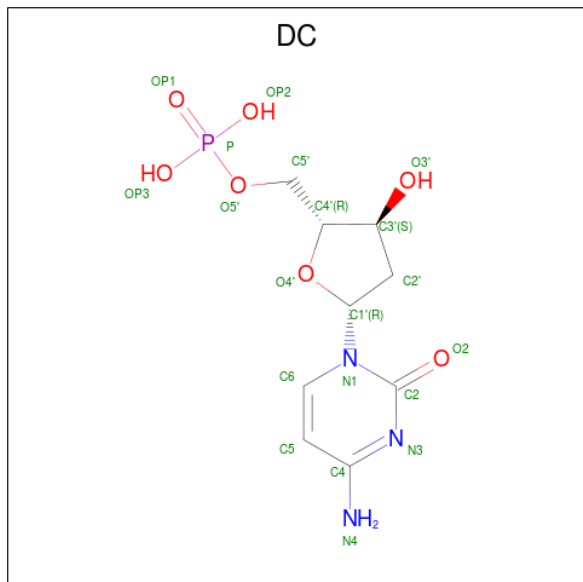
Chain	Residue	Modelled	Actual	Comment	Reference
S	315	ASN	SER	conflict	UNP B4Y886
S	417	GLN	THR	conflict	UNP B4Y886
T	315	ASN	SER	conflict	UNP B4Y886
T	417	GLN	THR	conflict	UNP B4Y886
U	315	ASN	SER	conflict	UNP B4Y886
U	417	GLN	THR	conflict	UNP B4Y886
V	315	ASN	SER	conflict	UNP B4Y886
V	417	GLN	THR	conflict	UNP B4Y886
W	315	ASN	SER	conflict	UNP B4Y886
W	417	GLN	THR	conflict	UNP B4Y886
X	315	ASN	SER	conflict	UNP B4Y886
X	417	GLN	THR	conflict	UNP B4Y886
Y	315	ASN	SER	conflict	UNP B4Y886
Y	417	GLN	THR	conflict	UNP B4Y886
Z	315	ASN	SER	conflict	UNP B4Y886
Z	417	GLN	THR	conflict	UNP B4Y886
a	315	ASN	SER	conflict	UNP B4Y886
a	417	GLN	THR	conflict	UNP B4Y886
b	315	ASN	SER	conflict	UNP B4Y886
b	417	GLN	THR	conflict	UNP B4Y886
c	315	ASN	SER	conflict	UNP B4Y886
c	417	GLN	THR	conflict	UNP B4Y886
d	315	ASN	SER	conflict	UNP B4Y886
d	417	GLN	THR	conflict	UNP B4Y886
e	315	ASN	SER	conflict	UNP B4Y886
e	417	GLN	THR	conflict	UNP B4Y886
f	315	ASN	SER	conflict	UNP B4Y886
f	417	GLN	THR	conflict	UNP B4Y886
g	315	ASN	SER	conflict	UNP B4Y886
g	417	GLN	THR	conflict	UNP B4Y886
h	315	ASN	SER	conflict	UNP B4Y886
h	417	GLN	THR	conflict	UNP B4Y886
i	315	ASN	SER	conflict	UNP B4Y886
i	417	GLN	THR	conflict	UNP B4Y886
j	315	ASN	SER	conflict	UNP B4Y886
j	417	GLN	THR	conflict	UNP B4Y886
k	315	ASN	SER	conflict	UNP B4Y886
k	417	GLN	THR	conflict	UNP B4Y886
l	315	ASN	SER	conflict	UNP B4Y886
l	417	GLN	THR	conflict	UNP B4Y886
m	315	ASN	SER	conflict	UNP B4Y886
m	417	GLN	THR	conflict	UNP B4Y886

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Chain	Residue	Modelled	Actual	Comment	Reference
n	315	ASN	SER	conflict	UNP B4Y886
n	417	GLN	THR	conflict	UNP B4Y886
o	315	ASN	SER	conflict	UNP B4Y886
o	417	GLN	THR	conflict	UNP B4Y886
p	315	ASN	SER	conflict	UNP B4Y886
p	417	GLN	THR	conflict	UNP B4Y886
q	315	ASN	SER	conflict	UNP B4Y886
q	417	GLN	THR	conflict	UNP B4Y886
r	315	ASN	SER	conflict	UNP B4Y886
r	417	GLN	THR	conflict	UNP B4Y886
s	315	ASN	SER	conflict	UNP B4Y886
s	417	GLN	THR	conflict	UNP B4Y886
t	315	ASN	SER	conflict	UNP B4Y886
t	417	GLN	THR	conflict	UNP B4Y886
u	315	ASN	SER	conflict	UNP B4Y886
u	417	GLN	THR	conflict	UNP B4Y886
v	315	ASN	SER	conflict	UNP B4Y886
v	417	GLN	THR	conflict	UNP B4Y886
w	315	ASN	SER	conflict	UNP B4Y886
w	417	GLN	THR	conflict	UNP B4Y886
x	315	ASN	SER	conflict	UNP B4Y886
x	417	GLN	THR	conflict	UNP B4Y886
y	315	ASN	SER	conflict	UNP B4Y886
y	417	GLN	THR	conflict	UNP B4Y886
z	315	ASN	SER	conflict	UNP B4Y886
z	417	GLN	THR	conflict	UNP B4Y886
1	315	ASN	SER	conflict	UNP B4Y886
1	417	GLN	THR	conflict	UNP B4Y886
2	315	ASN	SER	conflict	UNP B4Y886
2	417	GLN	THR	conflict	UNP B4Y886
3	315	ASN	SER	conflict	UNP B4Y886
3	417	GLN	THR	conflict	UNP B4Y886
4	315	ASN	SER	conflict	UNP B4Y886
4	417	GLN	THR	conflict	UNP B4Y886
5	315	ASN	SER	conflict	UNP B4Y886
5	417	GLN	THR	conflict	UNP B4Y886
6	315	ASN	SER	conflict	UNP B4Y886
6	417	GLN	THR	conflict	UNP B4Y886
7	315	ASN	SER	conflict	UNP B4Y886
7	417	GLN	THR	conflict	UNP B4Y886
8	315	ASN	SER	conflict	UNP B4Y886
8	417	GLN	THR	conflict	UNP B4Y886

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DC) (formula:  $C_9H_{14}N_3O_7P$ ).



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	
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	

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Mol	Chain	Residues	Atoms				AltConf
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	
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	

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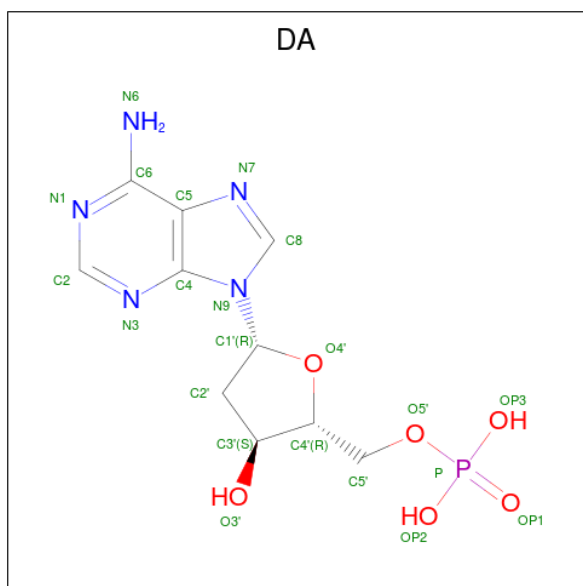
Mol	Chain	Residues	Atoms				AltConf
2	h	1	Total	C	N	O	0
			16	9	3	4	
2	i	1	Total	C	N	O	0
			16	9	3	4	
2	j	1	Total	C	N	O	0
			16	9	3	4	
2	k	1	Total	C	N	O	0
			16	9	3	4	
2	l	1	Total	C	N	O	0
			16	9	3	4	
2	m	1	Total	C	N	O	0
			16	9	3	4	
2	n	1	Total	C	N	O	0
			16	9	3	4	
2	o	1	Total	C	N	O	0
			16	9	3	4	
2	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	
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	

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Mol	Chain	Residues	Atoms				AltConf
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: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P).



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	

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Mol	Chain	Residues	Atoms					AltConf
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	
3	O	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	P	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	Q	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	R	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	S	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	T	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	U	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	V	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	W	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	X	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	Y	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	Z	1	Total	C	N	O	P	0
			21	10	5	5	1	

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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	
3	o	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	p	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	q	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	r	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	s	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	t	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	u	1	Total	C	N	O	P	0
			21	10	5	5	1	

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

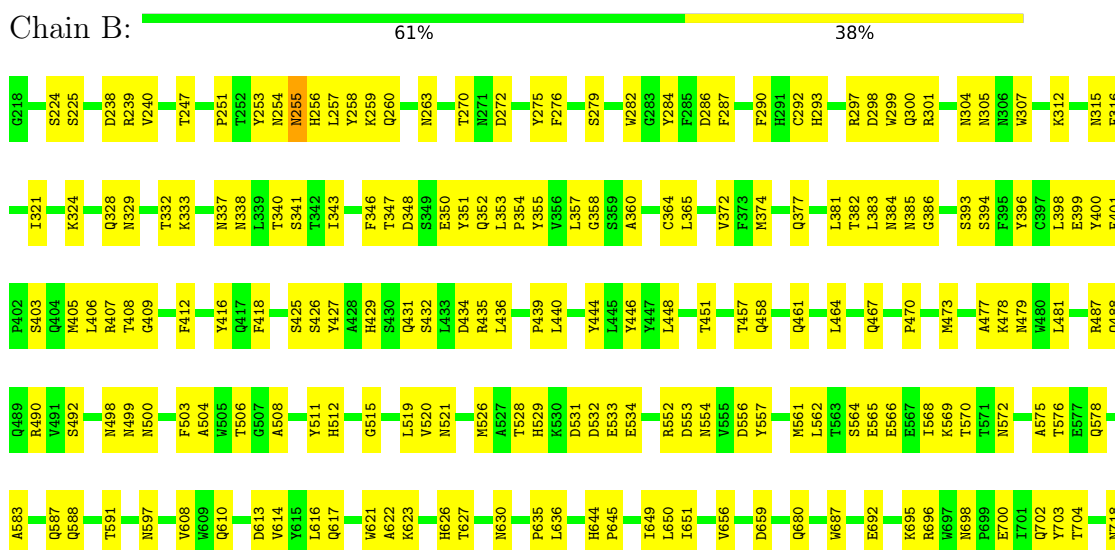
### 3 Residue-property plots

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.

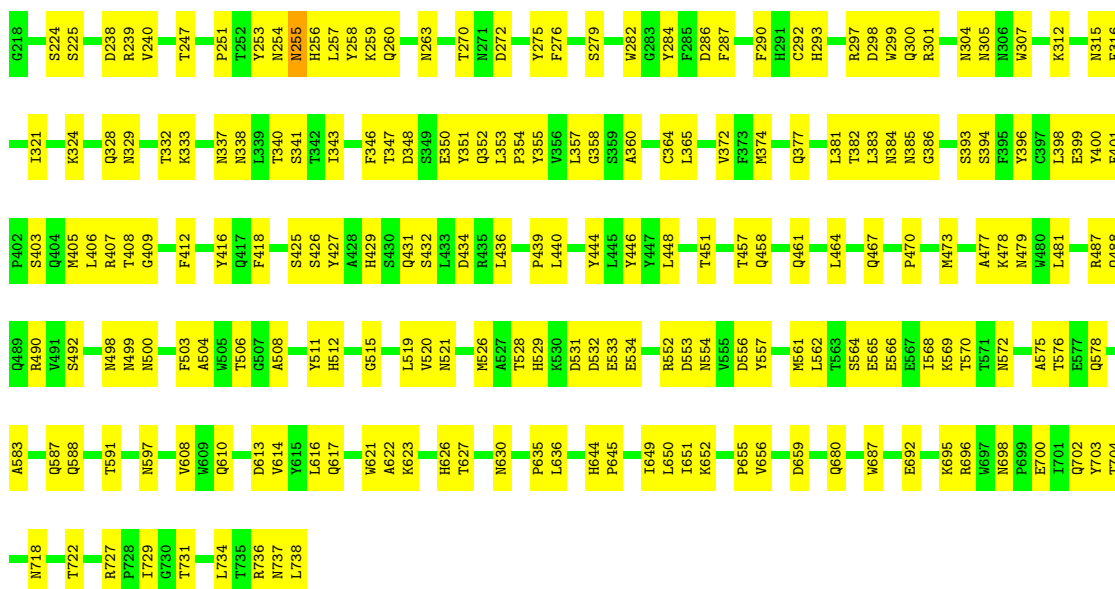
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

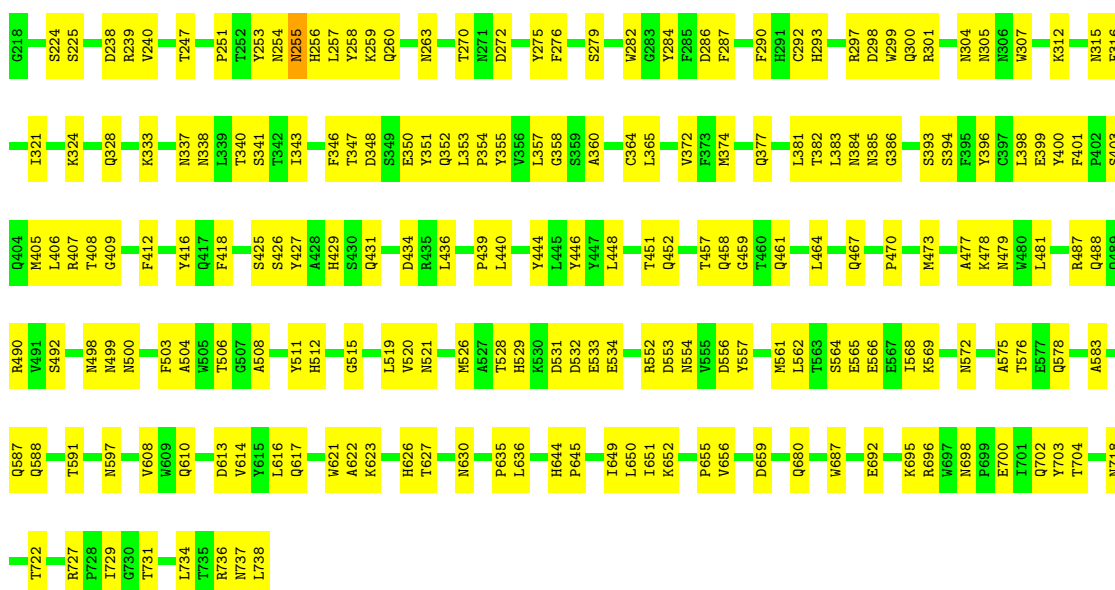






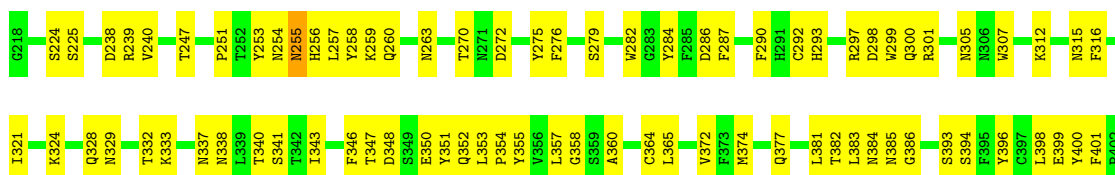
• Molecule 1: Capsid protein VP1

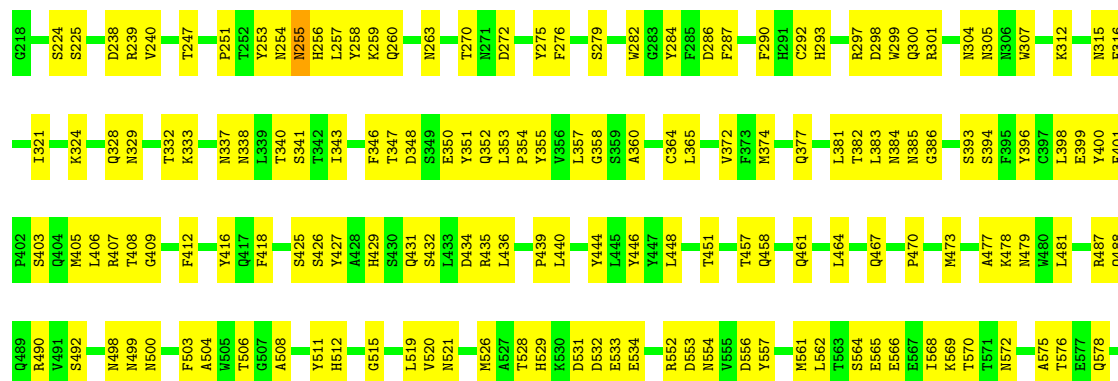
Chain F: 62% 38%



• Molecule 1: Capsid protein VP1

Chain G: 61% 39%

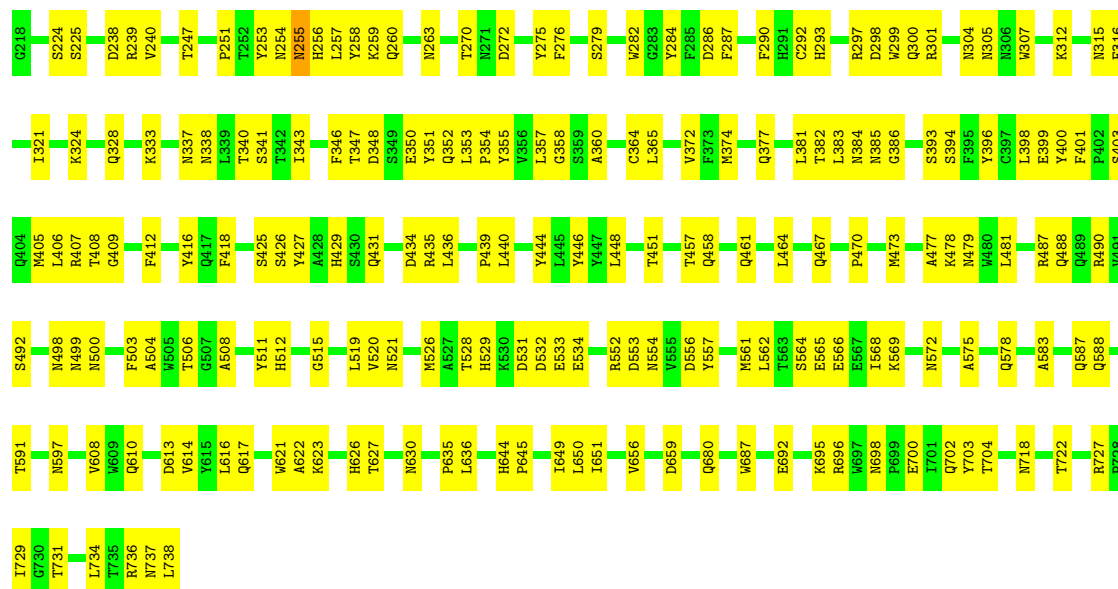






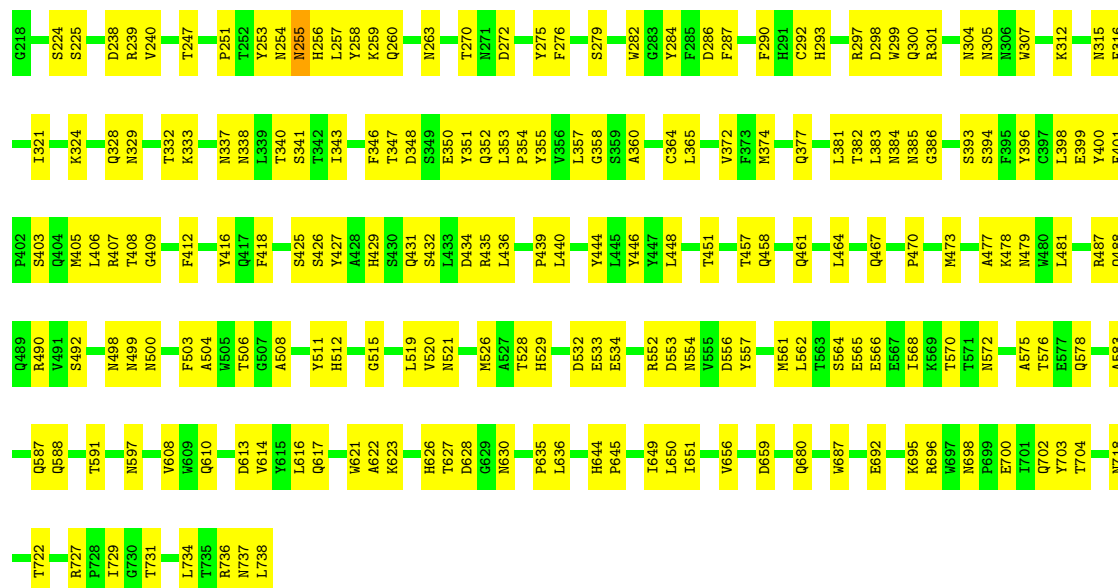
• Molecule 1: Capsid protein VP1

Chain J: 62% 37%

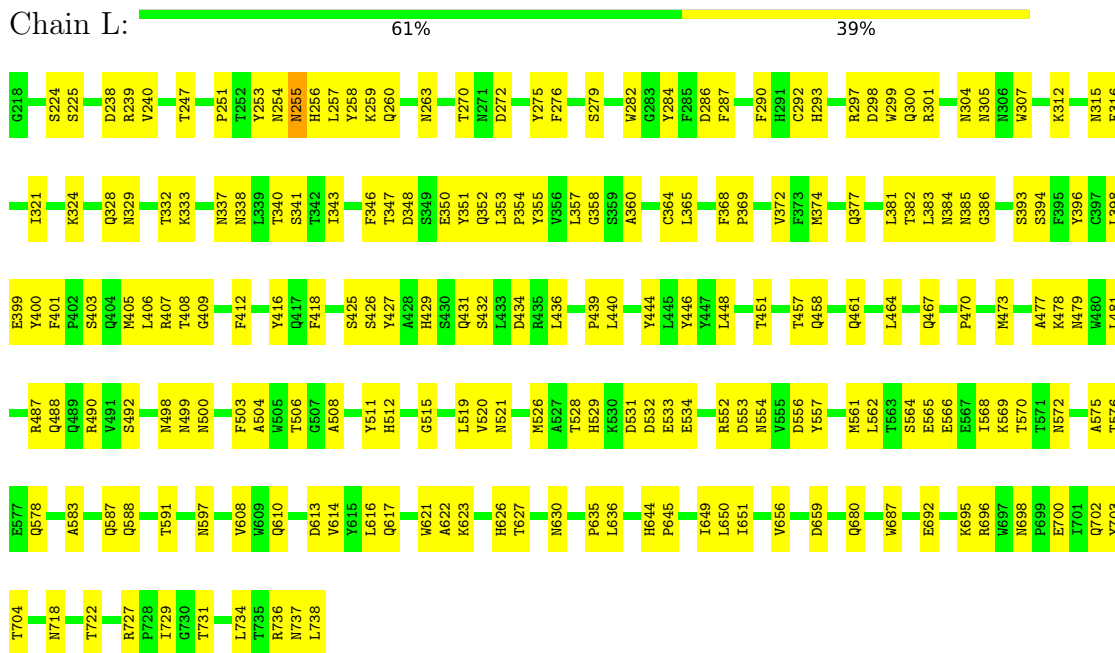


• Molecule 1: Capsid protein VP1

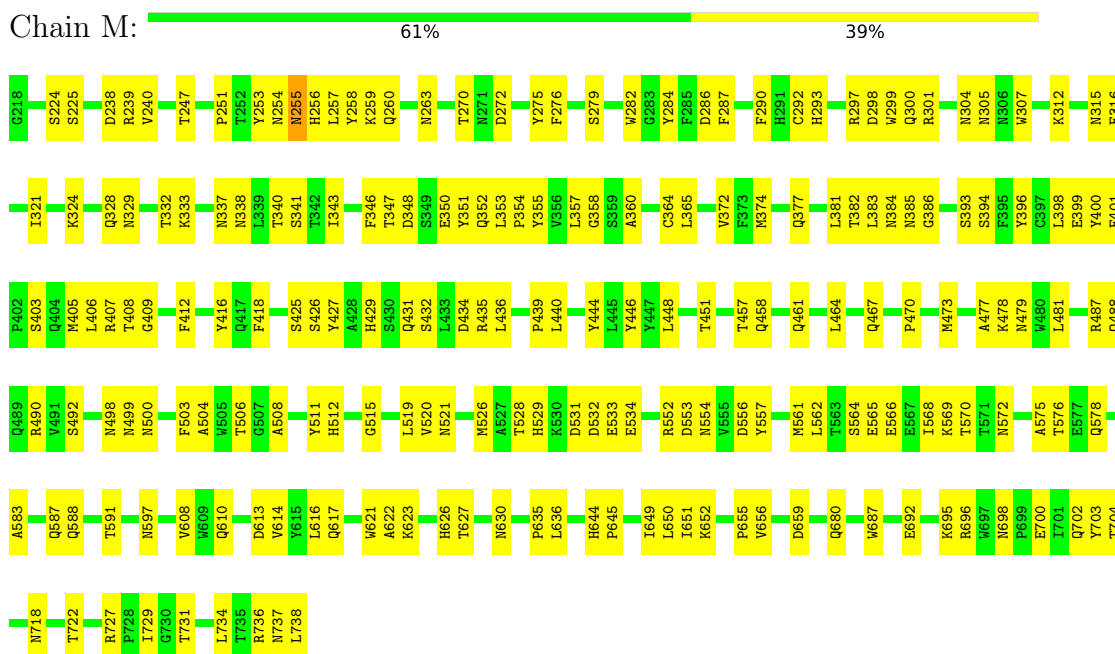
Chain K: 62% 38%



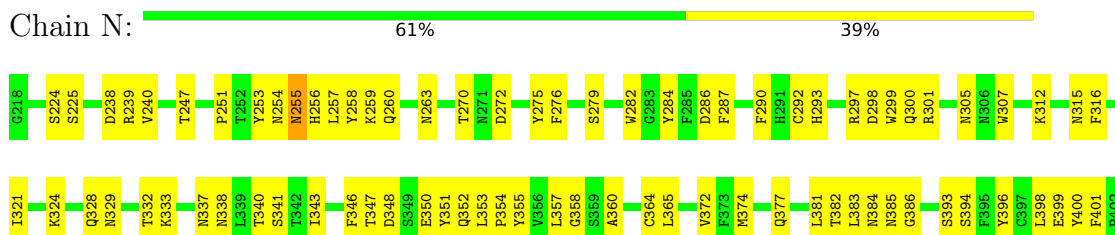
• Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

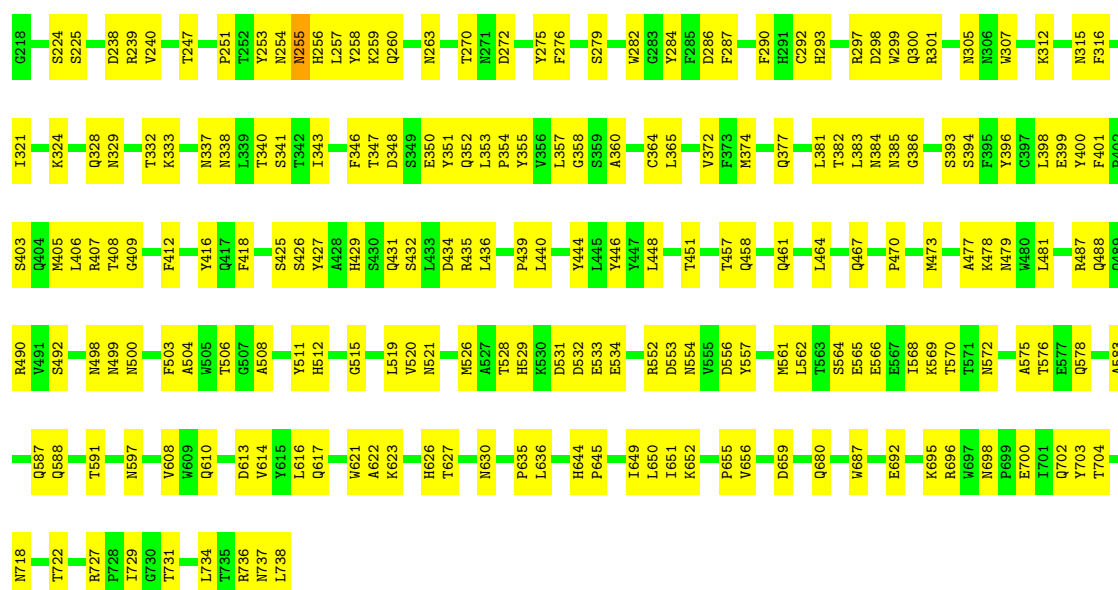






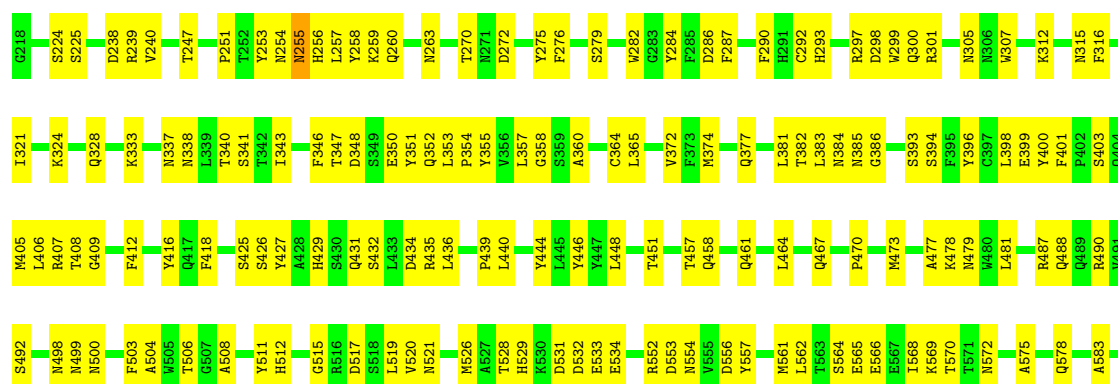
● Molecule 1: Capsid protein VP1

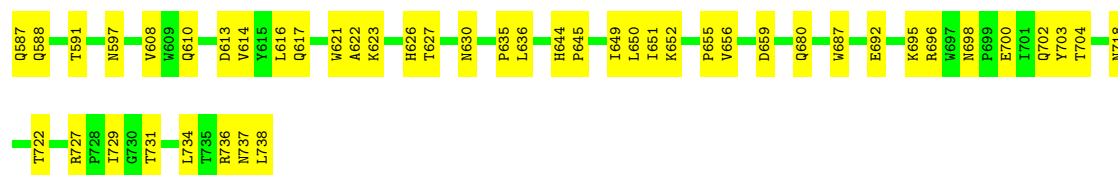
Chain O: 61% 39%



● Molecule 1: Capsid protein VP1

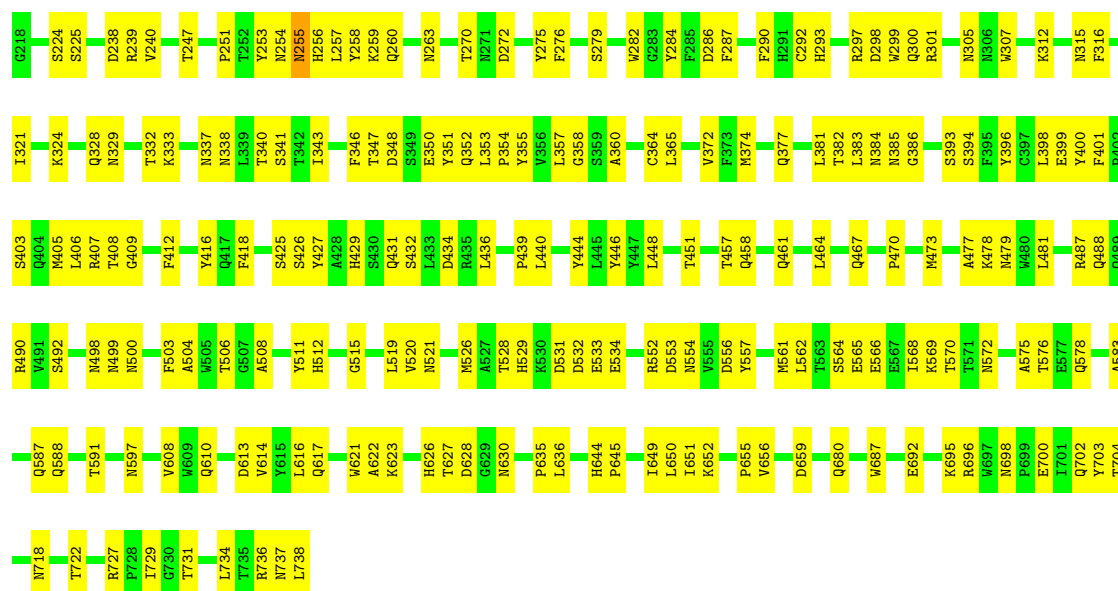
Chain P: 62% 38%





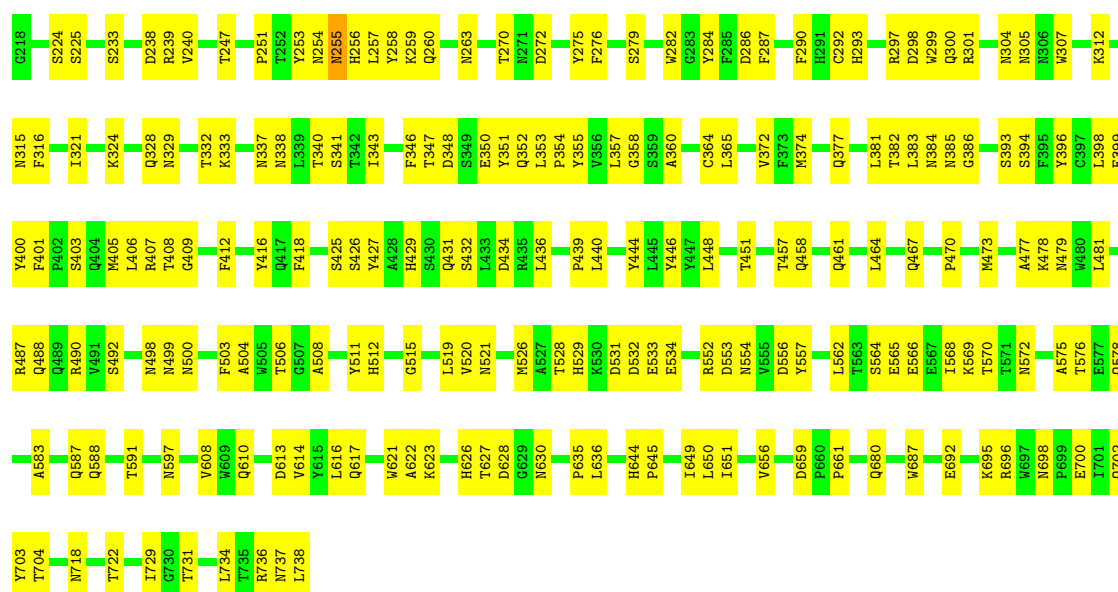
• Molecule 1: Capsid protein VP1

Chain Q: 61% 39%



• Molecule 1: Capsid protein VP1

Chain R: 61% 38%



• Molecule 1: Capsid protein VP1

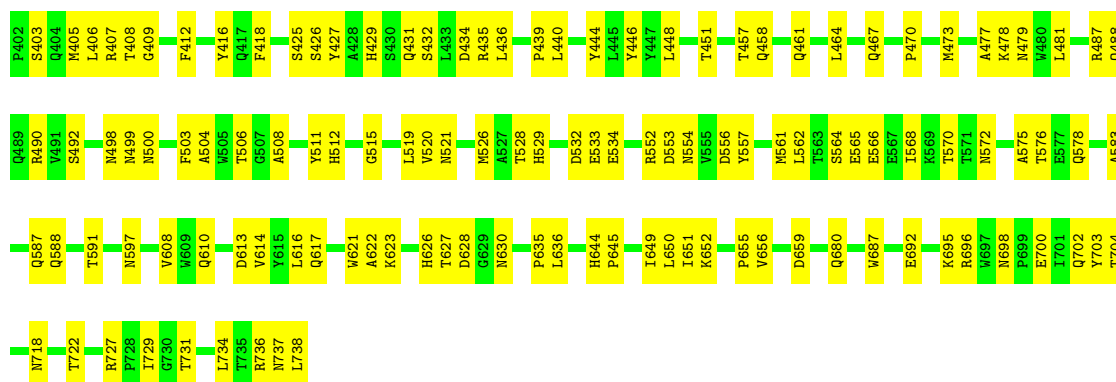
39%



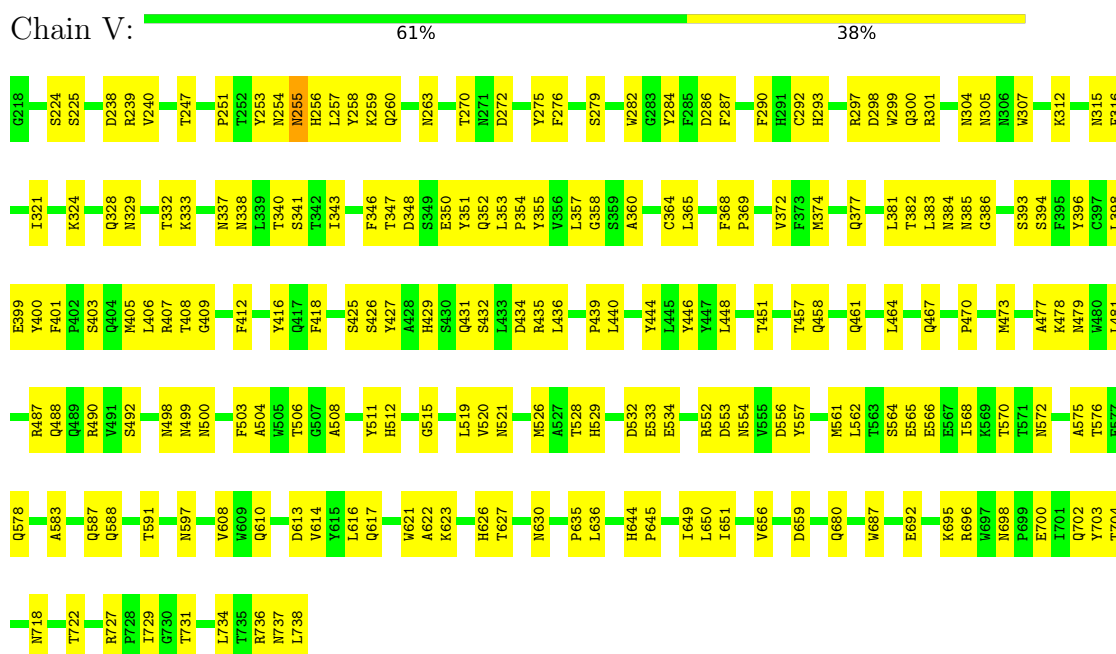
38%



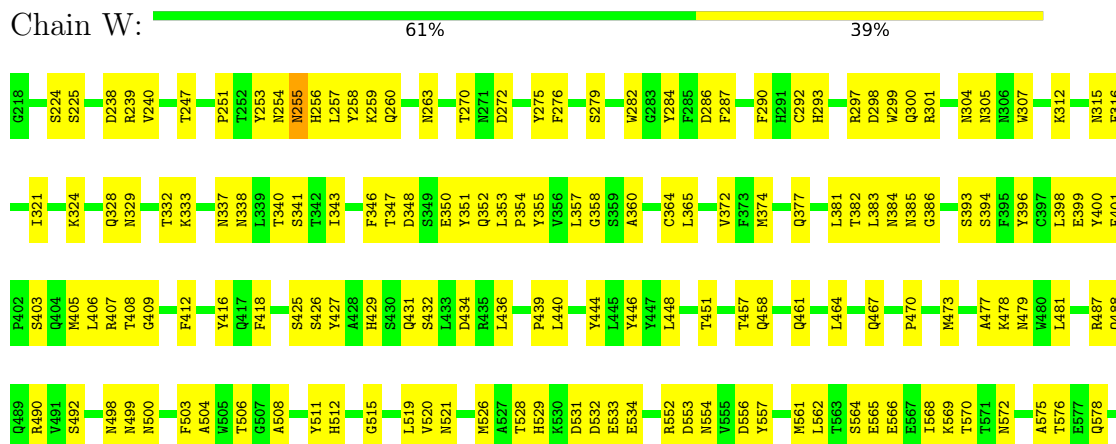
39%

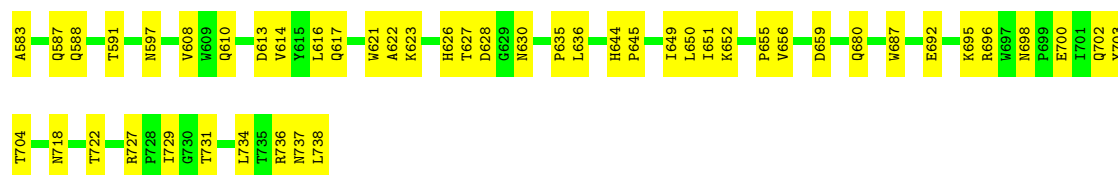


• Molecule 1: Capsid protein VP1



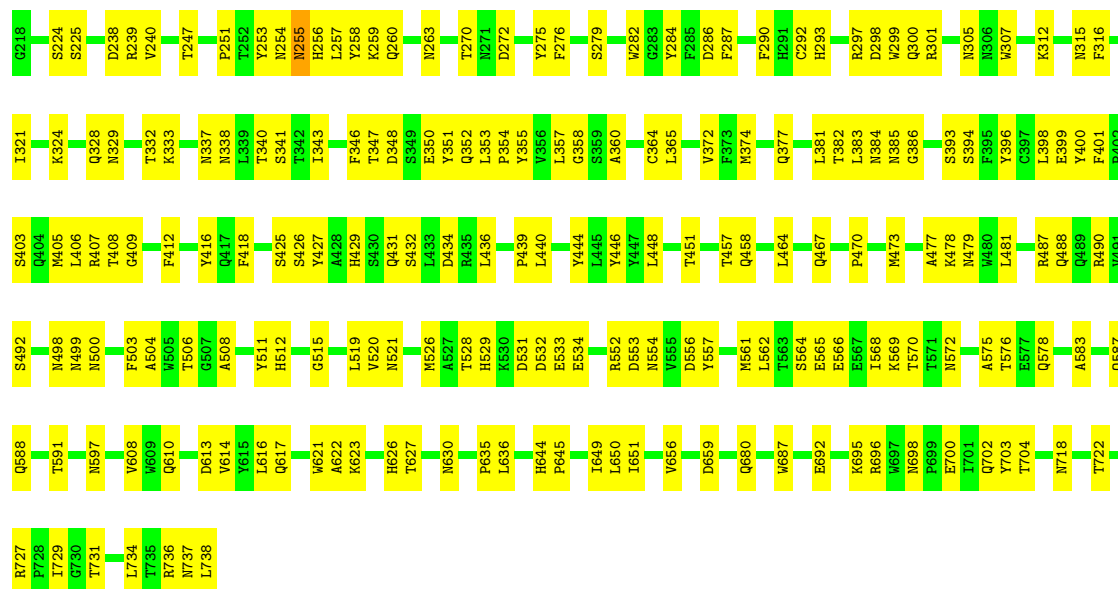
• Molecule 1: Capsid protein VP1





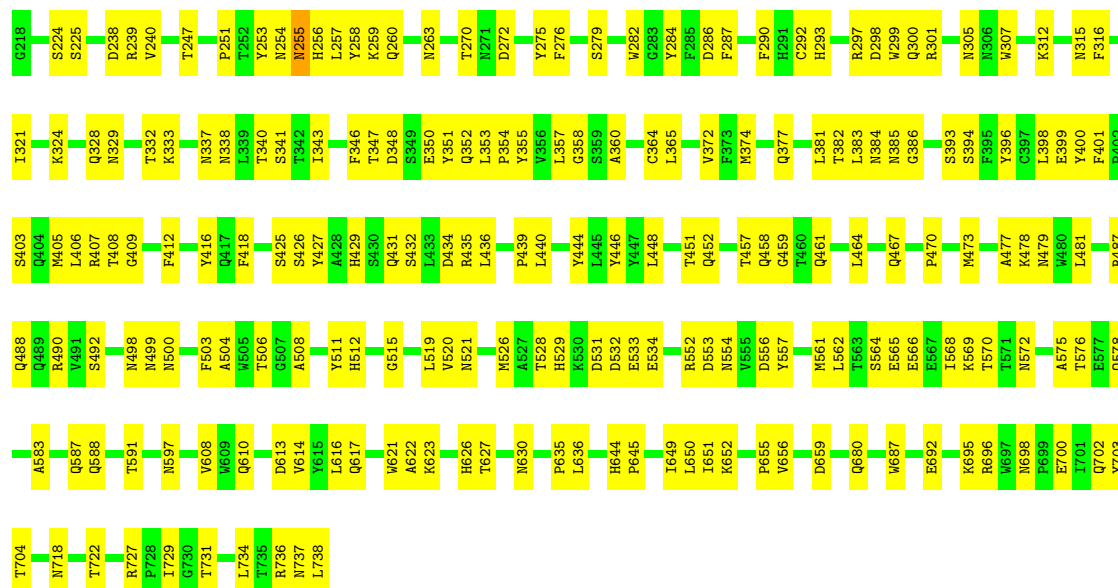
### • Molecule 1: Capsid protein VP1

Chain X:   62% 38%

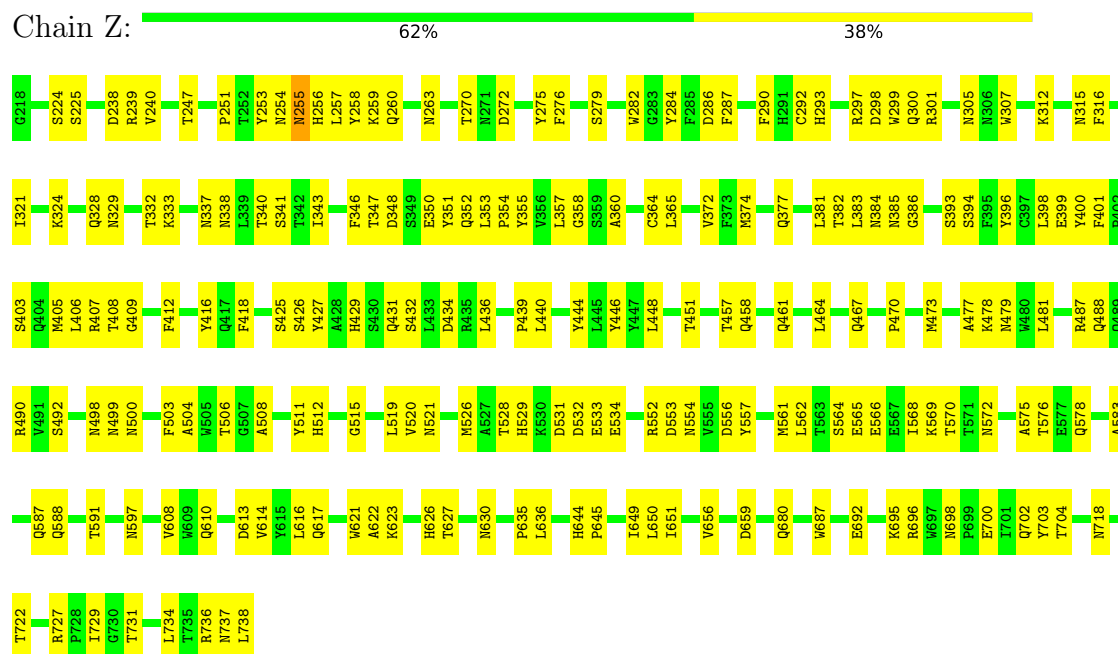


### • Molecule 1: Capsid protein VP1

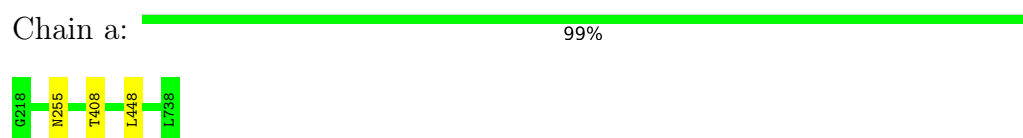
Chain Y:   61% 39%



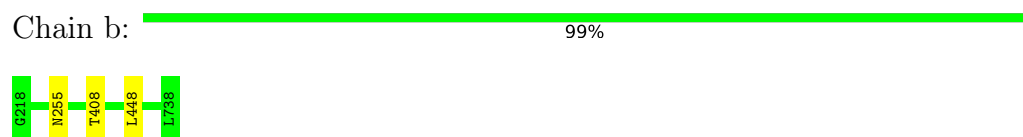
### • Molecule 1: Capsid protein VP1



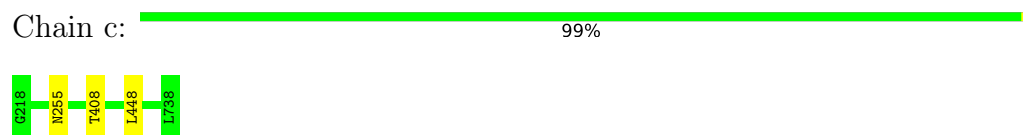
- Molecule 1: Capsid protein VP1



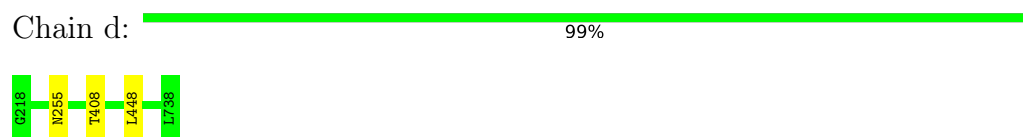
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1





- Molecule 1: Capsid protein VP1

Chain f:  99%



- Molecule 1: Capsid protein VP1

Chain g:  99%



- Molecule 1: Capsid protein VP1

Chain h:  99%



- Molecule 1: Capsid protein VP1

Chain i:  99%



- Molecule 1: Capsid protein VP1

Chain j:  99%



- Molecule 1: Capsid protein VP1

Chain k:  99%



- Molecule 1: Capsid protein VP1

Chain l:  99%



- Molecule 1: Capsid protein VP1

Chain m:  99%



- Molecule 1: Capsid protein VP1

Chain n:  99%



- Molecule 1: Capsid protein VP1

Chain o:  99%



- Molecule 1: Capsid protein VP1

Chain p:  99%



- Molecule 1: Capsid protein VP1

Chain q:  99%



- Molecule 1: Capsid protein VP1

Chain r:  99%



- Molecule 1: Capsid protein VP1

Chain s:  99%



- Molecule 1: Capsid protein VP1



Chain t:  99%



- Molecule 1: Capsid protein VP1

Chain u:  99%



- Molecule 1: Capsid protein VP1

Chain v:  99%



- Molecule 1: Capsid protein VP1

Chain w:  99%



- Molecule 1: Capsid protein VP1

Chain x:  99%



- Molecule 1: Capsid protein VP1

Chain y:  99%



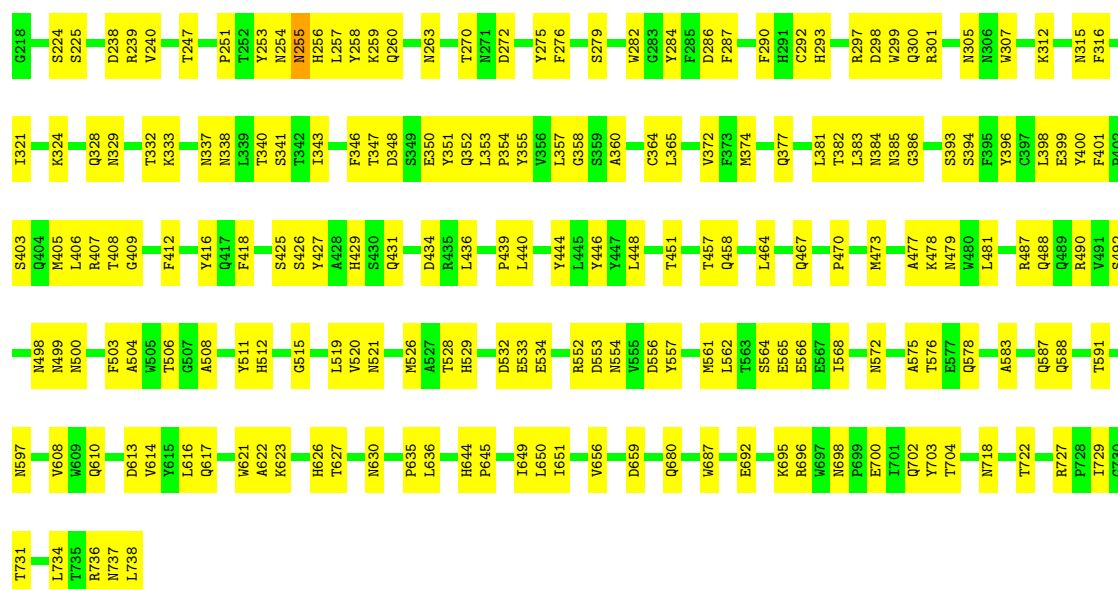
- Molecule 1: Capsid protein VP1

Chain z:  99%

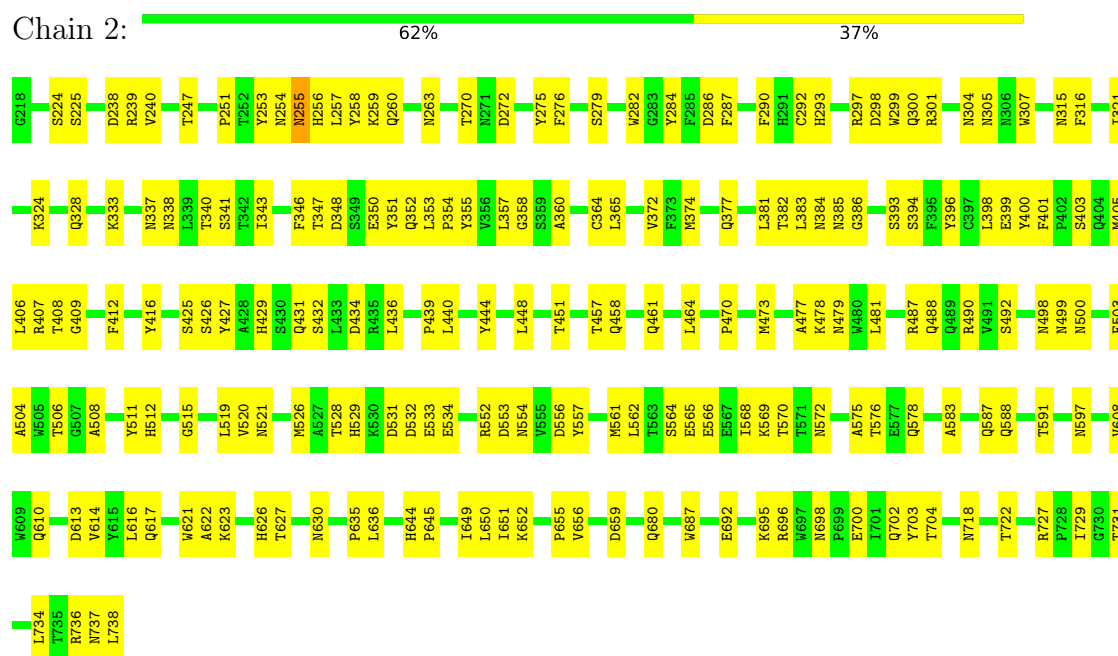


- Molecule 1: Capsid protein VP1

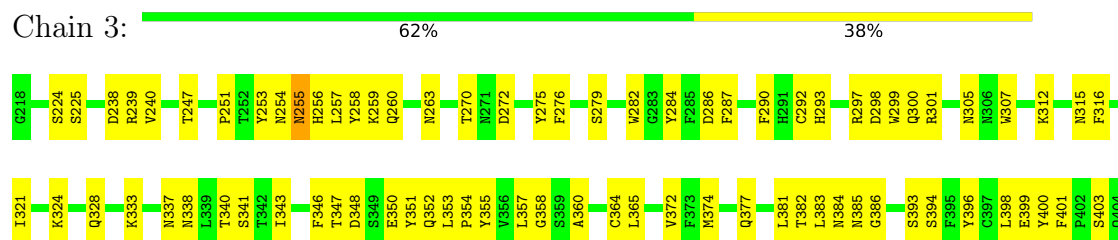
Chain 1:  63%  37%

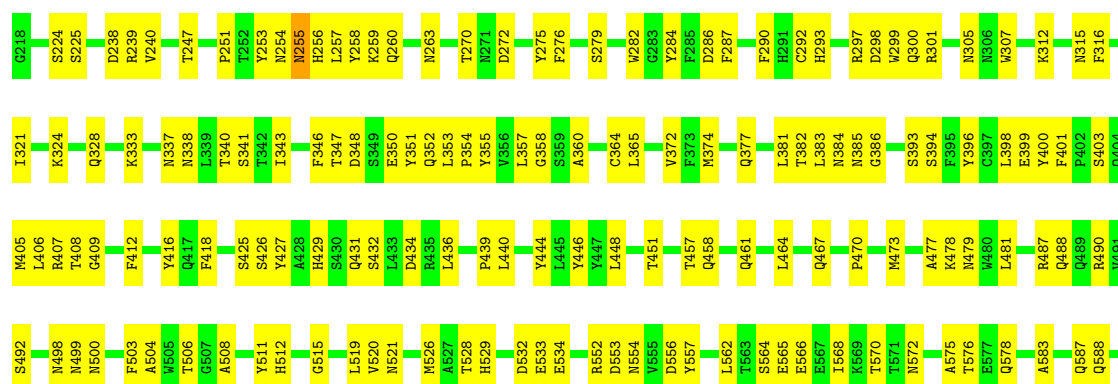


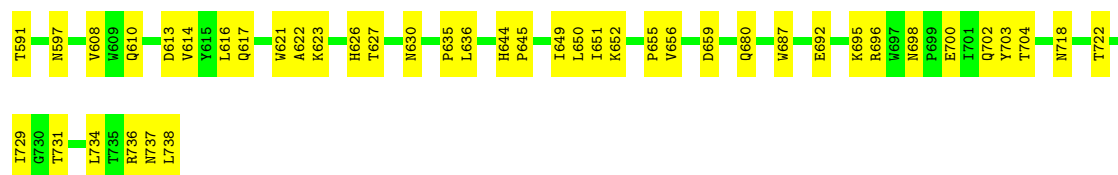
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

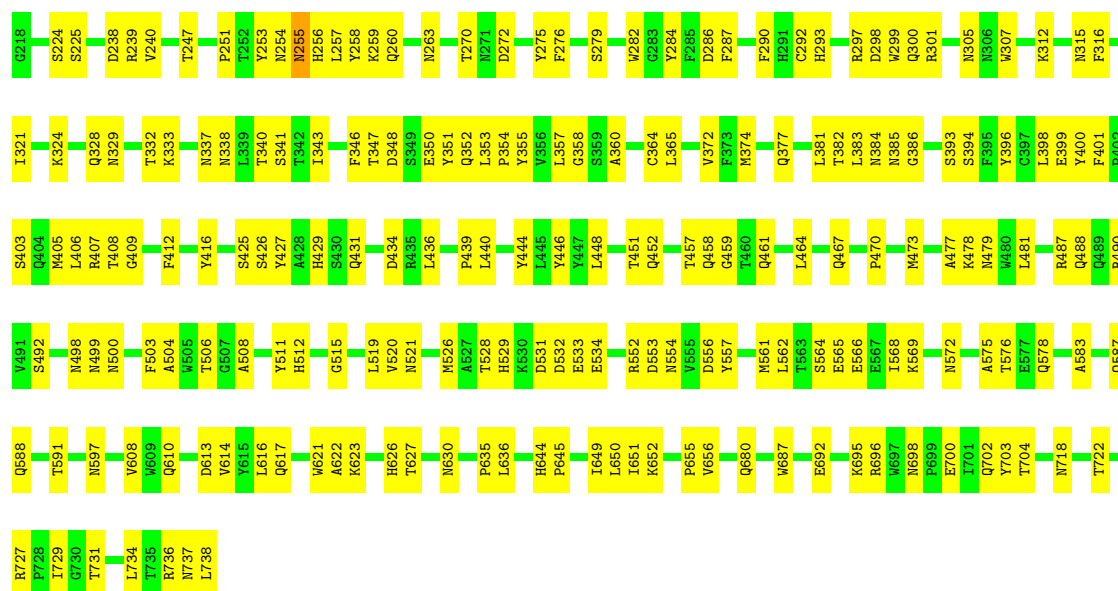






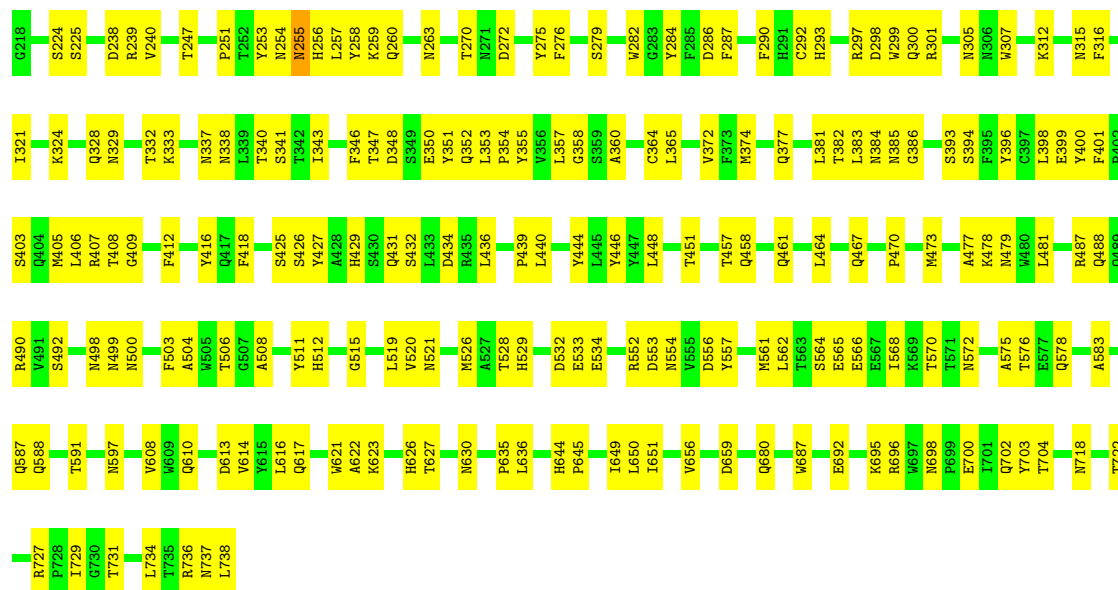
• Molecule 1: Capsid protein VP1

Chain 6: 62% 38%



• Molecule 1: Capsid protein VP1

Chain 7: 62% 38%

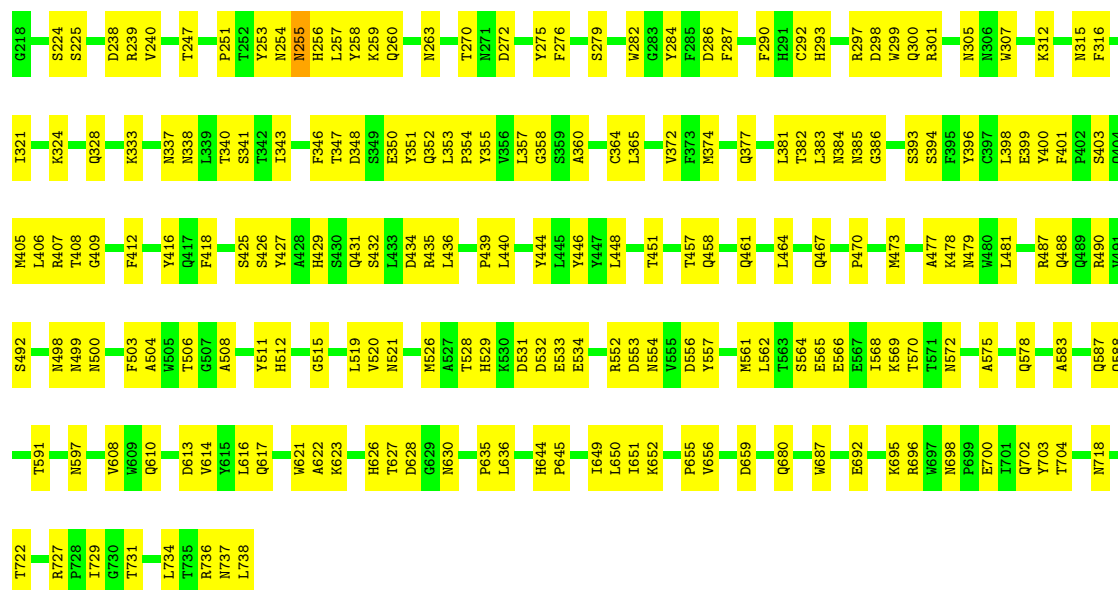


• Molecule 1: Capsid protein VP1

Chain 8:

62%

38%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1326	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 ( $e^-/\text{\AA}^2$ )	67	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	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	0.57	0/4272	0.56	0/5826
1	2	0.57	0/4272	0.56	0/5826
1	3	0.57	0/4272	0.56	0/5826
1	4	0.57	0/4272	0.56	0/5826
1	5	0.57	0/4272	0.56	0/5826
1	6	0.57	0/4272	0.56	0/5826
1	7	0.57	0/4272	0.56	0/5826
1	8	0.57	0/4272	0.56	0/5826
1	A	0.57	0/4272	0.56	0/5826
1	B	0.57	0/4272	0.56	0/5826
1	C	0.57	0/4272	0.56	0/5826
1	D	0.57	0/4272	0.56	0/5826
1	E	0.57	0/4272	0.56	0/5826
1	F	0.57	0/4272	0.56	0/5826
1	G	0.57	0/4272	0.56	0/5826
1	H	0.57	0/4272	0.56	0/5826
1	I	0.57	0/4272	0.56	0/5826
1	J	0.57	0/4272	0.56	0/5826
1	K	0.57	0/4272	0.56	0/5826
1	L	0.57	0/4272	0.56	0/5826
1	M	0.57	0/4272	0.56	0/5826
1	N	0.57	0/4272	0.56	0/5826
1	O	0.57	0/4272	0.56	0/5826
1	P	0.57	0/4272	0.56	0/5826
1	Q	0.57	0/4272	0.56	0/5826
1	R	0.57	0/4272	0.56	0/5826
1	S	0.57	0/4272	0.56	0/5826
1	T	0.57	0/4272	0.56	0/5826
1	U	0.57	0/4272	0.56	0/5826
1	V	0.57	0/4272	0.56	0/5826
1	W	0.57	0/4272	0.56	0/5826
1	X	0.57	0/4272	0.56	0/5826
1	Y	0.57	0/4272	0.56	0/5826
1	Z	0.57	0/4272	0.56	0/5826

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	a	0.57	0/4272	0.56	0/5826
1	b	0.57	0/4272	0.56	0/5826
1	c	0.57	0/4272	0.56	0/5826
1	d	0.57	0/4272	0.56	0/5826
1	e	0.57	0/4272	0.56	0/5826
1	f	0.57	0/4272	0.56	0/5826
1	g	0.57	0/4272	0.56	0/5826
1	h	0.57	0/4272	0.56	0/5826
1	i	0.57	0/4272	0.56	0/5826
1	j	0.57	0/4272	0.56	0/5826
1	k	0.57	0/4272	0.56	0/5826
1	l	0.57	0/4272	0.56	0/5826
1	m	0.57	0/4272	0.56	0/5826
1	n	0.57	0/4272	0.56	0/5826
1	o	0.57	0/4272	0.56	0/5826
1	p	0.57	0/4272	0.56	0/5826
1	q	0.57	0/4272	0.56	0/5826
1	r	0.57	0/4272	0.56	0/5826
1	s	0.57	0/4272	0.56	0/5826
1	t	0.57	0/4272	0.56	0/5826
1	u	0.57	0/4272	0.56	0/5826
1	v	0.57	0/4272	0.56	0/5826
1	w	0.57	0/4272	0.56	0/5826
1	x	0.57	0/4272	0.56	0/5826
1	y	0.57	0/4272	0.56	0/5826
1	z	0.57	0/4272	0.56	0/5826
All	All	0.57	0/256320	0.56	0/349560

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	4145	0	3907	173	0
1	2	4145	0	3907	172	0
1	3	4145	0	3907	172	0
1	4	4145	0	3907	174	0
1	5	4145	0	3907	172	0
1	6	4145	0	3907	174	0
1	7	4145	0	3907	171	0
1	8	4145	0	3907	177	0
1	A	4145	0	3907	247	0
1	B	4145	0	3907	246	0
1	C	4145	0	3907	244	0
1	D	4145	0	3907	246	0
1	E	4145	0	3907	247	0
1	F	4145	0	3907	245	0
1	G	4145	0	3907	243	0
1	H	4145	0	3907	240	0
1	I	4145	0	3907	238	0
1	J	4145	0	3907	243	0
1	K	4145	0	3907	245	0
1	L	4145	0	3907	245	0
1	M	4145	0	3907	248	0
1	N	4145	0	3907	247	0
1	O	4145	0	3907	244	0
1	P	4145	0	3907	233	0
1	Q	4145	0	3907	238	0
1	R	4145	0	3907	222	0
1	S	4145	0	3907	227	0
1	T	4145	0	3907	246	0
1	U	4145	0	3907	245	0
1	V	4145	0	3907	249	0
1	W	4145	0	3907	245	0
1	X	4145	0	3907	244	0
1	Y	4145	0	3907	247	0
1	Z	4145	0	3907	246	0
1	a	4145	0	3907	0	0
1	b	4145	0	3907	0	0
1	c	4145	0	3907	0	0
1	d	4145	0	3907	0	0
1	e	4145	0	3907	0	0
1	f	4145	0	3907	0	0
1	g	4145	0	3907	0	0
1	h	4145	0	3907	0	0
1	i	4145	0	3907	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4145	0	3907	0	0
1	k	4145	0	3907	0	0
1	l	4145	0	3907	0	0
1	m	4145	0	3907	0	0
1	n	4145	0	3907	0	0
1	o	4145	0	3907	0	0
1	p	4145	0	3907	0	0
1	q	4145	0	3907	0	0
1	r	4145	0	3907	0	0
1	s	4145	0	3907	0	0
1	t	4145	0	3907	0	0
1	u	4145	0	3907	0	0
1	v	4145	0	3907	0	0
1	w	4145	0	3907	0	0
1	x	4145	0	3907	0	0
1	y	4145	0	3907	0	0
1	z	4145	0	3907	0	0
2	1	16	0	12	0	0
2	2	16	0	12	0	0
2	3	16	0	12	0	0
2	4	16	0	12	0	0
2	5	16	0	12	0	0
2	6	16	0	12	0	0
2	7	16	0	12	0	0
2	8	16	0	12	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0	0
3	2	21	0	12	0	0
3	3	21	0	12	0	0
3	4	21	0	12	0	0
3	5	21	0	12	0	0
3	6	21	0	12	0	0
3	7	21	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8	21	0	12	0	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
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
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	250920	0	235860	5698	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 12.

All (5698) 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)
1:4:526:MET:HE2	1:4:575:ALA:HA	1.58	0.86
1:N:526:MET:HE2	1:N:575:ALA:HA	1.63	0.85
1:H:526:MET:HE2	1:H:575:ALA:HA	1.59	0.85
1:S:526:MET:HE2	1:S:575:ALA:HA	1.61	0.84
1:C:526:MET:HE2	1:C:575:ALA:HA	1.61	0.84
1:K:526:MET:HE2	1:K:575:ALA:HA	1.62	0.84
1:L:526:MET:HE2	1:L:575:ALA:HA	1.61	0.84
1:T:526:MET:HE2	1:T:575:ALA:HA	1.59	0.84
1:Z:526:MET:HE2	1:Z:575:ALA:HA	1.62	0.84
1:R:526:MET:HE2	1:R:575:ALA:HA	1.59	0.84
1:I:526:MET:HE2	1:I:575:ALA:HA	1.63	0.83
1:G:526:MET:HE2	1:G:575:ALA:HA	1.60	0.83
1:W:526:MET:HE2	1:W:575:ALA:HA	1.60	0.83
1:Q:526:MET:HE2	1:Q:575:ALA:HA	1.61	0.83
1:X:526:MET:HE2	1:X:575:ALA:HA	1.60	0.83
1:P:526:MET:HE2	1:P:575:ALA:HA	1.61	0.83
1:V:526:MET:HE2	1:V:575:ALA:HA	1.60	0.83
1:J:328:GLN:HE22	1:J:333:LYS:HG3	1.44	0.83
1:1:328:GLN:HE22	1:1:333:LYS:HG3	1.44	0.83
1:M:328:GLN:HE22	1:M:333:LYS:HG3	1.44	0.83
1:T:328:GLN:HE22	1:T:333:LYS:HG3	1.44	0.83
1:H:328:GLN:HE22	1:H:333:LYS:HG3	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:328:GLN:HE22	1:4:333:LYS:HG3	1.44	0.82
1:7:526:MET:HE2	1:7:575:ALA:HA	1.61	0.82
1:D:328:GLN:HE22	1:D:333:LYS:HG3	1.44	0.82
1:G:328:GLN:HE22	1:G:333:LYS:HG3	1.44	0.82
1:K:328:GLN:HE22	1:K:333:LYS:HG3	1.44	0.82
1:N:328:GLN:HE22	1:N:333:LYS:HG3	1.44	0.82
1:O:328:GLN:HE22	1:O:333:LYS:HG3	1.44	0.82
1:3:328:GLN:HE22	1:3:333:LYS:HG3	1.44	0.82
1:E:526:MET:HE2	1:E:575:ALA:HA	1.61	0.82
1:S:328:GLN:HE22	1:S:333:LYS:HG3	1.44	0.82
1:2:225:SER:HB3	1:3:407:ARG:HG3	1.61	0.82
1:C:328:GLN:HE22	1:C:333:LYS:HG3	1.44	0.82
1:I:328:GLN:HE22	1:I:333:LYS:HG3	1.44	0.82
1:L:328:GLN:HE22	1:L:333:LYS:HG3	1.44	0.82
1:R:328:GLN:HE22	1:R:333:LYS:HG3	1.44	0.82
1:Z:328:GLN:HE22	1:Z:333:LYS:HG3	1.44	0.82
1:2:225:SER:HA	1:3:407:ARG:HD2	1.61	0.82
1:6:328:GLN:HE22	1:6:333:LYS:HG3	1.44	0.82
1:6:526:MET:HE2	1:6:575:ALA:HA	1.61	0.82
1:Y:526:MET:HE2	1:Y:575:ALA:HA	1.60	0.82
1:F:526:MET:HE2	1:F:575:ALA:HA	1.61	0.82
1:G:225:SER:HB3	1:W:407:ARG:HG3	1.61	0.82
1:Y:328:GLN:HE22	1:Y:333:LYS:HG3	1.44	0.82
1:X:328:GLN:HE22	1:X:333:LYS:HG3	1.44	0.82
1:1:526:MET:HE2	1:1:575:ALA:HA	1.59	0.82
1:A:225:SER:HB3	1:E:407:ARG:HG3	1.61	0.82
1:F:328:GLN:HE22	1:F:333:LYS:HG3	1.44	0.82
1:E:407:ARG:HG3	1:U:225:SER:HB3	144.71	0.82
1:T:225:SER:HB3	1:6:407:ARG:HG3	164.64	0.81
1:8:328:GLN:HE22	1:8:333:LYS:HG3	1.44	0.81
1:8:526:MET:HE2	1:8:575:ALA:HA	1.60	0.81
1:A:328:GLN:HE22	1:A:333:LYS:HG3	1.44	0.81
1:O:526:MET:HE2	1:O:575:ALA:HA	1.59	0.81
1:P:328:GLN:HE22	1:P:333:LYS:HG3	1.44	0.81
1:F:407:ARG:HG3	1:R:225:SER:HB3	1.62	0.81
1:U:526:MET:HE2	1:U:575:ALA:HA	1.62	0.81
1:G:407:ARG:HG3	1:K:225:SER:HB3	144.01	0.81
1:M:225:SER:HB3	1:N:407:ARG:HG3	1.62	0.81
1:K:407:ARG:HG3	1:7:225:SER:HB3	1.62	0.81
1:A:407:ARG:HG3	1:J:225:SER:HB3	85.06	0.81
1:D:526:MET:HE2	1:D:575:ALA:HA	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:ARG:HG3	1:E:225:SER:HB3	1.63	0.81
1:J:407:ARG:HG3	1:L:225:SER:HB3	89.45	0.81
1:G:225:SER:HA	1:W:407:ARG:HD2	1.61	0.81
1:P:407:ARG:HD2	1:6:225:SER:HA	153.19	0.81
1:Y:225:SER:HB3	1:4:407:ARG:HG3	1.62	0.81
1:2:526:MET:HE2	1:2:575:ALA:HA	1.61	0.81
1:A:225:SER:HA	1:E:407:ARG:HD2	1.61	0.81
1:H:407:ARG:HG3	1:Z:225:SER:HB3	1.62	0.81
1:5:328:GLN:HE22	1:5:333:LYS:HG3	1.44	0.81
1:M:225:SER:HB3	1:S:407:ARG:HG3	101.95	0.81
1:V:225:SER:HB3	1:W:407:ARG:HG3	26.31	0.81
1:F:407:ARG:HG3	1:Z:225:SER:HB3	102.08	0.81
1:V:328:GLN:HE22	1:V:333:LYS:HG3	1.44	0.81
1:G:225:SER:HB3	1:1:407:ARG:HG3	153.11	0.81
1:2:328:GLN:HE22	1:2:333:LYS:HG3	1.44	0.81
1:C:407:ARG:HD2	1:D:225:SER:HA	1.63	0.81
1:H:225:SER:HB3	1:I:407:ARG:HG3	1.63	0.81
1:J:407:ARG:HD2	1:L:225:SER:HA	89.28	0.81
1:K:225:SER:HA	1:L:407:ARG:HD2	1.63	0.81
1:Q:328:GLN:HE22	1:Q:333:LYS:HG3	1.44	0.81
1:U:328:GLN:HE22	1:U:333:LYS:HG3	1.44	0.81
1:V:407:ARG:HG3	1:W:225:SER:HB3	1.62	0.81
1:A:526:MET:HE2	1:A:575:ALA:HA	1.64	0.81
1:G:407:ARG:HD2	1:K:225:SER:HA	145.51	0.81
1:L:407:ARG:HG3	1:N:225:SER:HB3	115.51	0.81
1:N:407:ARG:HG3	1:R:225:SER:HB3	144.01	0.81
1:Y:225:SER:HA	1:4:407:ARG:HD2	1.63	0.81
1:T:225:SER:HA	1:6:407:ARG:HD2	161.41	0.81
1:B:526:MET:HE2	1:B:575:ALA:HA	1.69	0.81
1:D:225:SER:HB3	1:O:407:ARG:HG3	102.80	0.81
1:G:225:SER:HA	1:1:407:ARG:HD2	153.20	0.81
1:Q:225:SER:HB3	1:Y:407:ARG:HG3	144.71	0.81
1:3:225:SER:HA	1:8:407:ARG:HD2	1.63	0.80
1:3:526:MET:HE2	1:3:575:ALA:HA	1.60	0.80
1:B:407:ARG:HD2	1:C:225:SER:HA	1.63	0.80
1:H:407:ARG:HD2	1:Z:225:SER:HA	1.62	0.80
1:L:407:ARG:HD2	1:N:225:SER:HA	113.06	0.80
1:T:407:ARG:HG3	1:Y:225:SER:HB3	118.17	0.80
1:N:407:ARG:HD2	1:R:225:SER:HA	145.50	0.80
1:P:225:SER:HB3	1:Q:407:ARG:HG3	1.63	0.80
1:T:407:ARG:HD2	1:Y:225:SER:HA	114.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:407:ARG:HG3	1:4:225:SER:HB3	89.45	0.80
1:B:407:ARG:HD2	1:L:225:SER:HA	74.92	0.80
1:F:407:ARG:HD2	1:R:225:SER:HA	1.63	0.80
1:I:225:SER:HA	1:T:407:ARG:HD2	164.39	0.80
1:I:225:SER:HB3	1:T:407:ARG:HG3	166.98	0.80
1:O:225:SER:HA	1:P:407:ARG:HD2	1.63	0.80
1:R:407:ARG:HD2	1:V:225:SER:HA	1.63	0.80
1:R:407:ARG:HG3	1:V:225:SER:HB3	1.63	0.80
1:W:328:GLN:HE22	1:W:333:LYS:HG3	1.44	0.80
1:F:407:ARG:HD2	1:Z:225:SER:HA	102.78	0.80
1:Z:407:ARG:HD2	1:4:225:SER:HA	89.29	0.80
1:5:526:MET:HE2	1:5:575:ALA:HA	1.60	0.80
1:D:225:SER:HA	1:O:407:ARG:HD2	101.00	0.80
1:F:225:SER:HA	1:G:407:ARG:HD2	1.63	0.80
1:U:225:SER:HA	1:2:407:ARG:HD2	154.12	0.80
1:O:225:SER:HB3	1:7:407:ARG:HG3	153.66	0.80
1:3:225:SER:HB3	1:8:407:ARG:HG3	1.62	0.80
1:E:328:GLN:HE22	1:E:333:LYS:HG3	1.44	0.80
1:H:225:SER:HA	1:I:407:ARG:HD2	1.63	0.80
1:M:225:SER:HA	1:S:407:ARG:HD2	101.38	0.80
1:V:407:ARG:HD2	1:W:225:SER:HA	1.63	0.80
1:Q:225:SER:HA	1:Y:407:ARG:HD2	145.00	0.80
1:K:407:ARG:HD2	1:7:225:SER:HA	1.62	0.80
1:A:407:ARG:HD2	1:J:225:SER:HA	83.68	0.80
1:C:407:ARG:HG3	1:D:225:SER:HB3	1.63	0.80
1:E:225:SER:HA	1:H:407:ARG:HD2	113.06	0.80
1:T:225:SER:HB3	1:U:407:ARG:HG3	1.63	0.80
1:U:225:SER:HB3	1:2:407:ARG:HG3	153.29	0.80
1:V:407:ARG:HG3	1:1:225:SER:HB3	154.35	0.80
1:D:407:ARG:HD2	1:E:225:SER:HA	1.63	0.80
1:K:225:SER:HB3	1:L:407:ARG:HG3	1.63	0.80
1:M:407:ARG:HG3	1:N:225:SER:HB3	26.31	0.80
1:O:225:SER:HA	1:7:407:ARG:HD2	152.54	0.80
1:P:225:SER:HA	1:Q:407:ARG:HD2	1.63	0.80
1:X:225:SER:HA	1:Y:407:ARG:HD2	1.63	0.80
1:X:225:SER:HB3	1:Y:407:ARG:HG3	1.62	0.80
1:B:328:GLN:HE22	1:B:333:LYS:HG3	1.44	0.80
1:B:407:ARG:HG3	1:C:225:SER:HB3	1.63	0.80
1:I:225:SER:HB3	1:J:407:ARG:HG3	1.63	0.80
1:O:225:SER:HB3	1:P:407:ARG:HG3	1.63	0.80
1:F:225:SER:HA	1:X:407:ARG:HD2	103.73	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:407:ARG:HG3	1:6:225:SER:HB3	153.10	0.80
1:K:407:ARG:HD2	1:W:225:SER:HA	159.35	0.80
1:B:407:ARG:HG3	1:L:225:SER:HB3	73.41	0.80
1:M:407:ARG:HD2	1:N:225:SER:HA	23.60	0.80
1:M:225:SER:HA	1:N:407:ARG:HD2	1.63	0.80
1:E:407:ARG:HD2	1:U:225:SER:HA	144.79	0.80
1:7:328:GLN:HE22	1:7:333:LYS:HG3	1.44	0.79
1:J:225:SER:HA	1:X:407:ARG:HD2	114.04	0.79
1:M:526:MET:HE2	1:M:575:ALA:HA	1.65	0.79
1:Q:225:SER:HB3	1:S:407:ARG:HG3	1.62	0.79
1:C:225:SER:HA	1:M:407:ARG:HD2	89.28	0.79
1:C:225:SER:HB3	1:M:407:ARG:HG3	89.45	0.79
1:I:225:SER:HA	1:J:407:ARG:HD2	1.63	0.79
1:T:225:SER:HA	1:U:407:ARG:HD2	1.63	0.79
1:V:407:ARG:HD2	1:1:225:SER:HA	153.02	0.79
1:A:225:SER:HB3	1:Z:407:ARG:HG3	106.72	0.79
1:R:407:ARG:HD2	1:X:225:SER:HA	83.07	0.79
1:1:431:GLN:HE22	1:2:354:PRO:HB3	1.48	0.79
1:U:407:ARG:HG3	1:5:225:SER:HB3	165.58	0.79
1:R:407:ARG:HG3	1:X:225:SER:HB3	84.23	0.79
1:A:225:SER:HA	1:Z:407:ARG:HD2	103.02	0.79
1:V:225:SER:HA	1:W:407:ARG:HD2	23.60	0.79
1:B:225:SER:HA	1:O:407:ARG:HD2	114.04	0.79
1:F:225:SER:HB3	1:G:407:ARG:HG3	1.63	0.79
1:Q:225:SER:HA	1:S:407:ARG:HD2	1.62	0.79
1:B:225:SER:HB3	1:O:407:ARG:HG3	115.11	0.79
1:D:407:ARG:HG3	1:S:225:SER:HB3	97.64	0.79
1:D:407:ARG:HD2	1:S:225:SER:HA	96.09	0.79
1:J:225:SER:HB3	1:X:407:ARG:HG3	115.11	0.79
1:J:526:MET:HE2	1:J:575:ALA:HA	1.64	0.79
1:C:407:ARG:HD2	1:S:225:SER:HA	104.26	0.79
1:5:407:ARG:HG3	1:8:225:SER:HB3	1.63	0.79
1:A:407:ARG:HD2	1:B:225:SER:HA	1.63	0.79
1:A:407:ARG:HG3	1:B:225:SER:HB3	1.63	0.79
1:C:407:ARG:HG3	1:S:225:SER:HB3	107.75	0.78
1:F:354:PRO:HB3	1:G:431:GLN:HE22	93.79	0.78
1:T:431:GLN:HE22	1:U:354:PRO:HB3	48.32	0.78
1:F:225:SER:HB3	1:X:407:ARG:HG3	103.10	0.78
1:3:354:PRO:HB3	1:4:431:GLN:HE22	1.49	0.78
1:U:407:ARG:HD2	1:5:225:SER:HA	164.45	0.78
1:5:407:ARG:HD2	1:8:225:SER:HA	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:431:GLN:HE22	1:N:354:PRO:HB3	48.31	0.78
1:N:431:GLN:HE22	1:O:354:PRO:HB3	49.98	0.78
1:Z:354:PRO:HB3	1:2:431:GLN:HE22	83.36	0.78
1:5:354:PRO:HB3	1:7:431:GLN:HE22	1.49	0.78
1:E:225:SER:HB3	1:H:407:ARG:HG3	115.50	0.78
1:O:431:GLN:HE22	1:P:354:PRO:HB3	48.31	0.78
1:O:610:GLN:HE21	1:P:627:THR:HG22	44.67	0.78
1:6:610:GLN:HE21	1:7:627:THR:HG22	1.49	0.78
1:E:431:GLN:HE22	1:Q:354:PRO:HB3	1.49	0.78
1:I:431:GLN:HE22	1:J:354:PRO:HB3	48.31	0.78
1:D:610:GLN:HE21	1:N:627:THR:HG22	1.49	0.78
1:R:431:GLN:HE22	1:S:354:PRO:HB3	1.49	0.78
1:B:610:GLN:HE21	1:M:627:THR:HG22	98.17	0.78
1:D:627:THR:HG22	1:P:610:GLN:HE21	1.49	0.78
1:F:354:PRO:HB3	1:Q:431:GLN:HE22	1.48	0.78
1:G:431:GLN:HE22	1:I:354:PRO:HB3	1.47	0.78
1:B:610:GLN:HE21	1:J:627:THR:HG22	1.49	0.78
1:K:627:THR:HG22	1:8:610:GLN:HE21	1.49	0.78
1:D:354:PRO:HB3	1:T:431:GLN:HE22	115.34	0.78
1:Z:431:GLN:HE22	1:4:354:PRO:HB3	1.49	0.78
1:A:627:THR:HG22	1:K:610:GLN:HE21	98.77	0.78
1:L:431:GLN:HE22	1:T:354:PRO:HB3	195.41	0.78
1:M:610:GLN:HE21	1:N:627:THR:HG22	44.67	0.78
1:E:610:GLN:HE21	1:X:627:THR:HG22	142.62	0.78
1:E:627:THR:HG22	1:F:610:GLN:HE21	1.49	0.78
1:A:431:GLN:HE22	1:G:354:PRO:HB3	1.48	0.78
1:K:407:ARG:HG3	1:W:225:SER:HB3	160.80	0.78
1:5:627:THR:HG22	1:7:610:GLN:HE21	1.49	0.78
1:M:354:PRO:HB3	1:O:431:GLN:HE22	80.94	0.78
1:V:627:THR:HG22	1:X:610:GLN:NE2	1.99	0.78
1:Z:610:GLN:HE21	1:4:627:THR:HG22	1.49	0.78
1:5:431:GLN:HE22	1:6:354:PRO:HB3	1.49	0.78
1:5:627:THR:HG22	1:7:610:GLN:NE2	1.99	0.78
1:F:627:THR:HG22	1:Q:610:GLN:HE21	1.49	0.78
1:E:610:GLN:HE21	1:Q:627:THR:HG22	1.49	0.78
1:E:610:GLN:NE2	1:Q:627:THR:HG22	1.99	0.78
1:X:610:GLN:NE2	1:Y:627:THR:HG22	44.09	0.78
1:1:610:GLN:HE21	1:2:627:THR:HG22	1.48	0.77
1:D:610:GLN:NE2	1:L:627:THR:HG22	119.95	0.77
1:A:610:GLN:HE21	1:G:627:THR:HG22	1.49	0.77
1:B:431:GLN:HE22	1:J:354:PRO:HB3	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:354:PRO:HB3	1:8:431:GLN:HE22	1.49	0.77
1:M:610:GLN:NE2	1:N:627:THR:HG22	44.09	0.77
1:T:610:GLN:HE21	1:U:627:THR:HG22	44.68	0.77
1:Z:431:GLN:HE22	1:1:354:PRO:HB3	94.97	0.77
1:Z:627:THR:HG22	1:2:610:GLN:NE2	71.50	0.77
1:Z:610:GLN:NE2	1:4:627:THR:HG22	2.00	0.77
1:B:627:THR:HG22	1:C:610:GLN:HE21	44.68	0.77
1:D:431:GLN:HE22	1:L:354:PRO:HB3	123.42	0.77
1:F:627:THR:HG22	1:Q:610:GLN:NE2	2.00	0.77
1:K:627:THR:HG22	1:8:610:GLN:NE2	1.99	0.77
1:W:610:GLN:HE21	1:X:627:THR:HG22	62.51	0.77
1:E:431:GLN:HE22	1:X:354:PRO:HB3	152.93	0.77
1:Z:354:PRO:HB3	1:3:431:GLN:HE22	1.49	0.77
1:B:431:GLN:HE22	1:M:354:PRO:HB3	121.72	0.77
1:H:354:PRO:HB3	1:Y:431:GLN:HE22	1.49	0.77
1:C:431:GLN:HE22	1:O:354:PRO:HB3	152.48	0.77
1:C:610:GLN:NE2	1:O:627:THR:HG22	141.54	0.77
1:R:610:GLN:HE21	1:S:627:THR:HG22	1.49	0.77
1:X:431:GLN:HE22	1:Y:354:PRO:HB3	48.31	0.77
1:V:627:THR:HG22	1:X:610:GLN:HE21	1.49	0.77
1:5:610:GLN:HE21	1:6:627:THR:HG22	1.49	0.77
1:B:354:PRO:HB3	1:L:431:GLN:HE22	1.49	0.77
1:C:627:THR:HG22	1:M:610:GLN:HE21	1.49	0.77
1:D:354:PRO:HB3	1:P:431:GLN:HE22	1.49	0.77
1:D:627:THR:HG22	1:P:610:GLN:NE2	1.99	0.77
1:F:627:THR:HG22	1:G:610:GLN:NE2	86.33	0.77
1:L:610:GLN:HE21	1:T:627:THR:HG22	194.98	0.77
1:N:431:GLN:HE22	1:P:354:PRO:HB3	1.49	0.77
1:C:354:PRO:HB3	1:P:431:GLN:HE22	50.13	0.77
1:W:431:GLN:HE22	1:Y:354:PRO:HB3	1.49	0.77
1:5:610:GLN:NE2	1:6:627:THR:HG22	2.00	0.77
1:6:610:GLN:NE2	1:7:627:THR:HG22	2.00	0.77
1:B:627:THR:HG22	1:L:610:GLN:HE21	1.49	0.77
1:C:354:PRO:HB3	1:M:431:GLN:HE22	1.49	0.77
1:B:627:THR:HG22	1:C:610:GLN:NE2	44.09	0.77
1:F:627:THR:HG22	1:G:610:GLN:HE21	86.91	0.77
1:G:627:THR:HG22	1:H:610:GLN:HE21	62.51	0.77
1:H:627:THR:HG22	1:Y:610:GLN:NE2	2.00	0.77
1:J:610:GLN:HE21	1:L:627:THR:HG22	1.49	0.77
1:O:610:GLN:NE2	1:P:627:THR:HG22	44.09	0.77
1:R:627:THR:HG22	1:U:610:GLN:HE21	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:610:GLN:HE21	1:Y:627:THR:HG22	1.49	0.77
1:X:610:GLN:HE21	1:Y:627:THR:HG22	44.67	0.77
1:Z:627:THR:HG22	1:2:610:GLN:HE21	72.12	0.77
1:Z:610:GLN:HE21	1:1:627:THR:HG22	88.91	0.77
1:A:431:GLN:HE22	1:8:354:PRO:HB3	151.45	0.77
1:B:610:GLN:NE2	1:M:627:THR:HG22	97.75	0.77
1:D:610:GLN:HE21	1:L:627:THR:HG22	120.76	0.77
1:E:627:THR:HG22	1:F:610:GLN:NE2	1.99	0.77
1:J:610:GLN:NE2	1:K:627:THR:HG22	62.15	0.77
1:B:610:GLN:NE2	1:J:627:THR:HG22	2.00	0.77
1:I:610:GLN:NE2	1:J:627:THR:HG22	44.09	0.77
1:Q:431:GLN:HE22	1:R:354:PRO:HB3	49.98	0.77
1:R:610:GLN:NE2	1:S:627:THR:HG22	2.00	0.77
1:Q:610:GLN:HE21	1:R:627:THR:HG22	62.51	0.77
1:S:431:GLN:HE22	1:U:354:PRO:HB3	1.48	0.77
1:W:431:GLN:HE22	1:X:354:PRO:HB3	49.98	0.77
1:V:354:PRO:HB3	1:X:431:GLN:HE22	1.49	0.77
1:B:627:THR:HG22	1:L:610:GLN:NE2	2.00	0.77
1:B:354:PRO:HB3	1:C:431:GLN:HE22	48.31	0.77
1:C:627:THR:HG22	1:M:610:GLN:NE2	1.99	0.77
1:G:354:PRO:HB3	1:H:431:GLN:HE22	49.99	0.77
1:G:627:THR:HG22	1:H:610:GLN:NE2	62.15	0.77
1:J:610:GLN:NE2	1:L:627:THR:HG22	1.99	0.77
1:N:610:GLN:HE21	1:P:627:THR:HG22	1.49	0.77
1:C:627:THR:HG22	1:P:610:GLN:NE2	64.27	0.77
1:G:610:GLN:NE2	1:I:627:THR:HG22	2.00	0.77
1:J:431:GLN:HE22	1:L:354:PRO:HB3	1.49	0.77
1:I:627:THR:HG22	1:K:610:GLN:HE21	101.90	0.77
1:T:354:PRO:HB3	1:V:431:GLN:HE22	80.94	0.77
1:T:627:THR:HG22	1:V:610:GLN:HE21	101.90	0.77
1:E:610:GLN:NE2	1:X:627:THR:HG22	142.70	0.77
1:A:610:GLN:NE2	1:8:627:THR:HG22	135.50	0.77
1:A:610:GLN:HE21	1:8:627:THR:HG22	135.65	0.77
1:E:627:THR:HG22	1:V:610:GLN:NE2	115.82	0.77
1:F:610:GLN:NE2	1:H:627:THR:HG22	119.95	0.77
1:D:431:GLN:HE22	1:N:354:PRO:HB3	1.49	0.77
1:Q:627:THR:HG22	1:S:610:GLN:NE2	86.33	0.77
1:R:354:PRO:HB3	1:U:431:GLN:HE22	1.49	0.77
1:U:610:GLN:HE21	1:V:627:THR:HG22	62.51	0.77
1:S:610:GLN:HE21	1:U:627:THR:HG22	1.49	0.77
1:H:610:GLN:NE2	1:W:627:THR:HG22	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:627:THR:HG22	1:Y:610:GLN:NE2	29.60	0.77
1:A:354:PRO:HB3	1:K:431:GLN:HE22	95.76	0.77
1:J:610:GLN:HE21	1:K:627:THR:HG22	62.51	0.77
1:I:610:GLN:HE21	1:J:627:THR:HG22	44.67	0.77
1:I:354:PRO:HB3	1:K:431:GLN:HE22	80.94	0.77
1:I:627:THR:HG22	1:K:610:GLN:NE2	101.86	0.77
1:N:610:GLN:NE2	1:P:627:THR:HG22	1.99	0.77
1:Q:610:GLN:NE2	1:R:627:THR:HG22	62.15	0.77
1:Q:354:PRO:HB3	1:S:431:GLN:HE22	93.79	0.77
1:T:610:GLN:NE2	1:U:627:THR:HG22	44.10	0.77
1:S:610:GLN:NE2	1:U:627:THR:HG22	1.99	0.77
1:W:610:GLN:NE2	1:X:627:THR:HG22	62.15	0.77
1:W:610:GLN:NE2	1:Y:627:THR:HG22	1.99	0.77
1:3:627:THR:HG22	1:4:610:GLN:NE2	2.00	0.76
1:F:610:GLN:HE21	1:H:627:THR:HG22	120.76	0.76
1:N:610:GLN:NE2	1:O:627:THR:HG22	62.15	0.76
1:T:627:THR:HG22	1:V:610:GLN:NE2	101.86	0.76
1:W:354:PRO:HB3	1:Y:431:GLN:HE22	47.34	0.76
1:A:627:THR:HG22	1:I:610:GLN:NE2	2.00	0.76
1:Q:627:THR:HG22	1:S:610:GLN:HE21	86.91	0.76
1:U:431:GLN:HE22	1:V:354:PRO:HB3	49.98	0.76
1:R:627:THR:HG22	1:U:610:GLN:NE2	1.99	0.76
1:H:431:GLN:HE22	1:W:354:PRO:HB3	1.49	0.76
1:E:354:PRO:HB3	1:V:431:GLN:HE22	134.56	0.76
1:A:610:GLN:NE2	1:G:627:THR:HG22	2.00	0.76
1:L:610:GLN:NE2	1:T:627:THR:HG22	194.63	0.76
1:D:610:GLN:NE2	1:N:627:THR:HG22	1.99	0.76
1:D:627:THR:HG22	1:T:610:GLN:HE21	115.79	0.76
1:Z:627:THR:HG22	1:3:610:GLN:HE21	1.49	0.76
1:Z:627:THR:HG22	1:3:610:GLN:NE2	1.99	0.76
1:H:627:THR:HG22	1:Y:610:GLN:HE21	1.49	0.76
1:J:431:GLN:HE22	1:K:354:PRO:HB3	49.98	0.76
1:1:610:GLN:NE2	1:2:627:THR:HG22	1.99	0.76
1:A:627:THR:HG22	1:K:610:GLN:NE2	98.54	0.76
1:M:627:THR:HG22	1:O:610:GLN:HE21	101.90	0.76
1:M:627:THR:HG22	1:O:610:GLN:NE2	101.86	0.76
1:U:610:GLN:NE2	1:V:627:THR:HG22	62.15	0.76
1:Z:610:GLN:NE2	1:1:627:THR:HG22	89.34	0.76
1:C:610:GLN:HE21	1:O:627:THR:HG22	141.85	0.76
1:G:343:ILE:HD12	1:G:651:ILE:HD11	1.68	0.76
1:M:343:ILE:HD12	1:M:651:ILE:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:343:ILE:HD12	1:2:651:ILE:HD11	1.68	0.76
1:3:627:THR:HG22	1:4:610:GLN:HE21	1.49	0.76
1:D:343:ILE:HD12	1:D:651:ILE:HD11	1.68	0.76
1:J:343:ILE:HD12	1:J:651:ILE:HD11	1.68	0.76
1:R:343:ILE:HD12	1:R:651:ILE:HD11	1.68	0.76
1:S:343:ILE:HD12	1:S:651:ILE:HD11	1.68	0.76
1:U:343:ILE:HD12	1:U:651:ILE:HD11	1.68	0.76
1:Y:343:ILE:HD12	1:Y:651:ILE:HD11	1.68	0.76
1:W:627:THR:HG22	1:Y:610:GLN:HE21	29.18	0.76
1:E:627:THR:HG22	1:V:610:GLN:HE21	116.67	0.76
1:N:610:GLN:HE21	1:O:627:THR:HG22	62.51	0.76
1:P:343:ILE:HD12	1:P:651:ILE:HD11	1.68	0.76
1:H:610:GLN:HE21	1:W:627:THR:HG22	1.49	0.76
1:F:343:ILE:HD12	1:F:651:ILE:HD11	1.68	0.76
1:F:431:GLN:HE22	1:H:354:PRO:HB3	123.41	0.76
1:D:627:THR:HG22	1:T:610:GLN:NE2	115.94	0.76
1:Z:343:ILE:HD12	1:Z:651:ILE:HD11	1.68	0.76
1:6:343:ILE:HD12	1:6:651:ILE:HD11	1.68	0.75
1:6:431:GLN:HE22	1:7:354:PRO:HB3	1.48	0.75
1:A:354:PRO:HB3	1:I:431:GLN:HE22	1.50	0.75
1:E:343:ILE:HD12	1:E:651:ILE:HD11	1.68	0.75
1:W:343:ILE:HD12	1:W:651:ILE:HD11	1.68	0.75
1:E:354:PRO:HB3	1:F:431:GLN:HE22	1.49	0.75
1:K:343:ILE:HD12	1:K:651:ILE:HD11	1.68	0.75
1:O:343:ILE:HD12	1:O:651:ILE:HD11	1.68	0.75
1:T:343:ILE:HD12	1:T:651:ILE:HD11	1.68	0.75
1:1:343:ILE:HD12	1:1:651:ILE:HD11	1.68	0.75
1:5:343:ILE:HD12	1:5:651:ILE:HD11	1.68	0.75
1:A:343:ILE:HD12	1:A:651:ILE:HD11	1.68	0.75
1:I:343:ILE:HD12	1:I:651:ILE:HD11	1.68	0.75
1:Q:343:ILE:HD12	1:Q:651:ILE:HD11	1.68	0.75
1:3:343:ILE:HD12	1:3:651:ILE:HD11	1.68	0.75
1:B:343:ILE:HD12	1:B:651:ILE:HD11	1.68	0.75
1:G:610:GLN:HE21	1:I:627:THR:HG22	1.49	0.75
1:X:343:ILE:HD12	1:X:651:ILE:HD11	1.68	0.75
1:C:627:THR:HG22	1:P:610:GLN:HE21	63.75	0.74
1:A:627:THR:HG22	1:I:610:GLN:HE21	1.51	0.74
1:N:343:ILE:HD12	1:N:651:ILE:HD11	1.68	0.74
1:C:343:ILE:HD12	1:C:651:ILE:HD11	1.68	0.74
1:L:343:ILE:HD12	1:L:651:ILE:HD11	1.68	0.74
1:7:343:ILE:HD12	1:7:651:ILE:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:343:ILE:HD12	1:H:651:ILE:HD11	1.68	0.74
1:V:343:ILE:HD12	1:V:651:ILE:HD11	1.68	0.74
1:8:343:ILE:HD12	1:8:651:ILE:HD11	1.68	0.73
1:4:343:ILE:HD12	1:4:651:ILE:HD11	1.68	0.73
1:A:298:ASP:OD2	1:E:400:TYR:OH	2.09	0.71
1:A:473:MET:HE1	1:G:275:TYR:HB3	1.74	0.70
1:1:568:ILE:HD12	1:1:572:ASN:HD22	1.57	0.69
1:6:556:ASP:OD1	1:6:557:TYR:N	2.26	0.69
1:N:499:ASN:OD1	1:N:500:ASN:N	2.26	0.69
1:P:568:ILE:HD12	1:P:572:ASN:HD22	1.58	0.69
1:T:298:ASP:OD2	1:6:400:TYR:OH	179.55	0.69
1:V:400:TYR:OH	1:W:298:ASP:OD2	2.11	0.69
1:4:499:ASN:OD1	1:4:500:ASN:N	2.26	0.69
1:G:499:ASN:OD1	1:G:500:ASN:N	2.26	0.69
1:G:568:ILE:HD12	1:G:572:ASN:HD22	1.58	0.69
1:H:568:ILE:HD12	1:H:572:ASN:HD22	1.58	0.69
1:I:499:ASN:OD1	1:I:500:ASN:N	2.26	0.69
1:K:568:ILE:HD12	1:K:572:ASN:HD22	1.58	0.69
1:J:400:TYR:OH	1:L:298:ASP:OD2	72.05	0.69
1:T:568:ILE:HD12	1:T:572:ASN:HD22	1.58	0.69
1:X:499:ASN:OD1	1:X:500:ASN:N	2.26	0.69
1:5:400:TYR:OH	1:8:298:ASP:OD2	2.11	0.69
1:K:275:TYR:HB3	1:8:473:MET:HE1	1.75	0.69
1:F:556:ASP:OD1	1:F:557:TYR:N	2.26	0.69
1:H:718:ASN:HD21	1:H:722:THR:HB	1.58	0.69
1:L:499:ASN:OD1	1:L:500:ASN:N	2.26	0.69
1:R:568:ILE:HD12	1:R:572:ASN:HD22	1.58	0.69
1:X:718:ASN:HD21	1:X:722:THR:HB	1.58	0.69
1:Y:568:ILE:HD12	1:Y:572:ASN:HD22	1.58	0.69
1:Z:499:ASN:OD1	1:Z:500:ASN:N	2.26	0.69
1:7:568:ILE:HD12	1:7:572:ASN:HD22	1.58	0.69
1:8:556:ASP:OD1	1:8:557:TYR:N	2.26	0.69
1:A:499:ASN:OD1	1:A:500:ASN:N	2.26	0.69
1:A:556:ASP:OD1	1:A:557:TYR:N	2.26	0.69
1:D:499:ASN:OD1	1:D:500:ASN:N	2.26	0.69
1:D:556:ASP:OD1	1:D:557:TYR:N	2.26	0.69
1:E:298:ASP:OD2	1:H:400:TYR:OH	145.83	0.69
1:E:568:ILE:HD12	1:E:572:ASN:HD22	1.58	0.69
1:E:718:ASN:HD21	1:E:722:THR:HB	1.58	0.69
1:J:556:ASP:OD1	1:J:557:TYR:N	2.26	0.69
1:K:499:ASN:OD1	1:K:500:ASN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:556:ASP:OD1	1:L:557:TYR:N	2.26	0.69
1:M:499:ASN:OD1	1:M:500:ASN:N	2.26	0.69
1:D:275:TYR:HB3	1:P:473:MET:HE1	1.74	0.69
1:Q:298:ASP:OD2	1:S:400:TYR:OH	2.11	0.69
1:Q:298:ASP:OD2	1:Y:400:TYR:OH	118.77	0.69
1:P:298:ASP:OD2	1:Q:400:TYR:OH	2.11	0.69
1:R:556:ASP:OD1	1:R:557:TYR:N	2.26	0.69
1:T:400:TYR:OH	1:Y:298:ASP:OD2	153.50	0.69
1:T:556:ASP:OD1	1:T:557:TYR:N	2.26	0.69
1:Z:568:ILE:HD12	1:Z:572:ASN:HD22	1.58	0.69
1:2:298:ASP:OD2	1:3:400:TYR:OH	2.10	0.69
1:2:556:ASP:OD1	1:2:557:TYR:N	2.26	0.69
1:7:718:ASN:HD21	1:7:722:THR:HB	1.58	0.69
1:8:499:ASN:OD1	1:8:500:ASN:N	2.26	0.69
1:B:400:TYR:OH	1:L:298:ASP:OD2	27.81	0.69
1:D:568:ILE:HD12	1:D:572:ASN:HD22	1.58	0.69
1:F:400:TYR:OH	1:R:298:ASP:OD2	2.11	0.69
1:H:556:ASP:OD1	1:H:557:TYR:N	2.26	0.69
1:J:499:ASN:OD1	1:J:500:ASN:N	2.26	0.69
1:L:568:ILE:HD12	1:L:572:ASN:HD22	1.58	0.69
1:O:499:ASN:OD1	1:O:500:ASN:N	2.26	0.69
1:O:718:ASN:HD21	1:O:722:THR:HB	1.58	0.69
1:P:556:ASP:OD1	1:P:557:TYR:N	2.26	0.69
1:D:400:TYR:OH	1:S:298:ASP:OD2	98.53	0.69
1:S:568:ILE:HD12	1:S:572:ASN:HD22	1.58	0.69
1:S:718:ASN:HD21	1:S:722:THR:HB	1.58	0.69
1:X:473:MET:HE1	1:Y:275:TYR:HB3	57.04	0.69
1:Y:499:ASN:OD1	1:Y:500:ASN:N	2.26	0.69
1:U:298:ASP:OD2	1:2:400:TYR:OH	157.57	0.69
1:A:718:ASN:HD21	1:A:722:THR:HB	1.58	0.69
1:B:400:TYR:OH	1:C:298:ASP:OD2	2.11	0.69
1:C:556:ASP:OD1	1:C:557:TYR:N	2.26	0.69
1:E:400:TYR:OH	1:U:298:ASP:OD2	117.93	0.69
1:G:298:ASP:OD2	1:W:400:TYR:OH	2.10	0.69
1:H:499:ASN:OD1	1:H:500:ASN:N	2.26	0.69
1:I:718:ASN:HD21	1:I:722:THR:HB	1.58	0.69
1:M:298:ASP:OD2	1:S:400:TYR:OH	113.30	0.69
1:M:556:ASP:OD1	1:M:557:TYR:N	2.26	0.69
1:O:298:ASP:OD2	1:7:400:TYR:OH	146.55	0.69
1:O:556:ASP:OD1	1:O:557:TYR:N	2.26	0.69
1:P:499:ASN:OD1	1:P:500:ASN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:499:ASN:OD1	1:R:500:ASN:N	2.26	0.69
1:U:568:ILE:HD12	1:U:572:ASN:HD22	1.58	0.69
1:R:400:TYR:OH	1:V:298:ASP:OD2	2.11	0.69
1:F:400:TYR:OH	1:Z:298:ASP:OD2	126.53	0.69
1:7:499:ASN:OD1	1:7:500:ASN:N	2.26	0.69
1:A:568:ILE:HD12	1:A:572:ASN:HD22	1.58	0.69
1:E:499:ASN:OD1	1:E:500:ASN:N	2.26	0.69
1:G:718:ASN:HD21	1:G:722:THR:HB	1.58	0.69
1:G:473:MET:HE1	1:I:275:TYR:HB3	1.75	0.69
1:M:568:ILE:HD12	1:M:572:ASN:HD22	1.58	0.69
1:Q:718:ASN:HD21	1:Q:722:THR:HB	1.58	0.69
1:S:499:ASN:OD1	1:S:500:ASN:N	2.26	0.69
1:S:556:ASP:OD1	1:S:557:TYR:N	2.26	0.69
1:T:499:ASN:OD1	1:T:500:ASN:N	2.26	0.69
1:V:499:ASN:OD1	1:V:500:ASN:N	2.26	0.69
1:W:718:ASN:HD21	1:W:722:THR:HB	1.58	0.69
1:Z:556:ASP:OD1	1:Z:557:TYR:N	2.26	0.69
1:1:499:ASN:OD1	1:1:500:ASN:N	2.26	0.69
1:8:568:ILE:HD12	1:8:572:ASN:HD22	1.58	0.69
1:B:499:ASN:OD1	1:B:500:ASN:N	2.26	0.69
1:F:499:ASN:OD1	1:F:500:ASN:N	2.26	0.69
1:G:556:ASP:OD1	1:G:557:TYR:N	2.26	0.69
1:I:556:ASP:OD1	1:I:557:TYR:N	2.26	0.69
1:J:568:ILE:HD12	1:J:572:ASN:HD22	1.58	0.69
1:K:556:ASP:OD1	1:K:557:TYR:N	2.26	0.69
1:N:568:ILE:HD12	1:N:572:ASN:HD22	1.58	0.69
1:P:718:ASN:HD21	1:P:722:THR:HB	1.58	0.69
1:U:499:ASN:OD1	1:U:500:ASN:N	2.26	0.69
1:U:400:TYR:OH	1:5:298:ASP:OD2	182.94	0.69
1:B:568:ILE:HD12	1:B:572:ASN:HD22	1.58	0.69
1:J:473:MET:HE1	1:K:275:TYR:HB3	57.07	0.69
1:K:718:ASN:HD21	1:K:722:THR:HB	1.58	0.69
1:R:718:ASN:HD21	1:R:722:THR:HB	1.58	0.69
1:X:298:ASP:OD2	1:Y:400:TYR:OH	2.11	0.69
1:Y:718:ASN:HD21	1:Y:722:THR:HB	1.58	0.69
1:H:400:TYR:OH	1:Z:298:ASP:OD2	2.11	0.69
1:2:347:THR:HG22	1:2:649:ILE:HG13	1.76	0.68
1:2:568:ILE:HD12	1:2:572:ASN:HD22	1.58	0.68
1:3:499:ASN:OD1	1:3:500:ASN:N	2.26	0.68
1:3:718:ASN:HD21	1:3:722:THR:HB	1.58	0.68
1:B:473:MET:HE1	1:J:275:TYR:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:ASN:OD1	1:C:500:ASN:N	2.26	0.68
1:E:347:THR:HG22	1:E:649:ILE:HG13	1.76	0.68
1:R:400:TYR:OH	1:X:298:ASP:OD2	63.89	0.68
1:V:556:ASP:OD1	1:V:557:TYR:N	2.26	0.68
1:W:568:ILE:HD12	1:W:572:ASN:HD22	1.58	0.68
1:Y:258:TYR:OH	1:Y:399:GLU:OE1	2.12	0.68
1:Z:347:THR:HG22	1:Z:649:ILE:HG13	1.76	0.68
1:2:499:ASN:OD1	1:2:500:ASN:N	2.26	0.68
1:7:347:THR:HG22	1:7:649:ILE:HG13	1.76	0.68
1:D:347:THR:HG22	1:D:649:ILE:HG13	1.76	0.68
1:D:718:ASN:HD21	1:D:722:THR:HB	1.58	0.68
1:G:347:THR:HG22	1:G:649:ILE:HG13	1.76	0.68
1:K:400:TYR:OH	1:W:298:ASP:OD2	163.01	0.68
1:M:347:THR:HG22	1:M:649:ILE:HG13	1.76	0.68
1:Q:692:GLU:HG3	1:Q:734:LEU:HD13	1.76	0.68
1:U:556:ASP:OD1	1:U:557:TYR:N	2.26	0.68
1:V:298:ASP:OD2	1:W:400:TYR:OH	72.95	0.68
1:W:692:GLU:HG3	1:W:734:LEU:HD13	1.76	0.68
1:X:347:THR:HG22	1:X:649:ILE:HG13	1.76	0.68
1:1:556:ASP:OD1	1:1:557:TYR:N	2.26	0.68
1:3:347:THR:HG22	1:3:649:ILE:HG13	1.76	0.68
1:6:499:ASN:OD1	1:6:500:ASN:N	2.26	0.68
1:F:568:ILE:HD12	1:F:572:ASN:HD22	1.58	0.68
1:H:298:ASP:OD2	1:I:400:TYR:OH	2.11	0.68
1:I:347:THR:HG22	1:I:649:ILE:HG13	1.76	0.68
1:J:718:ASN:HD21	1:J:722:THR:HB	1.58	0.68
1:K:298:ASP:OD2	1:L:400:TYR:OH	2.11	0.68
1:L:347:THR:HG22	1:L:649:ILE:HG13	1.76	0.68
1:L:718:ASN:HD21	1:L:722:THR:HB	1.58	0.68
1:M:718:ASN:HD21	1:M:722:THR:HB	1.58	0.68
1:O:347:THR:HG22	1:O:649:ILE:HG13	1.76	0.68
1:Q:556:ASP:OD1	1:Q:557:TYR:N	2.26	0.68
1:U:718:ASN:HD21	1:U:722:THR:HB	1.58	0.68
1:V:275:TYR:HB3	1:X:473:MET:HE1	1.75	0.68
1:V:568:ILE:HD12	1:V:572:ASN:HD22	1.58	0.68
1:W:499:ASN:OD1	1:W:500:ASN:N	2.26	0.68
1:W:556:ASP:OD1	1:W:557:TYR:N	2.26	0.68
1:X:568:ILE:HD12	1:X:572:ASN:HD22	1.58	0.68
1:2:718:ASN:HD21	1:2:722:THR:HB	1.58	0.68
1:6:568:ILE:HD12	1:6:572:ASN:HD22	1.58	0.68
1:C:347:THR:HG22	1:C:649:ILE:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ILE:HD12	1:C:572:ASN:HD22	1.58	0.68
1:C:718:ASN:HD21	1:C:722:THR:HB	1.58	0.68
1:F:692:GLU:HG3	1:F:734:LEU:HD13	1.76	0.68
1:F:718:ASN:HD21	1:F:722:THR:HB	1.58	0.68
1:H:692:GLU:HG3	1:H:734:LEU:HD13	1.76	0.68
1:K:347:THR:HG22	1:K:649:ILE:HG13	1.76	0.68
1:K:692:GLU:HG3	1:K:734:LEU:HD13	1.76	0.68
1:L:692:GLU:HG3	1:L:734:LEU:HD13	1.76	0.68
1:C:400:TYR:OH	1:S:298:ASP:OD2	128.13	0.68
1:T:718:ASN:HD21	1:T:722:THR:HB	1.58	0.68
1:U:347:THR:HG22	1:U:649:ILE:HG13	1.76	0.68
1:V:718:ASN:HD21	1:V:722:THR:HB	1.58	0.68
1:Z:718:ASN:HD21	1:Z:722:THR:HB	1.58	0.68
1:V:400:TYR:OH	1:I:298:ASP:OD2	146.53	0.68
1:5:499:ASN:OD1	1:5:500:ASN:N	2.26	0.68
1:3:298:ASP:OD2	1:8:400:TYR:OH	2.10	0.68
1:A:692:GLU:HG3	1:A:734:LEU:HD13	1.76	0.68
1:B:556:ASP:OD1	1:B:557:TYR:N	2.26	0.68
1:C:692:GLU:HG3	1:C:734:LEU:HD13	1.76	0.68
1:E:556:ASP:OD1	1:E:557:TYR:N	2.26	0.68
1:F:347:THR:HG22	1:F:649:ILE:HG13	1.76	0.68
1:H:347:THR:HG22	1:H:649:ILE:HG13	1.76	0.68
1:M:298:ASP:OD2	1:N:400:TYR:OH	2.11	0.68
1:O:473:MET:HE1	1:P:275:TYR:HB3	57.09	0.68
1:O:692:GLU:HG3	1:O:734:LEU:HD13	1.76	0.68
1:N:473:MET:HE1	1:P:275:TYR:HB3	1.76	0.68
1:Q:499:ASN:OD1	1:Q:500:ASN:N	2.26	0.68
1:Q:347:THR:HG22	1:Q:649:ILE:HG13	1.76	0.68
1:R:473:MET:HE1	1:S:275:TYR:HB3	1.76	0.68
1:T:473:MET:HE1	1:U:275:TYR:HB3	57.16	0.68
1:W:347:THR:HG22	1:W:649:ILE:HG13	1.76	0.68
1:3:556:ASP:OD1	1:3:557:TYR:N	2.26	0.68
1:6:347:THR:HG22	1:6:649:ILE:HG13	1.76	0.68
1:6:692:GLU:HG3	1:6:734:LEU:HD13	1.76	0.68
1:7:692:GLU:HG3	1:7:734:LEU:HD13	1.76	0.68
1:8:718:ASN:HD21	1:8:722:THR:HB	1.58	0.68
1:A:400:TYR:OH	1:J:298:ASP:OD2	64.82	0.68
1:A:400:TYR:OH	1:B:298:ASP:OD2	2.11	0.68
1:C:400:TYR:OH	1:D:298:ASP:OD2	2.11	0.68
1:D:298:ASP:OD2	1:O:400:TYR:OH	111.45	0.68
1:M:692:GLU:HG3	1:M:734:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:347:THR:HG22	1:S:649:ILE:HG13	1.76	0.68
1:J:298:ASP:OD2	1:X:400:TYR:OH	153.24	0.68
1:Y:556:ASP:OD1	1:Y:557:TYR:N	2.26	0.68
1:G:298:ASP:OD2	1:1:400:TYR:OH	147.24	0.68
1:4:692:GLU:HG3	1:4:734:LEU:HD13	1.76	0.68
1:8:692:GLU:HG3	1:8:734:LEU:HD13	1.76	0.68
1:A:347:THR:HG22	1:A:649:ILE:HG13	1.76	0.68
1:I:568:ILE:HD12	1:I:572:ASN:HD22	1.58	0.68
1:J:692:GLU:HG3	1:J:734:LEU:HD13	1.76	0.68
1:C:275:TYR:HB3	1:P:473:MET:HE1	55.00	0.68
1:X:556:ASP:OD1	1:X:557:TYR:N	2.26	0.68
1:P:400:TYR:OH	1:6:298:ASP:OD2	147.23	0.68
1:A:298:ASP:OD2	1:Z:400:TYR:OH	126.12	0.68
1:E:692:GLU:HG3	1:E:734:LEU:HD13	1.76	0.68
1:J:473:MET:HE1	1:L:275:TYR:HB3	1.76	0.68
1:M:473:MET:HE1	1:N:275:TYR:HB3	57.07	0.68
1:M:400:TYR:OH	1:N:298:ASP:OD2	72.95	0.68
1:P:692:GLU:HG3	1:P:734:LEU:HD13	1.76	0.68
1:U:692:GLU:HG3	1:U:734:LEU:HD13	1.76	0.68
1:V:692:GLU:HG3	1:V:734:LEU:HD13	1.76	0.68
1:Y:692:GLU:HG3	1:Y:734:LEU:HD13	1.76	0.68
1:Z:400:TYR:OH	1:4:298:ASP:OD2	72.05	0.68
1:4:718:ASN:HD21	1:4:722:THR:HB	1.58	0.68
1:B:718:ASN:HD21	1:B:722:THR:HB	1.58	0.68
1:F:473:MET:HE1	1:H:275:TYR:HB3	139.24	0.68
1:I:258:TYR:OH	1:I:399:GLU:OE1	2.12	0.68
1:C:275:TYR:HB3	1:M:473:MET:HE1	1.76	0.68
1:N:556:ASP:OD1	1:N:557:TYR:N	2.26	0.68
1:N:718:ASN:HD21	1:N:722:THR:HB	1.58	0.68
1:R:692:GLU:HG3	1:R:734:LEU:HD13	1.76	0.68
1:S:692:GLU:HG3	1:S:734:LEU:HD13	1.76	0.68
1:T:692:GLU:HG3	1:T:734:LEU:HD13	1.76	0.68
1:F:298:ASP:OD2	1:X:400:TYR:OH	126.79	0.68
1:X:692:GLU:HG3	1:X:734:LEU:HD13	1.76	0.68
1:Z:692:GLU:HG3	1:Z:734:LEU:HD13	1.76	0.68
1:1:692:GLU:HG3	1:1:734:LEU:HD13	1.76	0.68
1:3:568:ILE:HD12	1:3:572:ASN:HD22	1.58	0.68
1:5:692:GLU:HG3	1:5:734:LEU:HD13	1.76	0.68
1:6:718:ASN:HD21	1:6:722:THR:HB	1.58	0.68
1:N:692:GLU:HG3	1:N:734:LEU:HD13	1.76	0.68
1:O:298:ASP:OD2	1:P:400:TYR:OH	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:568:ILE:HD12	1:O:572:ASN:HD22	1.58	0.68
1:Q:568:ILE:HD12	1:Q:572:ASN:HD22	1.58	0.68
1:Z:258:TYR:OH	1:Z:399:GLU:OE1	2.12	0.68
1:1:347:THR:HG22	1:1:649:ILE:HG13	1.76	0.67
1:5:556:ASP:OD1	1:5:557:TYR:N	2.26	0.67
1:5:718:ASN:HD21	1:5:722:THR:HB	1.58	0.67
1:F:298:ASP:OD2	1:G:400:TYR:OH	2.11	0.67
1:L:258:TYR:OH	1:L:399:GLU:OE1	2.12	0.67
1:T:298:ASP:OD2	1:U:400:TYR:OH	2.11	0.67
1:V:347:THR:HG22	1:V:649:ILE:HG13	1.76	0.67
1:C:258:TYR:OH	1:C:399:GLU:OE1	2.12	0.67
1:B:473:MET:HE1	1:M:275:TYR:HB3	135.14	0.67
1:L:400:TYR:OH	1:N:298:ASP:OD2	145.83	0.67
1:R:258:TYR:OH	1:R:399:GLU:OE1	2.12	0.67
1:I:298:ASP:OD2	1:T:400:TYR:OH	182.29	0.67
1:T:347:THR:HG22	1:T:649:ILE:HG13	1.76	0.67
1:2:247:THR:HB	1:2:372:VAL:HG22	1.77	0.67
1:Y:298:ASP:OD2	1:4:400:TYR:OH	2.11	0.67
1:4:556:ASP:OD1	1:4:557:TYR:N	2.26	0.67
1:4:568:ILE:HD12	1:4:572:ASN:HD22	1.58	0.67
1:A:275:TYR:HB3	1:K:473:MET:HE1	109.39	0.67
1:F:275:TYR:HB3	1:Q:473:MET:HE1	1.76	0.67
1:V:350:GLU:OE1	1:V:352:GLN:NE2	2.28	0.67
1:W:275:TYR:HB3	1:Y:473:MET:HE1	50.75	0.67
1:Y:347:THR:HG22	1:Y:649:ILE:HG13	1.76	0.67
1:Z:275:TYR:HB3	1:2:473:MET:HE1	94.82	0.67
1:D:247:THR:HB	1:D:372:VAL:HG22	1.77	0.67
1:D:258:TYR:OH	1:D:399:GLU:OE1	2.12	0.67
1:E:247:THR:HB	1:E:372:VAL:HG22	1.77	0.67
1:K:258:TYR:OH	1:K:399:GLU:OE1	2.12	0.67
1:B:298:ASP:OD2	1:O:400:TYR:OH	153.24	0.67
1:T:258:TYR:OH	1:T:399:GLU:OE1	2.12	0.67
1:Y:350:GLU:OE1	1:Y:352:GLN:NE2	2.28	0.67
1:7:247:THR:HB	1:7:372:VAL:HG22	1.77	0.67
1:7:556:ASP:OD1	1:7:557:TYR:N	2.26	0.67
1:B:247:THR:HB	1:B:372:VAL:HG22	1.77	0.67
1:D:350:GLU:OE1	1:D:352:GLN:NE2	2.28	0.67
1:I:692:GLU:HG3	1:I:734:LEU:HD13	1.76	0.67
1:K:350:GLU:OE1	1:K:352:GLN:NE2	2.28	0.67
1:R:347:THR:HG22	1:R:649:ILE:HG13	1.76	0.67
1:6:473:MET:HE1	1:7:275:TYR:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:MET:HE1	1:Q:275:TYR:HB3	1.77	0.67
1:N:350:GLU:OE1	1:N:352:GLN:NE2	2.28	0.67
1:P:347:THR:HG22	1:P:649:ILE:HG13	1.76	0.67
1:Q:247:THR:HB	1:Q:372:VAL:HG22	1.77	0.67
1:Q:350:GLU:OE1	1:Q:352:GLN:NE2	2.28	0.67
1:W:350:GLU:OE1	1:W:352:GLN:NE2	2.28	0.67
1:X:350:GLU:OE1	1:X:352:GLN:NE2	2.28	0.67
1:2:258:TYR:OH	1:2:399:GLU:OE1	2.12	0.67
1:Z:473:MET:HE1	1:4:275:TYR:HB3	1.77	0.67
1:5:247:THR:HB	1:5:372:VAL:HG22	1.77	0.67
1:5:275:TYR:HB3	1:7:473:MET:HE1	1.77	0.67
1:5:350:GLU:OE1	1:5:352:GLN:NE2	2.28	0.67
1:7:350:GLU:OE1	1:7:352:GLN:NE2	2.28	0.67
1:A:350:GLU:OE1	1:A:352:GLN:NE2	2.28	0.67
1:E:350:GLU:OE1	1:E:352:GLN:NE2	2.28	0.67
1:F:350:GLU:OE1	1:F:352:GLN:NE2	2.28	0.67
1:G:692:GLU:HG3	1:G:734:LEU:HD13	1.76	0.67
1:I:298:ASP:OD2	1:J:400:TYR:OH	2.11	0.67
1:J:350:GLU:OE1	1:J:352:GLN:NE2	2.28	0.67
1:L:247:THR:HB	1:L:372:VAL:HG22	1.77	0.67
1:T:350:GLU:OE1	1:T:352:GLN:NE2	2.28	0.67
1:Z:247:THR:HB	1:Z:372:VAL:HG22	1.77	0.67
1:Z:275:TYR:HB3	1:3:473:MET:HE1	1.77	0.67
1:6:350:GLU:OE1	1:6:352:GLN:NE2	2.28	0.67
1:8:347:THR:HG22	1:8:649:ILE:HG13	1.76	0.67
1:A:473:MET:HE1	1:8:275:TYR:HB3	168.18	0.67
1:B:347:THR:HG22	1:B:649:ILE:HG13	1.76	0.67
1:G:247:THR:HB	1:G:372:VAL:HG22	1.77	0.67
1:H:258:TYR:OH	1:H:399:GLU:OE1	2.12	0.67
1:I:247:THR:HB	1:I:372:VAL:HG22	1.77	0.67
1:L:613:ASP:OD1	1:L:614:VAL:N	2.28	0.67
1:M:247:THR:HB	1:M:372:VAL:HG22	1.77	0.67
1:M:350:GLU:OE1	1:M:352:GLN:NE2	2.28	0.67
1:N:400:TYR:OH	1:R:298:ASP:OD2	126.42	0.67
1:T:247:THR:HB	1:T:372:VAL:HG22	1.77	0.67
1:V:247:THR:HB	1:V:372:VAL:HG22	1.77	0.67
1:Z:613:ASP:OD1	1:Z:614:VAL:N	2.28	0.67
1:1:350:GLU:OE1	1:1:352:GLN:NE2	2.28	0.67
1:1:247:THR:HB	1:1:372:VAL:HG22	1.77	0.67
1:1:718:ASN:HD21	1:1:722:THR:HB	1.58	0.67
1:4:347:THR:HG22	1:4:649:ILE:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:TYR:HB3	1:F:473:MET:HE1	1.77	0.67
1:F:613:ASP:OD1	1:F:614:VAL:N	2.28	0.67
1:H:350:GLU:OE1	1:H:352:GLN:NE2	2.28	0.67
1:I:613:ASP:OD1	1:I:614:VAL:N	2.28	0.67
1:C:298:ASP:OD2	1:M:400:TYR:OH	72.05	0.67
1:Q:613:ASP:OD1	1:Q:614:VAL:N	2.28	0.67
1:R:247:THR:HB	1:R:372:VAL:HG22	1.77	0.67
1:S:350:GLU:OE1	1:S:352:GLN:NE2	2.28	0.67
1:U:247:THR:HB	1:U:372:VAL:HG22	1.77	0.67
1:W:613:ASP:OD1	1:W:614:VAL:N	2.28	0.67
1:2:613:ASP:OD1	1:2:614:VAL:N	2.28	0.67
1:3:613:ASP:OD1	1:3:614:VAL:N	2.28	0.67
1:A:613:ASP:OD1	1:A:614:VAL:N	2.28	0.67
1:C:247:THR:HB	1:C:372:VAL:HG22	1.77	0.67
1:C:350:GLU:OE1	1:C:352:GLN:NE2	2.28	0.67
1:C:613:ASP:OD1	1:C:614:VAL:N	2.28	0.67
1:D:613:ASP:OD1	1:D:614:VAL:N	2.28	0.67
1:D:692:GLU:HG3	1:D:734:LEU:HD13	1.76	0.67
1:E:613:ASP:OD1	1:E:614:VAL:N	2.28	0.67
1:I:350:GLU:OE1	1:I:352:GLN:NE2	2.28	0.67
1:J:247:THR:HB	1:J:372:VAL:HG22	1.77	0.67
1:J:613:ASP:OD1	1:J:614:VAL:N	2.28	0.67
1:M:275:TYR:HB3	1:O:473:MET:HE1	91.03	0.67
1:N:347:THR:HG22	1:N:649:ILE:HG13	1.76	0.67
1:Z:350:GLU:OE1	1:Z:352:GLN:NE2	2.28	0.67
1:2:692:GLU:HG3	1:2:734:LEU:HD13	1.76	0.66
1:3:692:GLU:HG3	1:3:734:LEU:HD13	1.76	0.66
1:4:258:TYR:OH	1:4:399:GLU:OE1	2.12	0.66
1:5:473:MET:HE1	1:6:275:TYR:HB3	1.77	0.66
1:8:247:THR:HB	1:8:372:VAL:HG22	1.77	0.66
1:D:473:MET:HE1	1:N:275:TYR:HB3	1.77	0.66
1:J:347:THR:HG22	1:J:649:ILE:HG13	1.76	0.66
1:G:400:TYR:OH	1:K:298:ASP:OD2	126.42	0.66
1:L:350:GLU:OE1	1:L:352:GLN:NE2	2.28	0.66
1:M:258:TYR:OH	1:M:399:GLU:OE1	2.12	0.66
1:O:613:ASP:OD1	1:O:614:VAL:N	2.28	0.66
1:U:350:GLU:OE1	1:U:352:GLN:NE2	2.28	0.66
1:Y:247:THR:HB	1:Y:372:VAL:HG22	1.77	0.66
1:3:247:THR:HB	1:3:372:VAL:HG22	1.77	0.66
1:4:247:THR:HB	1:4:372:VAL:HG22	1.77	0.66
1:5:568:ILE:HD12	1:5:572:ASN:HD22	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:MET:HE1	1:L:275:TYR:HB3	139.26	0.66
1:G:258:TYR:OH	1:G:399:GLU:OE1	2.12	0.66
1:K:400:TYR:OH	1:7:298:ASP:OD2	2.11	0.66
1:I:275:TYR:HB3	1:K:473:MET:HE1	91.04	0.66
1:P:247:THR:HB	1:P:372:VAL:HG22	1.77	0.66
1:R:613:ASP:OD1	1:R:614:VAL:N	2.28	0.66
1:T:613:ASP:OD1	1:T:614:VAL:N	2.28	0.66
1:7:613:ASP:OD1	1:7:614:VAL:N	2.28	0.66
1:8:350:GLU:OE1	1:8:352:GLN:NE2	2.28	0.66
1:B:350:GLU:OE1	1:B:352:GLN:NE2	2.28	0.66
1:D:400:TYR:OH	1:E:298:ASP:OD2	2.11	0.66
1:N:258:TYR:OH	1:N:399:GLU:OE1	2.12	0.66
1:O:247:THR:HB	1:O:372:VAL:HG22	1.77	0.66
1:O:350:GLU:OE1	1:O:352:GLN:NE2	2.28	0.66
1:S:613:ASP:OD1	1:S:614:VAL:N	2.28	0.66
1:5:613:ASP:OD1	1:5:614:VAL:N	2.28	0.66
1:6:247:THR:HB	1:6:372:VAL:HG22	1.77	0.66
1:6:613:ASP:OD1	1:6:614:VAL:N	2.28	0.66
1:G:350:GLU:OE1	1:G:352:GLN:NE2	2.28	0.66
1:G:275:TYR:HB3	1:H:473:MET:HE1	57.07	0.66
1:H:613:ASP:OD1	1:H:614:VAL:N	2.28	0.66
1:K:247:THR:HB	1:K:372:VAL:HG22	1.77	0.66
1:P:350:GLU:OE1	1:P:352:GLN:NE2	2.28	0.66
1:U:613:ASP:OD1	1:U:614:VAL:N	2.28	0.66
1:3:350:GLU:OE1	1:3:352:GLN:NE2	2.28	0.66
1:8:613:ASP:OD1	1:8:614:VAL:N	2.28	0.66
1:A:247:THR:HB	1:A:372:VAL:HG22	1.77	0.66
1:F:247:THR:HB	1:F:372:VAL:HG22	1.77	0.66
1:K:613:ASP:OD1	1:K:614:VAL:N	2.28	0.66
1:N:247:THR:HB	1:N:372:VAL:HG22	1.77	0.66
1:P:613:ASP:OD1	1:P:614:VAL:N	2.28	0.66
1:S:473:MET:HE1	1:U:275:TYR:HB3	1.76	0.66
1:X:613:ASP:OD1	1:X:614:VAL:N	2.28	0.66
1:2:350:GLU:OE1	1:2:352:GLN:NE2	2.28	0.66
1:5:347:THR:HG22	1:5:649:ILE:HG13	1.76	0.66
1:A:258:TYR:OH	1:A:399:GLU:OE1	2.12	0.66
1:B:692:GLU:HG3	1:B:734:LEU:HD13	1.76	0.66
1:F:275:TYR:HB3	1:G:473:MET:HE1	104.57	0.66
1:H:247:THR:HB	1:H:372:VAL:HG22	1.77	0.66
1:J:258:TYR:OH	1:J:399:GLU:OE1	2.12	0.66
1:3:258:TYR:OH	1:3:399:GLU:OE1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:350:GLU:OE1	1:4:352:GLN:NE2	2.28	0.66
1:B:258:TYR:OH	1:B:399:GLU:OE1	2.12	0.66
1:O:258:TYR:OH	1:O:399:GLU:OE1	2.12	0.66
1:R:350:GLU:OE1	1:R:352:GLN:NE2	2.28	0.66
1:V:613:ASP:OD1	1:V:614:VAL:N	2.28	0.66
1:M:405:MET:C	1:M:406:LEU:HD12	2.17	0.66
1:P:405:MET:C	1:P:406:LEU:HD12	2.17	0.66
1:Y:613:ASP:OD1	1:Y:614:VAL:N	2.28	0.66
1:C:405:MET:C	1:C:406:LEU:HD12	2.17	0.66
1:F:258:TYR:OH	1:F:399:GLU:OE1	2.12	0.66
1:G:405:MET:C	1:G:406:LEU:HD12	2.17	0.66
1:H:405:MET:C	1:H:406:LEU:HD12	2.17	0.66
1:J:405:MET:C	1:J:406:LEU:HD12	2.17	0.66
1:M:613:ASP:OD1	1:M:614:VAL:N	2.28	0.66
1:N:613:ASP:OD1	1:N:614:VAL:N	2.28	0.66
1:S:405:MET:C	1:S:406:LEU:HD12	2.17	0.66
1:W:247:THR:HB	1:W:372:VAL:HG22	1.77	0.66
1:1:613:ASP:OD1	1:1:614:VAL:N	2.28	0.66
1:4:613:ASP:OD1	1:4:614:VAL:N	2.28	0.66
1:A:405:MET:C	1:A:406:LEU:HD12	2.17	0.66
1:C:473:MET:HE1	1:O:275:TYR:HB3	169.02	0.66
1:D:405:MET:C	1:D:406:LEU:HD12	2.17	0.66
1:E:473:MET:HE1	1:X:275:TYR:HB3	168.82	0.66
1:L:405:MET:C	1:L:406:LEU:HD12	2.17	0.66
1:S:247:THR:HB	1:S:372:VAL:HG22	1.77	0.66
1:X:247:THR:HB	1:X:372:VAL:HG22	1.77	0.66
1:I:405:MET:C	1:I:406:LEU:HD12	2.17	0.65
1:I:473:MET:HE1	1:J:275:TYR:HB3	57.12	0.65
1:K:405:MET:C	1:K:406:LEU:HD12	2.17	0.65
1:N:405:MET:C	1:N:406:LEU:HD12	2.17	0.65
1:O:405:MET:C	1:O:406:LEU:HD12	2.17	0.65
1:U:405:MET:C	1:U:406:LEU:HD12	2.17	0.65
1:E:275:TYR:HB3	1:V:473:MET:HE1	152.11	0.65
1:X:405:MET:C	1:X:406:LEU:HD12	2.17	0.65
1:6:258:TYR:OH	1:6:399:GLU:OE1	2.12	0.65
1:G:613:ASP:OD1	1:G:614:VAL:N	2.28	0.65
1:W:405:MET:C	1:W:406:LEU:HD12	2.17	0.65
1:4:405:MET:C	1:4:406:LEU:HD12	2.17	0.65
1:E:405:MET:C	1:E:406:LEU:HD12	2.17	0.65
1:V:405:MET:C	1:V:406:LEU:HD12	2.17	0.65
1:W:473:MET:HE1	1:Y:275:TYR:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:405:MET:C	1:3:406:LEU:HD12	2.17	0.65
1:6:405:MET:C	1:6:406:LEU:HD12	2.17	0.65
1:F:405:MET:C	1:F:406:LEU:HD12	2.17	0.65
1:Q:473:MET:HE1	1:R:275:TYR:HB3	57.07	0.65
1:W:258:TYR:OH	1:W:399:GLU:OE1	2.12	0.65
1:5:405:MET:C	1:5:406:LEU:HD12	2.17	0.65
1:7:405:MET:C	1:7:406:LEU:HD12	2.17	0.65
1:B:613:ASP:OD1	1:B:614:VAL:N	2.28	0.65
1:C:529:HIS:ND1	1:C:533:GLU:O	2.30	0.65
1:G:529:HIS:ND1	1:G:533:GLU:O	2.30	0.65
1:L:529:HIS:ND1	1:L:533:GLU:O	2.30	0.65
1:Q:405:MET:C	1:Q:406:LEU:HD12	2.17	0.65
1:X:529:HIS:ND1	1:X:533:GLU:O	2.30	0.65
1:Z:473:MET:HE1	1:1:275:TYR:HB3	104.21	0.65
1:1:405:MET:C	1:1:406:LEU:HD12	2.17	0.65
1:E:529:HIS:ND1	1:E:533:GLU:O	2.30	0.65
1:H:529:HIS:ND1	1:H:533:GLU:O	2.30	0.65
1:I:529:HIS:ND1	1:I:533:GLU:O	2.30	0.65
1:K:529:HIS:ND1	1:K:533:GLU:O	2.30	0.65
1:N:529:HIS:ND1	1:N:533:GLU:O	2.30	0.65
1:O:529:HIS:ND1	1:O:533:GLU:O	2.30	0.65
1:Q:258:TYR:OH	1:Q:399:GLU:OE1	2.12	0.65
1:Q:529:HIS:ND1	1:Q:533:GLU:O	2.30	0.65
1:R:529:HIS:ND1	1:R:533:GLU:O	2.30	0.65
1:W:529:HIS:ND1	1:W:533:GLU:O	2.30	0.65
1:A:529:HIS:ND1	1:A:533:GLU:O	2.30	0.65
1:I:251:PRO:HG3	1:I:374:MET:HE3	1.79	0.65
1:S:529:HIS:ND1	1:S:533:GLU:O	2.30	0.65
1:T:405:MET:C	1:T:406:LEU:HD12	2.17	0.65
1:V:529:HIS:ND1	1:V:533:GLU:O	2.30	0.65
1:Y:405:MET:C	1:Y:406:LEU:HD12	2.17	0.65
1:Y:529:HIS:ND1	1:Y:533:GLU:O	2.30	0.65
1:B:405:MET:C	1:B:406:LEU:HD12	2.17	0.65
1:D:529:HIS:ND1	1:D:533:GLU:O	2.30	0.65
1:U:529:HIS:ND1	1:U:533:GLU:O	2.30	0.65
1:2:529:HIS:ND1	1:2:533:GLU:O	2.30	0.65
1:3:529:HIS:ND1	1:3:533:GLU:O	2.30	0.65
1:E:492:SER:O	1:E:498:ASN:ND2	2.30	0.65
1:U:473:MET:HE1	1:V:275:TYR:HB3	57.06	0.65
1:2:405:MET:C	1:2:406:LEU:HD12	2.17	0.65
1:5:258:TYR:OH	1:5:399:GLU:OE1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:492:SER:O	1:7:498:ASN:ND2	2.31	0.65
1:7:529:HIS:ND1	1:7:533:GLU:O	2.30	0.65
1:Q:492:SER:O	1:Q:498:ASN:ND2	2.30	0.65
1:W:492:SER:O	1:W:498:ASN:ND2	2.30	0.65
1:Y:492:SER:O	1:Y:498:ASN:ND2	2.30	0.65
1:4:529:HIS:ND1	1:4:533:GLU:O	2.30	0.64
1:5:529:HIS:ND1	1:5:533:GLU:O	2.30	0.64
1:6:529:HIS:ND1	1:6:533:GLU:O	2.30	0.64
1:8:405:MET:C	1:8:406:LEU:HD12	2.17	0.64
1:R:405:MET:C	1:R:406:LEU:HD12	2.17	0.64
1:V:492:SER:O	1:V:498:ASN:ND2	2.31	0.64
1:6:492:SER:O	1:6:498:ASN:ND2	2.30	0.64
1:A:406:LEU:N	1:A:406:LEU:HD12	2.13	0.64
1:F:529:HIS:ND1	1:F:533:GLU:O	2.30	0.64
1:N:406:LEU:HD12	1:N:406:LEU:N	2.13	0.64
1:O:406:LEU:N	1:O:406:LEU:HD12	2.13	0.64
1:P:529:HIS:ND1	1:P:533:GLU:O	2.30	0.64
1:R:406:LEU:N	1:R:406:LEU:HD12	2.13	0.64
1:T:406:LEU:HD12	1:T:406:LEU:N	2.13	0.64
1:Z:405:MET:C	1:Z:406:LEU:HD12	2.17	0.64
1:Z:529:HIS:ND1	1:Z:533:GLU:O	2.30	0.64
1:1:406:LEU:N	1:1:406:LEU:HD12	2.13	0.64
1:3:406:LEU:HD12	1:3:406:LEU:N	2.13	0.64
1:4:406:LEU:HD12	1:4:406:LEU:N	2.13	0.64
1:B:529:HIS:ND1	1:B:533:GLU:O	2.30	0.64
1:S:406:LEU:HD12	1:S:406:LEU:N	2.13	0.64
1:T:529:HIS:ND1	1:T:533:GLU:O	2.30	0.64
1:U:258:TYR:OH	1:U:399:GLU:OE1	2.12	0.64
1:1:529:HIS:ND1	1:1:533:GLU:O	2.30	0.64
1:Z:396:TYR:OH	1:2:737:ASN:ND2	79.27	0.64
1:7:406:LEU:N	1:7:406:LEU:HD12	2.13	0.64
1:E:406:LEU:HD12	1:E:406:LEU:N	2.13	0.64
1:F:492:SER:O	1:F:498:ASN:ND2	2.31	0.64
1:G:406:LEU:HD12	1:G:406:LEU:N	2.13	0.64
1:H:406:LEU:HD12	1:H:406:LEU:N	2.13	0.64
1:J:529:HIS:ND1	1:J:533:GLU:O	2.30	0.64
1:L:473:MET:HE1	1:T:275:TYR:HB3	218.15	0.64
1:M:406:LEU:N	1:M:406:LEU:HD12	2.13	0.64
1:P:406:LEU:N	1:P:406:LEU:HD12	2.13	0.64
1:R:492:SER:O	1:R:498:ASN:ND2	2.30	0.64
1:8:529:HIS:ND1	1:8:533:GLU:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:LEU:N	1:F:406:LEU:HD12	2.13	0.64
1:A:275:TYR:HB3	1:I:473:MET:HE1	1.80	0.64
1:M:529:HIS:ND1	1:M:533:GLU:O	2.30	0.64
1:S:737:ASN:ND2	1:U:396:TYR:OH	2.31	0.64
1:X:258:TYR:OH	1:X:399:GLU:OE1	2.12	0.64
1:X:406:LEU:HD12	1:X:406:LEU:N	2.13	0.64
1:Y:406:LEU:HD12	1:Y:406:LEU:N	2.13	0.64
1:5:451:THR:HG21	1:6:503:PHE:CE2	2.33	0.64
1:8:696:ARG:HD3	1:8:700:GLU:OE2	1.98	0.64
1:G:696:ARG:HD3	1:G:700:GLU:OE2	1.98	0.64
1:J:406:LEU:N	1:J:406:LEU:HD12	2.13	0.64
1:N:696:ARG:HD3	1:N:700:GLU:OE2	1.98	0.64
1:P:696:ARG:HD3	1:P:700:GLU:OE2	1.98	0.64
1:S:258:TYR:OH	1:S:399:GLU:OE1	2.12	0.64
1:T:696:ARG:HD3	1:T:700:GLU:OE2	1.98	0.64
1:H:275:TYR:HB3	1:Y:473:MET:HE1	1.79	0.64
1:1:696:ARG:HD3	1:1:700:GLU:OE2	1.98	0.64
1:4:492:SER:O	1:4:498:ASN:ND2	2.30	0.64
1:4:696:ARG:HD3	1:4:700:GLU:OE2	1.98	0.64
1:D:696:ARG:HD3	1:D:700:GLU:OE2	1.98	0.64
1:I:696:ARG:HD3	1:I:700:GLU:OE2	1.98	0.64
1:J:696:ARG:HD3	1:J:700:GLU:OE2	1.98	0.64
1:N:492:SER:O	1:N:498:ASN:ND2	2.30	0.64
1:N:473:MET:HE1	1:O:275:TYR:HB3	57.07	0.64
1:S:492:SER:O	1:S:498:ASN:ND2	2.30	0.64
1:W:473:MET:HE1	1:X:275:TYR:HB3	57.07	0.64
1:Y:696:ARG:HD3	1:Y:700:GLU:OE2	1.98	0.64
1:Z:696:ARG:HD3	1:Z:700:GLU:OE2	1.98	0.64
1:C:406:LEU:N	1:C:406:LEU:HD12	2.13	0.64
1:H:492:SER:O	1:H:498:ASN:ND2	2.30	0.64
1:K:696:ARG:HD3	1:K:700:GLU:OE2	1.98	0.64
1:L:406:LEU:N	1:L:406:LEU:HD12	2.13	0.64
1:L:696:ARG:HD3	1:L:700:GLU:OE2	1.98	0.64
1:M:696:ARG:HD3	1:M:700:GLU:OE2	1.98	0.64
1:Q:696:ARG:HD3	1:Q:700:GLU:OE2	1.98	0.64
1:V:696:ARG:HD3	1:V:700:GLU:OE2	1.98	0.64
1:X:737:ASN:ND2	1:Y:396:TYR:OH	36.37	0.64
1:Z:251:PRO:HG3	1:Z:374:MET:HE3	1.80	0.64
1:Z:406:LEU:N	1:Z:406:LEU:HD12	2.13	0.64
1:5:696:ARG:HD3	1:5:700:GLU:OE2	1.98	0.64
1:B:696:ARG:HD3	1:B:700:GLU:OE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ASN:ND2	1:G:396:TYR:OH	2.29	0.64
1:I:492:SER:O	1:I:498:ASN:ND2	2.30	0.64
1:I:503:PHE:CE2	1:K:451:THR:HG21	120.32	0.64
1:K:492:SER:O	1:K:498:ASN:ND2	2.30	0.64
1:M:492:SER:O	1:M:498:ASN:ND2	2.30	0.64
1:W:406:LEU:HD12	1:W:406:LEU:N	2.13	0.64
1:X:251:PRO:HG3	1:X:374:MET:HE3	1.80	0.64
1:X:696:ARG:HD3	1:X:700:GLU:OE2	1.98	0.64
1:3:503:PHE:CE2	1:4:451:THR:HG21	2.33	0.64
1:5:492:SER:O	1:5:498:ASN:ND2	2.30	0.64
1:B:406:LEU:HD12	1:B:406:LEU:N	2.13	0.64
1:C:492:SER:O	1:C:498:ASN:ND2	2.30	0.64
1:D:737:ASN:ND2	1:L:396:TYR:OH	122.20	0.64
1:E:258:TYR:OH	1:E:399:GLU:OE1	2.12	0.64
1:M:251:PRO:HG3	1:M:374:MET:HE3	1.90	0.64
1:P:258:TYR:OH	1:P:399:GLU:OE1	2.12	0.64
1:Q:406:LEU:N	1:Q:406:LEU:HD12	2.13	0.64
1:1:737:ASN:ND2	1:2:396:TYR:OH	2.31	0.63
1:1:473:MET:HE1	1:2:275:TYR:HB3	1.80	0.63
1:I:406:LEU:N	1:I:406:LEU:HD12	2.13	0.63
1:M:737:ASN:ND2	1:N:396:TYR:OH	36.37	0.63
1:R:696:ARG:HD3	1:R:700:GLU:OE2	1.98	0.63
1:S:696:ARG:HD3	1:S:700:GLU:OE2	1.98	0.63
1:U:406:LEU:HD12	1:U:406:LEU:N	2.13	0.63
1:W:451:THR:HG21	1:X:503:PHE:CE2	74.86	0.63
1:Z:492:SER:O	1:Z:498:ASN:ND2	2.30	0.63
1:2:492:SER:O	1:2:498:ASN:ND2	2.30	0.63
1:Z:451:THR:HG21	1:4:503:PHE:CE2	2.33	0.63
1:B:737:ASN:ND2	1:M:396:TYR:OH	119.37	0.63
1:D:492:SER:O	1:D:498:ASN:ND2	2.31	0.63
1:G:503:PHE:CE2	1:H:451:THR:HG21	74.86	0.63
1:A:521:ASN:HB3	1:K:477:ALA:HA	125.29	0.63
1:L:737:ASN:ND2	1:T:396:TYR:OH	193.18	0.63
1:P:492:SER:O	1:P:498:ASN:ND2	2.30	0.63
1:U:451:THR:HG21	1:V:503:PHE:CE2	74.86	0.63
1:V:406:LEU:N	1:V:406:LEU:HD12	2.13	0.63
1:T:275:TYR:HB3	1:V:473:MET:HE1	91.02	0.63
1:A:451:THR:HG21	1:8:503:PHE:CE2	177.36	0.63
1:A:696:ARG:HD3	1:A:700:GLU:OE2	1.98	0.63
1:F:451:THR:HG21	1:H:503:PHE:CE2	155.07	0.63
1:H:696:ARG:HD3	1:H:700:GLU:OE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:406:LEU:HD12	1:K:406:LEU:N	2.13	0.63
1:R:477:ALA:HA	1:S:521:ASN:HB3	1.81	0.63
1:1:492:SER:O	1:1:498:ASN:ND2	2.30	0.63
1:2:406:LEU:N	1:2:406:LEU:HD12	2.13	0.63
1:8:406:LEU:HD12	1:8:406:LEU:N	2.13	0.63
1:D:396:TYR:OH	1:P:737:ASN:ND2	2.32	0.63
1:G:492:SER:O	1:G:498:ASN:ND2	2.30	0.63
1:K:251:PRO:HG3	1:K:374:MET:HE3	1.80	0.63
1:K:396:TYR:OH	1:8:737:ASN:ND2	2.32	0.63
1:O:451:THR:HG21	1:P:503:PHE:CE2	102.72	0.63
1:O:492:SER:O	1:O:498:ASN:ND2	2.31	0.63
1:R:396:TYR:OH	1:U:737:ASN:ND2	2.31	0.63
1:T:492:SER:O	1:T:498:ASN:ND2	2.30	0.63
1:U:696:ARG:HD3	1:U:700:GLU:OE2	1.98	0.63
1:V:396:TYR:OH	1:X:737:ASN:ND2	2.32	0.63
1:W:696:ARG:HD3	1:W:700:GLU:OE2	1.98	0.63
1:3:492:SER:O	1:3:498:ASN:ND2	2.30	0.63
1:8:492:SER:O	1:8:498:ASN:ND2	2.30	0.63
1:B:492:SER:O	1:B:498:ASN:ND2	2.31	0.63
1:D:251:PRO:HG3	1:D:374:MET:HE3	1.80	0.63
1:D:406:LEU:N	1:D:406:LEU:HD12	2.13	0.63
1:N:451:THR:HG21	1:O:503:PHE:CE2	74.86	0.63
1:Q:275:TYR:HB3	1:S:473:MET:HE1	104.56	0.63
1:5:477:ALA:HA	1:6:521:ASN:HB3	1.81	0.63
1:A:492:SER:O	1:A:498:ASN:ND2	2.30	0.63
1:B:275:TYR:HB3	1:C:473:MET:HE1	57.14	0.63
1:L:492:SER:O	1:L:498:ASN:ND2	2.30	0.63
1:F:503:PHE:CE2	1:Q:451:THR:HG21	2.34	0.63
1:R:251:PRO:HG3	1:R:374:MET:HE3	1.80	0.63
1:T:396:TYR:OH	1:V:737:ASN:ND2	83.14	0.63
1:E:521:ASN:HB3	1:V:477:ALA:HA	153.81	0.63
1:W:477:ALA:HA	1:X:521:ASN:HB3	60.61	0.63
1:H:521:ASN:HB3	1:Y:477:ALA:HA	1.81	0.63
1:2:251:PRO:HG3	1:2:374:MET:HE3	1.80	0.63
1:6:451:THR:HG21	1:7:503:PHE:CE2	2.34	0.63
1:C:696:ARG:HD3	1:C:700:GLU:OE2	1.98	0.63
1:D:477:ALA:HA	1:N:521:ASN:HB3	1.81	0.63
1:K:503:PHE:CE2	1:8:451:THR:HG21	2.34	0.63
1:R:451:THR:HG21	1:S:503:PHE:CE2	2.33	0.63
1:T:251:PRO:HG3	1:T:374:MET:HE3	1.83	0.63
1:V:258:TYR:OH	1:V:399:GLU:OE1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:521:ASN:HB3	1:Y:477:ALA:HA	37.37	0.63
1:Z:737:ASN:ND2	1:1:396:TYR:OH	95.03	0.63
1:2:696:ARG:HD3	1:2:700:GLU:OE2	1.98	0.63
1:3:696:ARG:HD3	1:3:700:GLU:OE2	1.98	0.63
1:5:521:ASN:HB3	1:7:477:ALA:HA	1.81	0.63
1:6:696:ARG:HD3	1:6:700:GLU:OE2	1.98	0.63
1:B:396:TYR:OH	1:C:737:ASN:ND2	36.37	0.63
1:B:477:ALA:HA	1:J:521:ASN:HB3	1.81	0.63
1:D:451:THR:HG21	1:L:503:PHE:CE2	155.08	0.63
1:E:503:PHE:CE2	1:F:451:THR:HG21	2.34	0.63
1:F:696:ARG:HD3	1:F:700:GLU:OE2	1.98	0.63
1:B:275:TYR:HB3	1:L:473:MET:HE1	1.80	0.63
1:F:396:TYR:OH	1:Q:737:ASN:ND2	2.31	0.63
1:T:737:ASN:ND2	1:U:396:TYR:OH	36.37	0.63
1:T:503:PHE:CE2	1:V:451:THR:HG21	120.33	0.63
1:3:275:TYR:HB3	1:4:473:MET:HE1	1.81	0.63
1:Z:521:ASN:HB3	1:3:477:ALA:HA	1.81	0.63
1:5:503:PHE:CE2	1:7:451:THR:HG21	2.34	0.63
1:B:396:TYR:OH	1:L:737:ASN:ND2	2.32	0.63
1:B:477:ALA:HA	1:M:521:ASN:HB3	120.02	0.63
1:C:503:PHE:CE2	1:M:451:THR:HG21	2.34	0.63
1:D:503:PHE:CE2	1:P:451:THR:HG21	2.34	0.63
1:E:521:ASN:HB3	1:F:477:ALA:HA	1.81	0.63
1:G:396:TYR:OH	1:H:737:ASN:ND2	52.74	0.63
1:H:451:THR:HG21	1:W:503:PHE:CE2	2.33	0.63
1:F:477:ALA:HA	1:H:521:ASN:HB3	134.50	0.63
1:A:503:PHE:CE2	1:K:451:THR:HG21	153.09	0.63
1:J:451:THR:HG21	1:L:503:PHE:CE2	2.34	0.63
1:M:521:ASN:HB3	1:O:477:ALA:HA	98.46	0.63
1:C:737:ASN:ND2	1:O:396:TYR:OH	153.84	0.63
1:Q:451:THR:HG21	1:R:503:PHE:CE2	74.87	0.63
1:W:396:TYR:OH	1:Y:737:ASN:ND2	48.56	0.63
1:W:451:THR:HG21	1:Y:503:PHE:CE2	2.34	0.63
1:A:477:ALA:HA	1:8:521:ASN:HB3	157.73	0.62
1:B:503:PHE:CE2	1:L:451:THR:HG21	2.33	0.62
1:N:451:THR:HG21	1:P:503:PHE:CE2	2.34	0.62
1:C:451:THR:HG21	1:O:503:PHE:CE2	157.73	0.62
1:O:696:ARG:HD3	1:O:700:GLU:OE2	1.98	0.62
1:R:275:TYR:HB3	1:U:473:MET:HE1	1.81	0.62
1:E:451:THR:HG21	1:X:503:PHE:CE2	156.52	0.62
1:Z:451:THR:HG21	1:1:503:PHE:CE2	95.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:737:ASN:ND2	1:4:396:TYR:OH	2.32	0.62
1:5:406:LEU:N	1:5:406:LEU:HD12	2.13	0.62
1:6:737:ASN:ND2	1:7:396:TYR:OH	2.31	0.62
1:6:477:ALA:HA	1:7:521:ASN:HB3	1.81	0.62
1:A:396:TYR:OH	1:I:737:ASN:ND2	2.32	0.62
1:B:503:PHE:CE2	1:C:451:THR:HG21	102.73	0.62
1:C:503:PHE:CE2	1:P:451:THR:HG21	73.61	0.62
1:D:503:PHE:CE2	1:T:451:THR:HG21	150.19	0.62
1:E:396:TYR:OH	1:V:737:ASN:ND2	125.99	0.62
1:E:696:ARG:HD3	1:E:700:GLU:OE2	1.98	0.62
1:I:521:ASN:HB3	1:K:477:ALA:HA	98.46	0.62
1:J:451:THR:HG21	1:K:503:PHE:CE2	74.86	0.62
1:D:737:ASN:ND2	1:N:396:TYR:OH	2.31	0.62
1:F:521:ASN:HB3	1:Q:477:ALA:HA	1.81	0.62
1:T:451:THR:HG21	1:U:503:PHE:CE2	102.73	0.62
1:U:492:SER:O	1:U:498:ASN:ND2	2.30	0.62
1:Z:503:PHE:CE2	1:3:451:THR:HG21	2.34	0.62
1:6:406:LEU:HD12	1:6:406:LEU:N	2.13	0.62
1:8:251:PRO:HG3	1:8:374:MET:HE3	1.81	0.62
1:A:521:ASN:HB3	1:I:477:ALA:HA	1.80	0.62
1:J:737:ASN:ND2	1:K:396:TYR:OH	52.73	0.62
1:M:503:PHE:CE2	1:O:451:THR:HG21	120.32	0.62
1:N:477:ALA:HA	1:P:521:ASN:HB3	1.81	0.62
1:T:477:ALA:HA	1:U:521:ASN:HB3	77.93	0.62
1:H:503:PHE:CE2	1:Y:451:THR:HG21	2.33	0.62
1:I:477:ALA:HA	1:J:521:ASN:HB3	77.92	0.62
1:M:451:THR:HG21	1:N:503:PHE:CE2	102.73	0.62
1:E:477:ALA:HA	1:Q:521:ASN:HB3	1.81	0.62
1:R:737:ASN:ND2	1:S:396:TYR:OH	2.32	0.62
1:S:451:THR:HG21	1:U:503:PHE:CE2	2.35	0.62
1:U:477:ALA:HA	1:V:521:ASN:HB3	60.61	0.62
1:W:251:PRO:HG3	1:W:374:MET:HE3	1.86	0.62
1:5:737:ASN:ND2	1:6:396:TYR:OH	2.32	0.62
1:A:396:TYR:OH	1:K:737:ASN:ND2	85.76	0.62
1:D:451:THR:HG21	1:N:503:PHE:CE2	2.34	0.62
1:Q:503:PHE:CE2	1:S:451:THR:HG21	98.72	0.62
1:3:521:ASN:HB3	1:4:477:ALA:HA	1.81	0.62
1:Z:396:TYR:OH	1:3:737:ASN:ND2	2.32	0.62
1:A:251:PRO:HG3	1:A:374:MET:HE3	1.80	0.62
1:D:521:ASN:HB3	1:P:477:ALA:HA	1.81	0.62
1:E:251:PRO:HG3	1:E:374:MET:HE3	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:521:ASN:HB3	1:H:477:ALA:HA	60.61	0.62
1:I:396:TYR:OH	1:K:737:ASN:ND2	83.14	0.62
1:M:396:TYR:OH	1:O:737:ASN:ND2	83.14	0.62
1:N:477:ALA:HA	1:O:521:ASN:HB3	60.61	0.62
1:E:451:THR:HG21	1:Q:503:PHE:CE2	2.34	0.62
1:R:503:PHE:CE2	1:U:451:THR:HG21	2.34	0.62
1:D:396:TYR:OH	1:T:737:ASN:ND2	110.09	0.62
1:U:659:ASP:OD2	1:5:333:LYS:NZ	208.65	0.62
1:Z:477:ALA:HA	1:1:521:ASN:HB3	90.19	0.62
1:B:251:PRO:HG3	1:B:374:MET:HE3	1.82	0.62
1:C:521:ASN:HB3	1:P:477:ALA:HA	61.28	0.62
1:D:521:ASN:HB3	1:T:477:ALA:HA	130.29	0.62
1:E:396:TYR:OH	1:F:737:ASN:ND2	2.32	0.62
1:E:503:PHE:CE2	1:V:451:THR:HG21	181.04	0.62
1:H:251:PRO:HG3	1:H:374:MET:HE3	1.83	0.62
1:I:451:THR:HG21	1:J:503:PHE:CE2	102.72	0.62
1:B:451:THR:HG21	1:J:503:PHE:CE2	2.34	0.62
1:O:477:ALA:HA	1:P:521:ASN:HB3	77.92	0.62
1:T:521:ASN:HB3	1:V:477:ALA:HA	98.46	0.62
1:1:451:THR:HG21	1:2:503:PHE:CE2	2.34	0.62
1:7:696:ARG:HD3	1:7:700:GLU:OE2	1.98	0.62
1:K:521:ASN:HB3	1:8:477:ALA:HA	1.81	0.62
1:B:451:THR:HG21	1:M:503:PHE:CE2	133.19	0.62
1:E:659:ASP:OD2	1:U:333:LYS:NZ	182.48	0.62
1:O:251:PRO:HG3	1:O:374:MET:HE3	1.87	0.62
1:Q:477:ALA:HA	1:R:521:ASN:HB3	60.61	0.62
1:V:503:PHE:CE2	1:X:451:THR:HG21	2.34	0.62
1:X:451:THR:HG21	1:Y:503:PHE:CE2	102.72	0.62
1:W:477:ALA:HA	1:Y:521:ASN:HB3	1.81	0.62
1:7:258:TYR:OH	1:7:399:GLU:OE1	2.12	0.62
1:8:258:TYR:OH	1:8:399:GLU:OE1	2.12	0.62
1:A:503:PHE:CE2	1:I:451:THR:HG21	2.34	0.62
1:B:521:ASN:HB3	1:C:477:ALA:HA	77.93	0.62
1:D:275:TYR:HB3	1:T:473:MET:HE1	129.07	0.62
1:E:477:ALA:HA	1:X:521:ASN:HB3	146.22	0.62
1:F:521:ASN:HB3	1:G:477:ALA:HA	90.69	0.62
1:F:396:TYR:OH	1:G:737:ASN:ND2	95.14	0.62
1:J:251:PRO:HG3	1:J:374:MET:HE3	1.81	0.62
1:W:503:PHE:CE2	1:Y:451:THR:HG21	41.30	0.62
1:Z:477:ALA:HA	1:4:521:ASN:HB3	1.80	0.62
1:B:521:ASN:HB3	1:L:477:ALA:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:477:ALA:HA	1:K:521:ASN:HB3	60.61	0.62
1:M:307:TRP:O	1:M:426:SER:OG	2.18	0.62
1:R:521:ASN:HB3	1:U:477:ALA:HA	1.81	0.62
1:T:307:TRP:O	1:T:426:SER:OG	2.18	0.62
1:S:477:ALA:HA	1:U:521:ASN:HB3	1.81	0.62
1:Z:307:TRP:O	1:Z:426:SER:OG	2.18	0.62
1:N:307:TRP:O	1:N:426:SER:OG	2.18	0.61
1:R:307:TRP:O	1:R:426:SER:OG	2.18	0.61
1:H:473:MET:HE1	1:W:275:TYR:HB3	1.82	0.61
1:A:307:TRP:O	1:A:426:SER:OG	2.18	0.61
1:C:477:ALA:HA	1:O:521:ASN:HB3	146.40	0.61
1:I:253:TYR:CE1	1:I:377:GLN:HB2	2.36	0.61
1:L:451:THR:HG21	1:T:503:PHE:CE2	235.46	0.61
1:C:521:ASN:HB3	1:M:477:ALA:HA	1.81	0.61
1:P:253:TYR:CE1	1:P:377:GLN:HB2	2.36	0.61
1:Q:253:TYR:CE1	1:Q:377:GLN:HB2	2.36	0.61
1:W:253:TYR:CE1	1:W:377:GLN:HB2	2.36	0.61
1:8:253:TYR:CE1	1:8:377:GLN:HB2	2.36	0.61
1:C:307:TRP:O	1:C:426:SER:OG	2.18	0.61
1:D:659:ASP:OD2	1:E:333:LYS:NZ	2.32	0.61
1:E:253:TYR:CE1	1:E:377:GLN:HB2	2.36	0.61
1:G:253:TYR:CE1	1:G:377:GLN:HB2	2.36	0.61
1:G:451:THR:HG21	1:I:503:PHE:CE2	2.36	0.61
1:H:253:TYR:CE1	1:H:377:GLN:HB2	2.36	0.61
1:I:737:ASN:ND2	1:J:396:TYR:OH	36.37	0.61
1:J:492:SER:O	1:J:498:ASN:ND2	2.30	0.61
1:K:253:TYR:CE1	1:K:377:GLN:HB2	2.36	0.61
1:L:307:TRP:O	1:L:426:SER:OG	2.18	0.61
1:L:477:ALA:HA	1:T:521:ASN:HB3	207.76	0.61
1:U:253:TYR:CE1	1:U:377:GLN:HB2	2.36	0.61
1:V:253:TYR:CE1	1:V:377:GLN:HB2	2.36	0.61
1:X:253:TYR:CE1	1:X:377:GLN:HB2	2.36	0.61
1:2:253:TYR:CE1	1:2:377:GLN:HB2	2.35	0.61
1:B:253:TYR:CE1	1:B:377:GLN:HB2	2.36	0.61
1:D:253:TYR:CE1	1:D:377:GLN:HB2	2.36	0.61
1:F:503:PHE:CE2	1:G:451:THR:HG21	98.72	0.61
1:L:253:TYR:CE1	1:L:377:GLN:HB2	2.36	0.61
1:J:477:ALA:HA	1:L:521:ASN:HB3	1.81	0.61
1:N:253:TYR:CE1	1:N:377:GLN:HB2	2.36	0.61
1:V:521:ASN:HB3	1:X:477:ALA:HA	1.81	0.61
1:C:253:TYR:CE1	1:C:377:GLN:HB2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:737:ASN:ND2	1:H:396:TYR:OH	122.20	0.61
1:H:396:TYR:OH	1:Y:737:ASN:ND2	2.32	0.61
1:K:659:ASP:OD2	1:7:333:LYS:NZ	2.32	0.61
1:A:253:TYR:CE1	1:A:377:GLN:HB2	2.36	0.61
1:G:737:ASN:ND2	1:I:396:TYR:OH	2.30	0.61
1:O:307:TRP:O	1:O:426:SER:OG	2.18	0.61
1:X:477:ALA:HA	1:Y:521:ASN:HB3	77.92	0.61
1:Z:253:TYR:CE1	1:Z:377:GLN:HB2	2.36	0.61
1:7:251:PRO:HG3	1:7:374:MET:HE3	1.83	0.61
1:C:251:PRO:HG3	1:C:374:MET:HE3	1.83	0.61
1:E:307:TRP:O	1:E:426:SER:OG	2.18	0.61
1:M:253:TYR:CE1	1:M:377:GLN:HB2	2.35	0.61
1:Q:333:LYS:NZ	1:S:659:ASP:OD2	2.32	0.61
1:Z:503:PHE:CE2	1:2:451:THR:HG21	110.88	0.61
1:3:396:TYR:OH	1:4:737:ASN:ND2	2.32	0.61
1:7:307:TRP:O	1:7:426:SER:OG	2.18	0.61
1:7:253:TYR:CE1	1:7:377:GLN:HB2	2.35	0.61
1:H:477:ALA:HA	1:W:521:ASN:HB3	1.80	0.61
1:J:253:TYR:CE1	1:J:377:GLN:HB2	2.36	0.61
1:J:307:TRP:O	1:J:426:SER:OG	2.18	0.61
1:M:477:ALA:HA	1:N:521:ASN:HB3	77.92	0.61
1:O:737:ASN:ND2	1:P:396:TYR:OH	36.37	0.61
1:S:307:TRP:O	1:S:426:SER:OG	2.18	0.61
1:S:253:TYR:CE1	1:S:377:GLN:HB2	2.36	0.61
1:W:737:ASN:ND2	1:Y:396:TYR:OH	2.32	0.61
1:X:307:TRP:O	1:X:426:SER:OG	2.18	0.61
1:5:253:TYR:CE1	1:5:377:GLN:HB2	2.35	0.61
1:D:477:ALA:HA	1:L:521:ASN:HB3	134.50	0.61
1:G:225:SER:CA	1:W:407:ARG:HD2	2.31	0.61
1:H:307:TRP:O	1:H:426:SER:OG	2.18	0.61
1:N:737:ASN:ND2	1:O:396:TYR:OH	52.73	0.61
1:R:253:TYR:CE1	1:R:377:GLN:HB2	2.36	0.61
1:T:253:TYR:CE1	1:T:377:GLN:HB2	2.35	0.61
1:X:492:SER:O	1:X:498:ASN:ND2	2.31	0.61
1:1:477:ALA:HA	1:2:521:ASN:HB3	1.82	0.61
1:6:307:TRP:O	1:6:426:SER:OG	2.18	0.61
1:S:251:PRO:HG3	1:S:374:MET:HE3	1.86	0.61
1:Y:253:TYR:CE1	1:Y:377:GLN:HB2	2.36	0.61
1:Y:307:TRP:O	1:Y:426:SER:OG	2.18	0.61
1:Y:407:ARG:O	1:Y:409:GLY:N	2.34	0.61
1:1:253:TYR:CE1	1:1:377:GLN:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:407:ARG:O	1:7:409:GLY:N	2.34	0.60
1:D:307:TRP:O	1:D:426:SER:OG	2.18	0.60
1:E:407:ARG:O	1:E:409:GLY:N	2.34	0.60
1:E:737:ASN:ND2	1:Q:396:TYR:OH	2.31	0.60
1:F:307:TRP:O	1:F:426:SER:OG	2.18	0.60
1:M:407:ARG:O	1:M:409:GLY:N	2.34	0.60
1:Q:737:ASN:ND2	1:R:396:TYR:OH	52.73	0.60
1:T:407:ARG:O	1:T:409:GLY:N	2.34	0.60
1:U:251:PRO:HG3	1:U:374:MET:HE3	1.83	0.60
1:U:307:TRP:O	1:U:426:SER:OG	2.18	0.60
1:V:407:ARG:O	1:V:409:GLY:N	2.34	0.60
1:6:253:TYR:CE1	1:6:377:GLN:HB2	2.36	0.60
1:G:477:ALA:HA	1:I:521:ASN:HB3	1.83	0.60
1:S:407:ARG:O	1:S:409:GLY:N	2.34	0.60
1:U:407:ARG:O	1:U:409:GLY:N	2.34	0.60
1:Z:407:ARG:O	1:Z:409:GLY:N	2.34	0.60
1:3:407:ARG:O	1:3:409:GLY:N	2.34	0.60
1:4:407:ARG:O	1:4:409:GLY:N	2.34	0.60
1:5:396:TYR:OH	1:7:737:ASN:ND2	2.32	0.60
1:A:451:THR:HG21	1:G:503:PHE:CE2	2.36	0.60
1:B:307:TRP:O	1:B:426:SER:OG	2.18	0.60
1:F:253:TYR:CE1	1:F:377:GLN:HB2	2.36	0.60
1:G:407:ARG:O	1:G:409:GLY:N	2.34	0.60
1:O:407:ARG:O	1:O:409:GLY:N	2.34	0.60
1:Q:521:ASN:HB3	1:S:477:ALA:HA	90.69	0.60
1:R:407:ARG:O	1:R:409:GLY:N	2.34	0.60
1:3:253:TYR:CE1	1:3:377:GLN:HB2	2.36	0.60
1:C:407:ARG:O	1:C:409:GLY:N	2.34	0.60
1:H:407:ARG:O	1:H:409:GLY:N	2.34	0.60
1:N:407:ARG:O	1:N:409:GLY:N	2.34	0.60
1:N:737:ASN:ND2	1:P:396:TYR:OH	2.32	0.60
1:O:253:TYR:CE1	1:O:377:GLN:HB2	2.35	0.60
1:P:407:ARG:O	1:P:409:GLY:N	2.34	0.60
1:C:396:TYR:OH	1:P:737:ASN:ND2	49.22	0.60
1:1:407:ARG:O	1:1:409:GLY:N	2.34	0.60
1:4:253:TYR:CE1	1:4:377:GLN:HB2	2.36	0.60
1:L:407:ARG:O	1:L:409:GLY:N	2.34	0.60
1:Z:521:ASN:HB3	1:2:477:ALA:HA	94.48	0.60
1:4:307:TRP:O	1:4:426:SER:OG	2.18	0.60
1:I:407:ARG:O	1:I:409:GLY:N	2.34	0.60
1:E:737:ASN:ND2	1:X:396:TYR:OH	153.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:258:TYR:OH	1:1:399:GLU:OE1	2.12	0.60
1:B:407:ARG:O	1:B:409:GLY:N	2.34	0.60
1:J:407:ARG:O	1:J:409:GLY:N	2.34	0.60
1:Q:407:ARG:O	1:Q:409:GLY:N	2.34	0.60
1:F:333:LYS:NZ	1:X:659:ASP:OD2	139.16	0.60
1:2:407:ARG:O	1:2:409:GLY:N	2.34	0.60
1:5:407:ARG:O	1:5:409:GLY:N	2.34	0.60
1:D:407:ARG:O	1:D:409:GLY:N	2.34	0.60
1:A:440:LEU:HD11	1:G:279:SER:HB2	1.84	0.60
1:N:251:PRO:HG3	1:N:374:MET:HE3	1.88	0.60
1:O:333:LYS:NZ	1:P:659:ASP:OD2	2.32	0.60
1:X:407:ARG:O	1:X:409:GLY:N	2.34	0.60
1:3:511:TYR:HD2	1:3:520:VAL:HG22	1.67	0.60
1:G:307:TRP:O	1:G:426:SER:OG	2.18	0.60
1:N:511:TYR:HD2	1:N:520:VAL:HG22	1.67	0.60
1:O:511:TYR:HD2	1:O:520:VAL:HG22	1.67	0.60
1:P:307:TRP:O	1:P:426:SER:OG	2.18	0.60
1:V:511:TYR:HD2	1:V:520:VAL:HG22	1.67	0.60
1:4:511:TYR:HD2	1:4:520:VAL:HG22	1.67	0.60
1:A:737:ASN:ND2	1:8:396:TYR:OH	146.71	0.60
1:8:407:ARG:O	1:8:409:GLY:N	2.34	0.60
1:A:407:ARG:O	1:A:409:GLY:N	2.34	0.60
1:A:477:ALA:HA	1:G:521:ASN:HB3	1.83	0.60
1:P:251:PRO:HG3	1:P:374:MET:HE3	1.86	0.60
1:W:407:ARG:O	1:W:409:GLY:N	2.34	0.60
1:X:254:ASN:O	1:X:257:LEU:N	2.35	0.60
1:J:333:LYS:NZ	1:X:659:ASP:OD2	149.17	0.60
1:Y:511:TYR:HD2	1:Y:520:VAL:HG22	1.67	0.60
1:G:251:PRO:HG3	1:G:374:MET:HE3	1.84	0.59
1:G:511:TYR:HD2	1:G:520:VAL:HG22	1.67	0.59
1:I:511:TYR:HD2	1:I:520:VAL:HG22	1.67	0.59
1:K:407:ARG:O	1:K:409:GLY:N	2.34	0.59
1:3:333:LYS:NZ	1:8:659:ASP:OD2	2.32	0.59
1:A:511:TYR:HD2	1:A:520:VAL:HG22	1.67	0.59
1:F:407:ARG:O	1:F:409:GLY:N	2.34	0.59
1:G:355:TYR:CZ	1:G:357:LEU:HB2	2.38	0.59
1:M:254:ASN:O	1:M:257:LEU:N	2.35	0.59
1:P:355:TYR:CZ	1:P:357:LEU:HB2	2.38	0.59
1:P:511:TYR:HD2	1:P:520:VAL:HG22	1.67	0.59
1:T:531:ASP:OD1	1:T:569:LYS:NZ	2.28	0.59
1:Y:531:ASP:OD1	1:Y:569:LYS:NZ	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:355:TYR:CZ	1:4:357:LEU:HB2	2.38	0.59
1:6:407:ARG:O	1:6:409:GLY:N	2.34	0.59
1:A:355:TYR:CZ	1:A:357:LEU:HB2	2.38	0.59
1:B:355:TYR:CZ	1:B:357:LEU:HB2	2.38	0.59
1:F:588:GLN:N	1:F:591:THR:OG1	2.36	0.59
1:K:307:TRP:O	1:K:426:SER:OG	2.18	0.59
1:N:355:TYR:CZ	1:N:357:LEU:HB2	2.38	0.59
1:O:254:ASN:O	1:O:257:LEU:N	2.35	0.59
1:O:355:TYR:CZ	1:O:357:LEU:HB2	2.38	0.59
1:Q:355:TYR:CZ	1:Q:357:LEU:HB2	2.38	0.59
1:Q:511:TYR:HD2	1:Q:520:VAL:HG22	1.67	0.59
1:T:588:GLN:N	1:T:591:THR:OG1	2.36	0.59
1:U:254:ASN:O	1:U:257:LEU:N	2.35	0.59
1:V:307:TRP:O	1:V:426:SER:OG	2.18	0.59
1:W:355:TYR:CZ	1:W:357:LEU:HB2	2.38	0.59
1:W:511:TYR:HD2	1:W:520:VAL:HG22	1.67	0.59
1:W:588:GLN:N	1:W:591:THR:OG1	2.36	0.59
1:1:307:TRP:O	1:1:426:SER:OG	2.18	0.59
1:4:588:GLN:N	1:4:591:THR:OG1	2.36	0.59
1:5:588:GLN:N	1:5:591:THR:OG1	2.36	0.59
1:6:588:GLN:N	1:6:591:THR:OG1	2.36	0.59
1:E:588:GLN:N	1:E:591:THR:OG1	2.36	0.59
1:I:355:TYR:CZ	1:I:357:LEU:HB2	2.38	0.59
1:J:254:ASN:O	1:J:257:LEU:N	2.35	0.59
1:J:588:GLN:N	1:J:591:THR:OG1	2.36	0.59
1:Q:588:GLN:N	1:Q:591:THR:OG1	2.36	0.59
1:R:355:TYR:CZ	1:R:357:LEU:HB2	2.38	0.59
1:T:355:TYR:CZ	1:T:357:LEU:HB2	2.38	0.59
1:T:511:TYR:HD2	1:T:520:VAL:HG22	1.67	0.59
1:U:588:GLN:N	1:U:591:THR:OG1	2.36	0.59
1:V:254:ASN:O	1:V:257:LEU:N	2.35	0.59
1:1:588:GLN:N	1:1:591:THR:OG1	2.36	0.59
1:3:588:GLN:N	1:3:591:THR:OG1	2.36	0.59
1:5:511:TYR:HD2	1:5:520:VAL:HG22	1.67	0.59
1:7:588:GLN:N	1:7:591:THR:OG1	2.36	0.59
1:8:254:ASN:O	1:8:257:LEU:N	2.35	0.59
1:A:254:ASN:O	1:A:257:LEU:N	2.35	0.59
1:B:254:ASN:O	1:B:257:LEU:N	2.35	0.59
1:C:396:TYR:OH	1:M:737:ASN:ND2	2.32	0.59
1:F:300:GLN:NE2	1:F:703:TYR:O	2.36	0.59
1:G:588:GLN:N	1:G:591:THR:OG1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:511:TYR:HD2	1:H:520:VAL:HG22	1.67	0.59
1:I:588:GLN:N	1:I:591:THR:OG1	2.36	0.59
1:J:511:TYR:HD2	1:J:520:VAL:HG22	1.67	0.59
1:K:511:TYR:HD2	1:K:520:VAL:HG22	1.67	0.59
1:L:251:PRO:HG3	1:L:374:MET:HE3	1.84	0.59
1:M:588:GLN:N	1:M:591:THR:OG1	2.36	0.59
1:N:588:GLN:N	1:N:591:THR:OG1	2.36	0.59
1:O:588:GLN:N	1:O:591:THR:OG1	2.36	0.59
1:Q:307:TRP:O	1:Q:426:SER:OG	2.18	0.59
1:Q:396:TYR:OH	1:S:737:ASN:ND2	95.14	0.59
1:R:254:ASN:O	1:R:257:LEU:N	2.35	0.59
1:R:588:GLN:N	1:R:591:THR:OG1	2.36	0.59
1:S:300:GLN:NE2	1:S:703:TYR:O	2.36	0.59
1:S:355:TYR:CZ	1:S:357:LEU:HB2	2.38	0.59
1:U:300:GLN:NE2	1:U:703:TYR:O	2.36	0.59
1:U:355:TYR:CZ	1:U:357:LEU:HB2	2.38	0.59
1:V:588:GLN:N	1:V:591:THR:OG1	2.36	0.59
1:X:511:TYR:HD2	1:X:520:VAL:HG22	1.67	0.59
1:Y:254:ASN:O	1:Y:257:LEU:N	2.35	0.59
1:Z:355:TYR:CZ	1:Z:357:LEU:HB2	2.38	0.59
1:Z:531:ASP:OD1	1:Z:569:LYS:NZ	2.28	0.59
1:U:225:SER:CA	1:2:407:ARG:HD2	153.30	0.59
1:2:307:TRP:O	1:2:426:SER:OG	2.18	0.59
1:8:300:GLN:NE2	1:8:703:TYR:O	2.36	0.59
1:A:588:GLN:N	1:A:591:THR:OG1	2.36	0.59
1:A:659:ASP:OD2	1:J:333:LYS:NZ	96.58	0.59
1:C:355:TYR:CZ	1:C:357:LEU:HB2	2.38	0.59
1:D:588:GLN:N	1:D:591:THR:OG1	2.36	0.59
1:D:300:GLN:NE2	1:D:703:TYR:O	2.36	0.59
1:J:355:TYR:CZ	1:J:357:LEU:HB2	2.38	0.59
1:K:300:GLN:NE2	1:K:703:TYR:O	2.36	0.59
1:L:355:TYR:CZ	1:L:357:LEU:HB2	2.38	0.59
1:L:531:ASP:OD1	1:L:569:LYS:NZ	2.28	0.59
1:M:355:TYR:CZ	1:M:357:LEU:HB2	2.38	0.59
1:N:254:ASN:O	1:N:257:LEU:N	2.35	0.59
1:P:225:SER:CA	1:Q:407:ARG:HD2	2.33	0.59
1:P:254:ASN:O	1:P:257:LEU:N	2.35	0.59
1:R:511:TYR:HD2	1:R:520:VAL:HG22	1.67	0.59
1:V:300:GLN:NE2	1:V:703:TYR:O	2.36	0.59
1:W:307:TRP:O	1:W:426:SER:OG	2.18	0.59
1:X:355:TYR:CZ	1:X:357:LEU:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:355:TYR:CZ	1:Y:357:LEU:HB2	2.38	0.59
1:Y:300:GLN:NE2	1:Y:703:TYR:O	2.36	0.59
1:2:254:ASN:O	1:2:257:LEU:N	2.35	0.59
1:3:225:SER:CA	1:8:407:ARG:HD2	2.33	0.59
1:4:254:ASN:O	1:4:257:LEU:N	2.35	0.59
1:6:300:GLN:NE2	1:6:703:TYR:O	2.36	0.59
1:F:511:TYR:HD2	1:F:520:VAL:HG22	1.67	0.59
1:H:254:ASN:O	1:H:257:LEU:N	2.35	0.59
1:I:254:ASN:O	1:I:257:LEU:N	2.35	0.59
1:H:225:SER:CA	1:I:407:ARG:HD2	2.33	0.59
1:B:333:LYS:NZ	1:O:659:ASP:OD2	149.18	0.59
1:P:300:GLN:NE2	1:P:703:TYR:O	2.36	0.59
1:S:588:GLN:N	1:S:591:THR:OG1	2.36	0.59
1:V:355:TYR:CZ	1:V:357:LEU:HB2	2.38	0.59
1:2:588:GLN:N	1:2:591:THR:OG1	2.36	0.59
1:2:225:SER:CA	1:3:407:ARG:HD2	2.31	0.59
1:4:300:GLN:NE2	1:4:703:TYR:O	2.36	0.59
1:8:511:TYR:HD2	1:8:520:VAL:HG22	1.67	0.59
1:D:254:ASN:O	1:D:257:LEU:N	2.35	0.59
1:F:355:TYR:CZ	1:F:357:LEU:HB2	2.38	0.59
1:G:254:ASN:O	1:G:257:LEU:N	2.35	0.59
1:H:588:GLN:N	1:H:591:THR:OG1	2.36	0.59
1:J:737:ASN:ND2	1:L:396:TYR:OH	2.32	0.59
1:N:300:GLN:NE2	1:N:703:TYR:O	2.36	0.59
1:S:254:ASN:O	1:S:257:LEU:N	2.35	0.59
1:X:588:GLN:N	1:X:591:THR:OG1	2.36	0.59
1:2:254:ASN:O	1:2:255:ASN:C	2.42	0.59
1:A:300:GLN:NE2	1:A:703:TYR:O	2.36	0.59
1:B:511:TYR:HD2	1:B:520:VAL:HG22	1.67	0.59
1:C:300:GLN:NE2	1:C:703:TYR:O	2.36	0.59
1:F:531:ASP:OD1	1:F:569:LYS:NZ	2.28	0.59
1:H:254:ASN:O	1:H:255:ASN:C	2.42	0.59
1:H:300:GLN:NE2	1:H:703:TYR:O	2.36	0.59
1:L:511:TYR:HD2	1:L:520:VAL:HG22	1.67	0.59
1:L:300:GLN:NE2	1:L:703:TYR:O	2.36	0.59
1:M:511:TYR:HD2	1:M:520:VAL:HG22	1.67	0.59
1:O:225:SER:CA	1:P:407:ARG:HD2	2.33	0.59
1:U:511:TYR:HD2	1:U:520:VAL:HG22	1.67	0.59
1:W:254:ASN:O	1:W:257:LEU:N	2.35	0.59
1:W:737:ASN:ND2	1:X:396:TYR:OH	52.73	0.59
1:Y:254:ASN:O	1:Y:255:ASN:C	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:588:GLN:N	1:Y:591:THR:OG1	2.36	0.59
1:Z:588:GLN:N	1:Z:591:THR:OG1	2.36	0.59
1:1:511:TYR:HD2	1:1:520:VAL:HG22	1.67	0.59
1:3:300:GLN:NE2	1:3:703:TYR:O	2.36	0.59
1:8:355:TYR:CZ	1:8:357:LEU:HB2	2.37	0.59
1:A:254:ASN:O	1:A:255:ASN:C	2.42	0.59
1:D:254:ASN:O	1:D:255:ASN:C	2.42	0.59
1:D:511:TYR:HD2	1:D:520:VAL:HG22	1.67	0.59
1:E:254:ASN:O	1:E:257:LEU:N	2.35	0.59
1:G:300:GLN:NE2	1:G:703:TYR:O	2.36	0.59
1:K:254:ASN:O	1:K:255:ASN:C	2.42	0.59
1:K:588:GLN:N	1:K:591:THR:OG1	2.36	0.59
1:N:254:ASN:O	1:N:255:ASN:C	2.42	0.59
1:P:588:GLN:N	1:P:591:THR:OG1	2.36	0.59
1:R:254:ASN:O	1:R:255:ASN:C	2.42	0.59
1:C:407:ARG:HD2	1:S:225:SER:CA	104.34	0.59
1:S:511:TYR:HD2	1:S:520:VAL:HG22	1.67	0.59
1:T:407:ARG:HD2	1:Y:225:SER:CA	114.33	0.59
1:U:736:ARG:HH21	1:V:626:HIS:CD2	53.66	0.59
1:Z:254:ASN:O	1:Z:257:LEU:N	2.35	0.59
1:1:251:PRO:HG3	1:1:374:MET:HE3	1.84	0.58
1:2:355:TYR:CZ	1:2:357:LEU:HB2	2.38	0.58
1:6:355:TYR:CZ	1:6:357:LEU:HB2	2.38	0.58
1:8:588:GLN:N	1:8:591:THR:OG1	2.36	0.58
1:A:479:ASN:ND2	1:G:358:GLY:O	2.35	0.58
1:C:588:GLN:N	1:C:591:THR:OG1	2.36	0.58
1:D:355:TYR:CZ	1:D:357:LEU:HB2	2.38	0.58
1:F:254:ASN:O	1:F:257:LEU:N	2.35	0.58
1:H:737:ASN:ND2	1:W:396:TYR:OH	2.32	0.58
1:G:440:LEU:HD11	1:I:279:SER:HB2	1.85	0.58
1:J:300:GLN:NE2	1:J:703:TYR:O	2.36	0.58
1:L:254:ASN:O	1:L:255:ASN:C	2.42	0.58
1:L:588:GLN:N	1:L:591:THR:OG1	2.36	0.58
1:M:300:GLN:NE2	1:M:703:TYR:O	2.36	0.58
1:M:407:ARG:HD2	1:N:225:SER:CA	24.05	0.58
1:O:300:GLN:NE2	1:O:703:TYR:O	2.36	0.58
1:Q:736:ARG:HH21	1:R:626:HIS:CD2	53.67	0.58
1:X:300:GLN:NE2	1:X:703:TYR:O	2.36	0.58
1:Z:300:GLN:NE2	1:Z:703:TYR:O	2.36	0.58
1:Z:511:TYR:HD2	1:Z:520:VAL:HG22	1.67	0.58
1:2:511:TYR:HD2	1:2:520:VAL:HG22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:254:ASN:O	1:6:257:LEU:N	2.35	0.58
1:6:511:TYR:HD2	1:6:520:VAL:HG22	1.67	0.58
1:8:254:ASN:O	1:8:255:ASN:C	2.42	0.58
1:A:626:HIS:CD2	1:K:736:ARG:HH21	87.80	0.58
1:C:511:TYR:HD2	1:C:520:VAL:HG22	1.67	0.58
1:K:254:ASN:O	1:K:257:LEU:N	2.35	0.58
1:L:407:ARG:HD2	1:N:225:SER:CA	113.14	0.58
1:M:333:LYS:NZ	1:N:659:ASP:OD2	2.32	0.58
1:R:407:ARG:HD2	1:V:225:SER:CA	2.33	0.58
1:R:736:ARG:HH21	1:S:626:HIS:CD2	2.22	0.58
1:A:225:SER:CA	1:Z:407:ARG:HD2	103.06	0.58
1:1:254:ASN:O	1:1:257:LEU:N	2.35	0.58
1:1:355:TYR:CZ	1:1:357:LEU:HB2	2.38	0.58
1:3:355:TYR:CZ	1:3:357:LEU:HB2	2.38	0.58
1:4:251:PRO:HG3	1:4:374:MET:HE3	1.84	0.58
1:5:355:TYR:CZ	1:5:357:LEU:HB2	2.38	0.58
1:A:324:LYS:NZ	1:A:337:ASN:OD1	2.36	0.58
1:B:588:GLN:N	1:B:591:THR:OG1	2.36	0.58
1:B:626:HIS:CD2	1:L:736:ARG:HH21	2.21	0.58
1:B:626:HIS:CD2	1:C:736:ARG:HH21	39.37	0.58
1:I:307:TRP:O	1:I:426:SER:OG	2.18	0.58
1:I:300:GLN:NE2	1:I:703:TYR:O	2.36	0.58
1:N:324:LYS:NZ	1:N:337:ASN:OD1	2.37	0.58
1:P:254:ASN:O	1:P:255:ASN:C	2.42	0.58
1:Q:225:SER:CA	1:Y:407:ARG:HD2	144.09	0.58
1:T:254:ASN:O	1:T:257:LEU:N	2.35	0.58
1:1:254:ASN:O	1:1:256:HIS:N	2.37	0.58
1:2:300:GLN:NE2	1:2:703:TYR:O	2.36	0.58
1:3:254:ASN:O	1:3:257:LEU:N	2.35	0.58
1:5:659:ASP:OD2	1:8:333:LYS:NZ	2.31	0.58
1:7:511:TYR:HD2	1:7:520:VAL:HG22	1.67	0.58
1:8:307:TRP:O	1:8:426:SER:OG	2.18	0.58
1:C:324:LYS:NZ	1:C:337:ASN:OD1	2.36	0.58
1:D:626:HIS:CD2	1:T:736:ARG:HH21	104.59	0.58
1:E:511:TYR:HD2	1:E:520:VAL:HG22	1.67	0.58
1:G:407:ARG:HD2	1:K:225:SER:CA	144.57	0.58
1:H:355:TYR:CZ	1:H:357:LEU:HB2	2.38	0.58
1:I:324:LYS:NZ	1:I:337:ASN:OD1	2.36	0.58
1:I:736:ARG:HH21	1:J:626:HIS:CD2	39.37	0.58
1:J:479:ASN:ND2	1:K:358:GLY:O	53.78	0.58
1:R:254:ASN:O	1:R:256:HIS:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:324:LYS:NZ	1:R:337:ASN:OD1	2.36	0.58
1:D:407:ARG:HD2	1:S:225:SER:CA	96.25	0.58
1:S:254:ASN:O	1:S:255:ASN:C	2.42	0.58
1:T:254:ASN:O	1:T:256:HIS:N	2.37	0.58
1:T:300:GLN:NE2	1:T:703:TYR:O	2.36	0.58
1:U:254:ASN:O	1:U:255:ASN:C	2.42	0.58
1:Y:254:ASN:O	1:Y:256:HIS:N	2.37	0.58
1:4:254:ASN:O	1:4:256:HIS:N	2.37	0.58
1:A:254:ASN:O	1:A:256:HIS:N	2.37	0.58
1:C:254:ASN:O	1:C:256:HIS:N	2.37	0.58
1:F:254:ASN:O	1:F:255:ASN:C	2.42	0.58
1:E:626:HIS:CD2	1:F:736:ARG:HH21	2.22	0.58
1:F:736:ARG:HH21	1:H:626:HIS:CD2	111.64	0.58
1:G:324:LYS:NZ	1:G:337:ASN:OD1	2.36	0.58
1:F:626:HIS:CD2	1:G:736:ARG:HH21	83.68	0.58
1:H:254:ASN:O	1:H:256:HIS:N	2.37	0.58
1:H:626:HIS:CD2	1:Y:736:ARG:HH21	2.22	0.58
1:I:254:ASN:O	1:I:255:ASN:C	2.42	0.58
1:G:479:ASN:ND2	1:I:358:GLY:O	2.36	0.58
1:I:626:HIS:CD2	1:K:736:ARG:HH21	88.36	0.58
1:M:254:ASN:O	1:M:256:HIS:N	2.37	0.58
1:N:254:ASN:O	1:N:256:HIS:N	2.37	0.58
1:O:324:LYS:NZ	1:O:337:ASN:OD1	2.36	0.58
1:P:324:LYS:NZ	1:P:337:ASN:OD1	2.36	0.58
1:R:300:GLN:NE2	1:R:703:TYR:O	2.36	0.58
1:Q:225:SER:CA	1:S:407:ARG:HD2	2.33	0.58
1:T:324:LYS:NZ	1:T:337:ASN:OD1	2.36	0.58
1:I:333:LYS:NZ	1:T:659:ASP:OD2	202.37	0.58
1:V:407:ARG:HD2	1:W:225:SER:CA	2.33	0.58
1:V:659:ASP:OD2	1:1:333:LYS:NZ	188.72	0.58
1:Z:254:ASN:O	1:Z:256:HIS:N	2.37	0.58
1:Z:407:ARG:HD2	1:4:225:SER:CA	89.32	0.58
1:Z:736:ARG:HH21	1:1:626:HIS:CD2	82.32	0.58
1:3:254:ASN:O	1:3:255:ASN:C	2.42	0.58
1:3:324:LYS:NZ	1:3:337:ASN:OD1	2.36	0.58
1:Z:736:ARG:HH21	1:4:626:HIS:CD2	2.21	0.58
1:7:300:GLN:NE2	1:7:703:TYR:O	2.36	0.58
1:7:355:TYR:CZ	1:7:357:LEU:HB2	2.37	0.58
1:B:321:ILE:HD13	1:B:343:ILE:HD11	1.86	0.58
1:C:254:ASN:O	1:C:257:LEU:N	2.35	0.58
1:E:300:GLN:NE2	1:E:703:TYR:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:TYR:CZ	1:E:357:LEU:HB2	2.38	0.58
1:G:254:ASN:O	1:G:255:ASN:C	2.42	0.58
1:F:333:LYS:NZ	1:G:659:ASP:OD2	2.30	0.58
1:J:254:ASN:O	1:J:255:ASN:C	2.42	0.58
1:K:254:ASN:O	1:K:256:HIS:N	2.37	0.58
1:K:355:TYR:CZ	1:K:357:LEU:HB2	2.38	0.58
1:N:321:ILE:HD13	1:N:343:ILE:HD11	1.86	0.58
1:O:254:ASN:O	1:O:256:HIS:N	2.37	0.58
1:Q:254:ASN:O	1:Q:257:LEU:N	2.35	0.58
1:Q:300:GLN:NE2	1:Q:703:TYR:O	2.36	0.58
1:E:407:ARG:HD2	1:U:225:SER:CA	144.24	0.58
1:W:300:GLN:NE2	1:W:703:TYR:O	2.36	0.58
1:1:254:ASN:O	1:1:255:ASN:C	2.42	0.58
1:3:254:ASN:O	1:3:256:HIS:N	2.37	0.58
1:5:254:ASN:O	1:5:257:LEU:N	2.35	0.58
1:5:300:GLN:NE2	1:5:703:TYR:O	2.36	0.58
1:K:407:ARG:HD2	1:7:225:SER:CA	2.33	0.58
1:7:254:ASN:O	1:7:255:ASN:C	2.42	0.58
1:7:254:ASN:O	1:7:257:LEU:N	2.35	0.58
1:B:254:ASN:O	1:B:256:HIS:N	2.37	0.58
1:D:736:ARG:HH21	1:N:626:HIS:CD2	2.22	0.58
1:E:254:ASN:O	1:E:255:ASN:C	2.42	0.58
1:K:321:ILE:HD13	1:K:343:ILE:HD11	1.86	0.58
1:L:254:ASN:O	1:L:256:HIS:N	2.37	0.58
1:N:736:ARG:HH21	1:O:626:HIS:CD2	53.66	0.58
1:O:254:ASN:O	1:O:255:ASN:C	2.42	0.58
1:Q:358:GLY:O	1:S:479:ASN:ND2	83.84	0.58
1:T:254:ASN:O	1:T:255:ASN:C	2.42	0.58
1:U:254:ASN:O	1:U:256:HIS:N	2.37	0.58
1:V:251:PRO:HG3	1:V:374:MET:HE3	1.88	0.58
1:W:736:ARG:HH21	1:Y:626:HIS:CD2	2.22	0.58
1:W:626:HIS:CD2	1:Y:736:ARG:HH21	31.21	0.58
1:Z:254:ASN:O	1:Z:255:ASN:C	2.42	0.58
1:4:324:LYS:NZ	1:4:337:ASN:OD1	2.36	0.58
1:5:736:ARG:HH21	1:6:626:HIS:CD2	2.21	0.58
1:6:736:ARG:HH21	1:7:626:HIS:CD2	2.22	0.58
1:A:321:ILE:HD13	1:A:343:ILE:HD11	1.86	0.58
1:D:407:ARG:HD2	1:E:225:SER:CA	2.33	0.58
1:H:321:ILE:HD13	1:H:343:ILE:HD11	1.86	0.58
1:M:479:ASN:ND2	1:N:358:GLY:O	70.01	0.58
1:C:279:SER:HB2	1:P:440:LEU:HD11	39.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:254:ASN:O	1:X:255:ASN:C	2.42	0.58
1:X:321:ILE:HD13	1:X:343:ILE:HD11	1.86	0.58
1:3:321:ILE:HD13	1:3:343:ILE:HD11	1.86	0.58
1:4:321:ILE:HD13	1:4:343:ILE:HD11	1.86	0.58
1:6:254:ASN:O	1:6:256:HIS:N	2.37	0.58
1:B:300:GLN:NE2	1:B:703:TYR:O	2.36	0.58
1:D:254:ASN:O	1:D:256:HIS:N	2.37	0.58
1:F:254:ASN:O	1:F:256:HIS:N	2.37	0.58
1:G:321:ILE:HD13	1:G:343:ILE:HD11	1.86	0.58
1:L:321:ILE:HD13	1:L:343:ILE:HD11	1.86	0.58
1:M:254:ASN:O	1:M:255:ASN:C	2.42	0.58
1:M:321:ILE:HD13	1:M:343:ILE:HD11	1.86	0.58
1:O:321:ILE:HD13	1:O:343:ILE:HD11	1.86	0.58
1:P:321:ILE:HD13	1:P:343:ILE:HD11	1.86	0.58
1:L:736:ARG:HH21	1:T:626:HIS:CD2	179.08	0.58
1:T:333:LYS:NZ	1:U:659:ASP:OD2	2.32	0.58
1:V:254:ASN:O	1:V:256:HIS:N	2.37	0.58
1:W:254:ASN:O	1:W:256:HIS:N	2.37	0.58
1:X:254:ASN:O	1:X:256:HIS:N	2.37	0.58
1:E:479:ASN:ND2	1:X:358:GLY:O	138.71	0.58
1:X:479:ASN:ND2	1:Y:358:GLY:O	70.01	0.58
1:Y:321:ILE:HD13	1:Y:343:ILE:HD11	1.86	0.58
1:2:254:ASN:O	1:2:256:HIS:N	2.37	0.58
1:3:626:HIS:CD2	1:4:736:ARG:HH21	2.22	0.58
1:6:324:LYS:NZ	1:6:337:ASN:OD1	2.36	0.58
1:7:254:ASN:O	1:7:256:HIS:N	2.37	0.58
1:C:321:ILE:HD13	1:C:343:ILE:HD11	1.86	0.58
1:C:358:GLY:O	1:P:479:ASN:ND2	54.36	0.58
1:E:254:ASN:O	1:E:256:HIS:N	2.37	0.58
1:E:626:HIS:CD2	1:V:736:ARG:HH21	110.66	0.58
1:H:358:GLY:O	1:Y:479:ASN:ND2	2.37	0.58
1:I:225:SER:CA	1:J:407:ARG:HD2	2.33	0.58
1:L:324:LYS:NZ	1:L:337:ASN:OD1	2.37	0.58
1:B:225:SER:CA	1:O:407:ARG:HD2	113.62	0.58
1:Q:254:ASN:O	1:Q:256:HIS:N	2.37	0.58
1:Q:321:ILE:HD13	1:Q:343:ILE:HD11	1.86	0.58
1:V:324:LYS:NZ	1:V:337:ASN:OD1	2.36	0.58
1:V:321:ILE:HD13	1:V:343:ILE:HD11	1.86	0.58
1:W:321:ILE:HD13	1:W:343:ILE:HD11	1.86	0.58
1:6:251:PRO:HG3	1:6:374:MET:HE3	1.86	0.57
1:8:254:ASN:O	1:8:256:HIS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:324:LYS:NZ	1:8:337:ASN:OD1	2.37	0.57
1:B:659:ASP:OD2	1:L:333:LYS:NZ	96.43	0.57
1:B:737:ASN:ND2	1:J:396:TYR:OH	2.32	0.57
1:H:324:LYS:NZ	1:H:337:ASN:OD1	2.36	0.57
1:J:321:ILE:HD13	1:J:343:ILE:HD11	1.86	0.57
1:L:254:ASN:O	1:L:257:LEU:N	2.35	0.57
1:R:321:ILE:HD13	1:R:343:ILE:HD11	1.86	0.57
1:S:254:ASN:O	1:S:256:HIS:N	2.37	0.57
1:M:333:LYS:NZ	1:S:659:ASP:OD2	128.80	0.57
1:U:324:LYS:NZ	1:U:337:ASN:OD1	2.36	0.57
1:U:737:ASN:ND2	1:V:396:TYR:OH	52.73	0.57
1:H:479:ASN:ND2	1:W:358:GLY:O	2.37	0.57
1:V:358:GLY:O	1:X:479:ASN:ND2	2.37	0.57
1:W:736:ARG:HH21	1:X:626:HIS:CD2	53.66	0.57
1:H:407:ARG:HD2	1:Z:225:SER:CA	2.33	0.57
1:Z:324:LYS:NZ	1:Z:337:ASN:OD1	2.36	0.57
1:Z:626:HIS:CD2	1:2:736:ARG:HH21	67.04	0.57
1:1:300:GLN:NE2	1:1:703:TYR:O	2.36	0.57
1:T:225:SER:CA	1:6:407:ARG:HD2	161.12	0.57
1:A:407:ARG:HD2	1:B:225:SER:CA	2.33	0.57
1:C:225:SER:CA	1:M:407:ARG:HD2	89.32	0.57
1:F:324:LYS:NZ	1:F:337:ASN:OD1	2.36	0.57
1:F:479:ASN:ND2	1:H:358:GLY:O	124.35	0.57
1:M:324:LYS:NZ	1:M:337:ASN:OD1	2.36	0.57
1:P:254:ASN:O	1:P:256:HIS:N	2.37	0.57
1:L:440:LEU:HD11	1:T:279:SER:HB2	204.87	0.57
1:U:407:ARG:HD2	1:5:225:SER:CA	163.60	0.57
1:Y:225:SER:CA	1:4:407:ARG:HD2	2.33	0.57
1:Z:279:SER:HB2	1:2:440:LEU:HD11	97.73	0.57
1:G:333:LYS:NZ	1:1:659:ASP:OD2	193.58	0.57
1:5:254:ASN:O	1:5:256:HIS:N	2.37	0.57
1:B:324:LYS:NZ	1:B:337:ASN:OD1	2.37	0.57
1:C:254:ASN:O	1:C:255:ASN:C	2.42	0.57
1:C:626:HIS:CD2	1:P:736:ARG:HH21	56.16	0.57
1:C:736:ARG:HH21	1:O:626:HIS:CD2	134.53	0.57
1:D:324:LYS:NZ	1:D:337:ASN:OD1	2.36	0.57
1:F:251:PRO:HG3	1:F:374:MET:HE3	1.86	0.57
1:F:626:HIS:CD2	1:Q:736:ARG:HH21	2.22	0.57
1:G:626:HIS:CD2	1:H:736:ARG:HH21	53.67	0.57
1:I:321:ILE:HD13	1:I:343:ILE:HD11	1.86	0.57
1:K:324:LYS:NZ	1:K:337:ASN:OD1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:736:ARG:HH21	1:N:626:HIS:CD2	39.37	0.57
1:R:659:ASP:OD2	1:X:333:LYS:NZ	96.34	0.57
1:S:321:ILE:HD13	1:S:343:ILE:HD11	1.86	0.57
1:W:254:ASN:O	1:W:255:ASN:C	2.42	0.57
1:W:324:LYS:NZ	1:W:337:ASN:OD1	2.36	0.57
1:V:225:SER:CA	1:W:407:ARG:HD2	24.05	0.57
1:V:626:HIS:CD2	1:X:736:ARG:HH21	2.22	0.57
1:7:321:ILE:HD13	1:7:343:ILE:HD11	1.86	0.57
1:5:626:HIS:CD2	1:7:736:ARG:HH21	2.22	0.57
1:8:321:ILE:HD13	1:8:343:ILE:HD11	1.86	0.57
1:C:626:HIS:CD2	1:M:736:ARG:HH21	2.22	0.57
1:F:225:SER:CA	1:X:407:ARG:HD2	103.39	0.57
1:H:659:ASP:OD2	1:Z:333:LYS:NZ	2.32	0.57
1:K:487:ARG:HG2	1:K:488:GLN:N	2.20	0.57
1:M:225:SER:CA	1:S:407:ARG:HD2	100.45	0.57
1:P:407:ARG:HD2	1:6:225:SER:CA	152.32	0.57
1:P:659:ASP:OD2	1:6:333:LYS:NZ	193.57	0.57
1:Q:254:ASN:O	1:Q:255:ASN:C	2.42	0.57
1:Q:324:LYS:NZ	1:Q:337:ASN:OD1	2.37	0.57
1:R:479:ASN:ND2	1:S:358:GLY:O	2.37	0.57
1:T:736:ARG:HH21	1:U:626:HIS:CD2	39.37	0.57
1:1:487:ARG:HG2	1:1:488:GLN:N	2.20	0.57
1:1:736:ARG:HH21	1:2:626:HIS:CD2	2.22	0.57
1:7:324:LYS:NZ	1:7:337:ASN:OD1	2.36	0.57
1:B:736:ARG:HH21	1:J:626:HIS:CD2	2.21	0.57
1:E:321:ILE:HD13	1:E:343:ILE:HD11	1.86	0.57
1:E:487:ARG:HG2	1:E:488:GLN:N	2.20	0.57
1:G:736:ARG:HH21	1:I:626:HIS:CD2	2.22	0.57
1:H:487:ARG:HG2	1:H:488:GLN:N	2.20	0.57
1:J:254:ASN:O	1:J:256:HIS:N	2.37	0.57
1:J:324:LYS:NZ	1:J:337:ASN:OD1	2.36	0.57
1:J:736:ARG:HH21	1:K:626:HIS:CD2	53.67	0.57
1:J:440:LEU:HD11	1:K:279:SER:HB2	42.58	0.57
1:D:736:ARG:HH21	1:L:626:HIS:CD2	111.64	0.57
1:O:736:ARG:HH21	1:P:626:HIS:CD2	39.36	0.57
1:S:736:ARG:HH21	1:U:626:HIS:CD2	2.22	0.57
1:T:479:ASN:ND2	1:U:358:GLY:O	70.02	0.57
1:T:487:ARG:HG2	1:T:488:GLN:N	2.20	0.57
1:Y:324:LYS:NZ	1:Y:337:ASN:OD1	2.37	0.57
1:Z:626:HIS:CD2	1:3:736:ARG:HH21	2.22	0.57
1:2:696:ARG:NE	1:2:698:ASN:OD1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:254:ASN:O	1:6:255:ASN:C	2.42	0.57
1:B:358:GLY:O	1:C:479:ASN:ND2	70.02	0.57
1:E:324:LYS:NZ	1:E:337:ASN:OD1	2.36	0.57
1:G:254:ASN:O	1:G:256:HIS:N	2.37	0.57
1:J:225:SER:CA	1:X:407:ARG:HD2	113.62	0.57
1:J:736:ARG:HH21	1:L:626:HIS:CD2	2.22	0.57
1:B:358:GLY:O	1:L:479:ASN:ND2	2.37	0.57
1:N:487:ARG:HG2	1:N:488:GLN:N	2.20	0.57
1:D:333:LYS:NZ	1:O:659:ASP:OD2	125.46	0.57
1:O:479:ASN:ND2	1:P:358:GLY:O	70.01	0.57
1:D:626:HIS:CD2	1:P:736:ARG:HH21	2.22	0.57
1:S:487:ARG:HG2	1:S:488:GLN:N	2.20	0.57
1:L:479:ASN:ND2	1:T:358:GLY:O	192.71	0.57
1:T:626:HIS:CD2	1:V:736:ARG:HH21	88.36	0.57
1:U:321:ILE:HD13	1:U:343:ILE:HD11	1.86	0.57
1:U:487:ARG:HG2	1:U:488:GLN:N	2.20	0.57
1:R:626:HIS:CD2	1:U:736:ARG:HH21	2.22	0.57
1:V:254:ASN:O	1:V:255:ASN:C	2.42	0.57
1:Z:487:ARG:HG2	1:Z:488:GLN:N	2.20	0.57
1:7:487:ARG:HG2	1:7:488:GLN:N	2.20	0.57
1:A:487:ARG:HG2	1:A:488:GLN:N	2.20	0.57
1:C:479:ASN:ND2	1:O:358:GLY:O	137.53	0.57
1:F:407:ARG:HD2	1:R:225:SER:CA	2.33	0.57
1:I:254:ASN:O	1:I:256:HIS:N	2.37	0.57
1:L:487:ARG:HG2	1:L:488:GLN:N	2.20	0.57
1:B:736:ARG:HH21	1:M:626:HIS:CD2	96.85	0.57
1:Q:251:PRO:HG3	1:Q:374:MET:HE3	1.87	0.57
1:Q:487:ARG:HG2	1:Q:488:GLN:N	2.20	0.57
1:R:659:ASP:OD2	1:V:333:LYS:NZ	2.31	0.57
1:T:440:LEU:HD11	1:U:279:SER:HB2	63.35	0.57
1:W:279:SER:HB2	1:Y:440:LEU:HD11	65.62	0.57
1:W:479:ASN:ND2	1:X:358:GLY:O	53.78	0.57
1:Z:358:GLY:O	1:2:479:ASN:ND2	89.67	0.57
1:Z:439:PRO:O	1:Z:470:PRO:HG3	2.05	0.57
1:1:479:ASN:ND2	1:2:358:GLY:O	2.37	0.57
1:2:487:ARG:HG2	1:2:488:GLN:N	2.20	0.57
1:Z:479:ASN:ND2	1:4:358:GLY:O	2.38	0.57
1:4:487:ARG:HG2	1:4:488:GLN:N	2.20	0.57
1:5:251:PRO:HG3	1:5:374:MET:HE3	1.87	0.57
1:D:487:ARG:HG2	1:D:488:GLN:N	2.20	0.57
1:F:279:SER:HB2	1:G:440:LEU:HD11	105.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:487:ARG:HG2	1:J:488:GLN:N	2.20	0.57
1:K:626:HIS:CD2	1:8:736:ARG:HH21	2.22	0.57
1:L:439:PRO:O	1:L:470:PRO:HG3	2.05	0.57
1:D:440:LEU:HD11	1:N:279:SER:HB2	1.87	0.57
1:N:439:PRO:O	1:N:470:PRO:HG3	2.05	0.57
1:P:439:PRO:O	1:P:470:PRO:HG3	2.05	0.57
1:N:407:ARG:HD2	1:R:225:SER:CA	144.56	0.57
1:X:736:ARG:HH21	1:Y:626:HIS:CD2	39.37	0.57
1:U:333:LYS:NZ	1:2:659:ASP:OD2	199.79	0.57
1:5:487:ARG:HG2	1:5:488:GLN:N	2.20	0.57
1:6:321:ILE:HD13	1:6:343:ILE:HD11	1.86	0.57
1:8:439:PRO:O	1:8:470:PRO:HG3	2.05	0.57
1:A:439:PRO:O	1:A:470:PRO:HG3	2.05	0.57
1:A:626:HIS:CD2	1:I:736:ARG:HH21	2.23	0.57
1:E:736:ARG:HH21	1:Q:626:HIS:CD2	2.22	0.57
1:F:321:ILE:HD13	1:F:343:ILE:HD11	1.86	0.57
1:F:487:ARG:HG2	1:F:488:GLN:N	2.20	0.57
1:F:358:GLY:O	1:G:479:ASN:ND2	83.84	0.57
1:E:225:SER:CA	1:H:407:ARG:HD2	113.14	0.57
1:A:279:SER:HB2	1:K:440:LEU:HD11	101.67	0.57
1:M:439:PRO:O	1:M:470:PRO:HG3	2.05	0.57
1:F:279:SER:HB2	1:Q:440:LEU:HD11	1.87	0.57
1:T:321:ILE:HD13	1:T:343:ILE:HD11	1.86	0.57
1:R:279:SER:HB2	1:U:440:LEU:HD11	1.87	0.57
1:R:358:GLY:O	1:U:479:ASN:ND2	2.37	0.57
1:W:439:PRO:O	1:W:470:PRO:HG3	2.05	0.57
1:X:225:SER:CA	1:Y:407:ARG:HD2	2.33	0.57
1:1:324:LYS:NZ	1:1:337:ASN:OD1	2.36	0.57
1:2:324:LYS:NZ	1:2:337:ASN:OD1	2.36	0.57
1:5:254:ASN:O	1:5:255:ASN:C	2.42	0.57
1:6:440:LEU:HD11	1:7:279:SER:HB2	1.87	0.57
1:A:358:GLY:O	1:I:479:ASN:ND2	2.37	0.57
1:A:736:ARG:HH21	1:8:626:HIS:CD2	129.42	0.57
1:B:487:ARG:HG2	1:B:488:GLN:N	2.20	0.57
1:D:225:SER:CA	1:O:407:ARG:HD2	100.99	0.57
1:A:225:SER:CA	1:E:407:ARG:HD2	2.32	0.57
1:F:439:PRO:O	1:F:470:PRO:HG3	2.05	0.57
1:F:225:SER:CA	1:G:407:ARG:HD2	2.34	0.57
1:B:440:LEU:HD11	1:J:279:SER:HB2	1.87	0.57
1:B:440:LEU:HD11	1:M:279:SER:HB2	146.04	0.57
1:M:696:ARG:HH21	1:M:698:ASN:HD21	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:626:HIS:CD2	1:O:736:ARG:HH21	88.35	0.57
1:P:487:ARG:HG2	1:P:488:GLN:N	2.20	0.57
1:S:439:PRO:O	1:S:470:PRO:HG3	2.05	0.57
1:S:440:LEU:HD11	1:U:279:SER:HB2	1.87	0.57
1:T:439:PRO:O	1:T:470:PRO:HG3	2.05	0.57
1:T:696:ARG:NE	1:T:698:ASN:OD1	2.36	0.57
1:2:696:ARG:HH21	1:2:698:ASN:HD21	1.54	0.56
1:6:487:ARG:HG2	1:6:488:GLN:N	2.20	0.56
1:B:439:PRO:O	1:B:470:PRO:HG3	2.05	0.56
1:D:696:ARG:HH21	1:D:698:ASN:HD21	1.53	0.56
1:E:439:PRO:O	1:E:470:PRO:HG3	2.05	0.56
1:E:736:ARG:HH21	1:X:626:HIS:CD2	134.02	0.56
1:H:439:PRO:O	1:H:470:PRO:HG3	2.05	0.56
1:J:439:PRO:O	1:J:470:PRO:HG3	2.05	0.56
1:J:696:ARG:HH21	1:J:698:ASN:HD21	1.54	0.56
1:L:696:ARG:NE	1:L:698:ASN:OD1	2.36	0.56
1:O:440:LEU:HD11	1:P:279:SER:HB2	63.35	0.56
1:F:358:GLY:O	1:Q:479:ASN:ND2	2.37	0.56
1:R:439:PRO:O	1:R:470:PRO:HG3	2.05	0.56
1:T:279:SER:HB2	1:V:440:LEU:HD11	67.07	0.56
1:E:279:SER:HB2	1:V:440:LEU:HD11	156.38	0.56
1:H:736:ARG:HH21	1:W:626:HIS:CD2	2.21	0.56
1:X:487:ARG:HG2	1:X:488:GLN:N	2.20	0.56
1:X:696:ARG:HH21	1:X:698:ASN:HD21	1.53	0.56
1:Z:279:SER:HB2	1:3:440:LEU:HD11	1.87	0.56
1:1:321:ILE:HD13	1:1:343:ILE:HD11	1.86	0.56
1:1:696:ARG:HH21	1:1:698:ASN:HD21	1.53	0.56
1:5:279:SER:HB2	1:7:440:LEU:HD11	1.87	0.56
1:8:487:ARG:HG2	1:8:488:GLN:N	2.20	0.56
1:E:440:LEU:HD11	1:Q:279:SER:HB2	1.87	0.56
1:G:487:ARG:HG2	1:G:488:GLN:N	2.20	0.56
1:N:479:ASN:ND2	1:O:358:GLY:O	53.78	0.56
1:N:696:ARG:NE	1:N:698:ASN:OD1	2.36	0.56
1:O:439:PRO:O	1:O:470:PRO:HG3	2.05	0.56
1:O:487:ARG:HG2	1:O:488:GLN:N	2.20	0.56
1:R:696:ARG:NE	1:R:698:ASN:OD1	2.36	0.56
1:Z:440:LEU:HD11	1:1:279:SER:HB2	103.98	0.56
1:Z:479:ASN:ND2	1:1:358:GLY:O	86.91	0.56
1:1:439:PRO:O	1:1:470:PRO:HG3	2.05	0.56
1:2:321:ILE:HD13	1:2:343:ILE:HD11	1.86	0.56
1:3:358:GLY:O	1:4:479:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:439:PRO:O	1:6:470:PRO:HG3	2.05	0.56
1:C:696:ARG:HH21	1:C:698:ASN:HD21	1.53	0.56
1:D:321:ILE:HD13	1:D:343:ILE:HD11	1.86	0.56
1:E:279:SER:HB2	1:F:440:LEU:HD11	1.87	0.56
1:I:439:PRO:O	1:I:470:PRO:HG3	2.05	0.56
1:I:479:ASN:ND2	1:J:358:GLY:O	70.01	0.56
1:J:407:ARG:HD2	1:L:225:SER:CA	89.32	0.56
1:D:479:ASN:ND2	1:L:358:GLY:O	124.35	0.56
1:L:696:ARG:HH21	1:L:698:ASN:HD21	1.54	0.56
1:M:487:ARG:HG2	1:M:488:GLN:N	2.20	0.56
1:T:659:ASP:OD2	1:Y:333:LYS:NZ	135.34	0.56
1:T:696:ARG:HH21	1:T:698:ASN:HD21	1.54	0.56
1:E:440:LEU:HD11	1:X:279:SER:HB2	168.91	0.56
1:Y:696:ARG:NE	1:Y:698:ASN:OD1	2.36	0.56
1:Z:696:ARG:NE	1:Z:698:ASN:OD1	2.36	0.56
1:3:307:TRP:O	1:3:426:SER:OG	2.18	0.56
1:B:254:ASN:O	1:B:255:ASN:C	2.42	0.56
1:F:696:ARG:NE	1:F:698:ASN:OD1	2.36	0.56
1:G:358:GLY:O	1:H:479:ASN:ND2	53.79	0.56
1:G:439:PRO:O	1:G:470:PRO:HG3	2.05	0.56
1:A:407:ARG:HD2	1:J:225:SER:CA	83.81	0.56
1:N:736:ARG:HH21	1:P:626:HIS:CD2	2.22	0.56
1:R:440:LEU:HD11	1:S:279:SER:HB2	1.87	0.56
1:T:358:GLY:O	1:V:479:ASN:ND2	87.33	0.56
1:V:439:PRO:O	1:V:470:PRO:HG3	2.05	0.56
1:V:696:ARG:NE	1:V:698:ASN:OD1	2.36	0.56
1:Z:321:ILE:HD13	1:Z:343:ILE:HD11	1.86	0.56
1:3:251:PRO:HG3	1:3:374:MET:HE3	1.87	0.56
1:4:696:ARG:NE	1:4:698:ASN:OD1	2.36	0.56
1:5:440:LEU:HD11	1:6:279:SER:HB2	1.87	0.56
1:C:440:LEU:HD11	1:O:279:SER:HB2	169.32	0.56
1:G:225:SER:CA	1:I:407:ARG:HD2	152.34	0.56
1:I:487:ARG:HG2	1:I:488:GLN:N	2.20	0.56
1:K:439:PRO:O	1:K:470:PRO:HG3	2.05	0.56
1:M:225:SER:CA	1:N:407:ARG:HD2	2.33	0.56
1:N:479:ASN:ND2	1:P:358:GLY:O	2.37	0.56
1:M:279:SER:HB2	1:O:440:LEU:HD11	67.07	0.56
1:R:487:ARG:HG2	1:R:488:GLN:N	2.20	0.56
1:S:324:LYS:NZ	1:S:337:ASN:OD1	2.36	0.56
1:K:407:ARG:HD2	1:W:225:SER:CA	159.06	0.56
1:Y:439:PRO:O	1:Y:470:PRO:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:439:PRO:O	1:3:470:PRO:HG3	2.05	0.56
1:4:439:PRO:O	1:4:470:PRO:HG3	2.05	0.56
1:D:439:PRO:O	1:D:470:PRO:HG3	2.05	0.56
1:F:407:ARG:HD2	1:Z:225:SER:CA	101.87	0.56
1:I:696:ARG:HH21	1:I:698:ASN:HD21	1.54	0.56
1:M:329:ASN:O	1:M:332:THR:OG1	2.21	0.56
1:N:659:ASP:OD2	1:R:333:LYS:NZ	189.62	0.56
1:Q:439:PRO:O	1:Q:470:PRO:HG3	2.05	0.56
1:U:439:PRO:O	1:U:470:PRO:HG3	2.05	0.56
1:H:279:SER:HB2	1:Y:440:LEU:HD11	1.87	0.56
1:Y:487:ARG:HG2	1:Y:488:GLN:N	2.20	0.56
1:1:348:ASP:OD2	1:1:352:GLN:N	2.39	0.56
1:2:348:ASP:OD2	1:2:352:GLN:N	2.39	0.56
1:2:439:PRO:O	1:2:470:PRO:HG3	2.05	0.56
1:3:487:ARG:HG2	1:3:488:GLN:N	2.20	0.56
1:4:348:ASP:OD2	1:4:352:GLN:N	2.39	0.56
1:Y:333:LYS:NZ	1:4:659:ASP:OD2	2.32	0.56
1:D:348:ASP:OD2	1:D:352:GLN:N	2.39	0.56
1:I:440:LEU:HD11	1:J:279:SER:HB2	63.35	0.56
1:C:358:GLY:O	1:M:479:ASN:ND2	2.37	0.56
1:N:696:ARG:HH21	1:N:698:ASN:HD21	1.53	0.56
1:E:479:ASN:ND2	1:Q:358:GLY:O	2.37	0.56
1:R:407:ARG:HD2	1:X:225:SER:CA	82.54	0.56
1:T:348:ASP:OD2	1:T:352:GLN:N	2.39	0.56
1:W:487:ARG:HG2	1:W:488:GLN:N	2.20	0.56
1:5:439:PRO:O	1:5:470:PRO:HG3	2.05	0.56
1:A:696:ARG:HH21	1:A:698:ASN:HD21	1.53	0.56
1:C:487:ARG:HG2	1:C:488:GLN:N	2.20	0.56
1:D:358:GLY:O	1:P:479:ASN:ND2	2.37	0.56
1:F:440:LEU:HD11	1:H:279:SER:HB2	131.51	0.56
1:I:358:GLY:O	1:K:479:ASN:ND2	87.33	0.56
1:N:348:ASP:OD2	1:N:352:GLN:N	2.39	0.56
1:Q:626:HIS:CD2	1:S:736:ARG:HH21	83.68	0.56
1:U:348:ASP:OD2	1:U:352:GLN:N	2.39	0.56
1:T:225:SER:CA	1:U:407:ARG:HD2	2.33	0.56
1:X:531:ASP:OD1	1:X:569:LYS:NZ	2.28	0.56
1:5:321:ILE:HD13	1:5:343:ILE:HD11	1.86	0.56
1:5:324:LYS:NZ	1:5:337:ASN:OD1	2.37	0.56
1:5:479:ASN:ND2	1:6:358:GLY:O	2.38	0.56
1:7:696:ARG:HH21	1:7:698:ASN:HD21	1.53	0.56
1:C:531:ASP:OD1	1:C:569:LYS:NZ	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:GLY:O	1:T:479:ASN:ND2	121.89	0.56
1:I:531:ASP:OD1	1:I:569:LYS:NZ	2.28	0.56
1:L:348:ASP:OD2	1:L:352:GLN:N	2.39	0.56
1:J:479:ASN:ND2	1:L:358:GLY:O	2.37	0.56
1:M:348:ASP:OD2	1:M:352:GLN:N	2.39	0.56
1:O:348:ASP:OD2	1:O:352:GLN:N	2.39	0.56
1:Q:696:ARG:HH21	1:Q:698:ASN:HD21	1.54	0.56
1:V:487:ARG:HG2	1:V:488:GLN:N	2.20	0.56
1:W:696:ARG:HH21	1:W:698:ASN:HD21	1.54	0.56
1:1:315:ASN:OD1	1:1:316:PHE:N	2.39	0.56
1:3:348:ASP:OD2	1:3:352:GLN:N	2.39	0.56
1:B:348:ASP:OD2	1:B:352:GLN:N	2.39	0.56
1:E:696:ARG:HH21	1:E:698:ASN:HD21	1.54	0.56
1:F:315:ASN:OD1	1:F:316:PHE:N	2.39	0.56
1:G:348:ASP:OD2	1:G:352:GLN:N	2.39	0.56
1:G:696:ARG:HH21	1:G:698:ASN:HD21	1.53	0.56
1:J:315:ASN:OD1	1:J:316:PHE:N	2.39	0.56
1:J:348:ASP:OD2	1:J:352:GLN:N	2.39	0.56
1:K:348:ASP:OD2	1:K:352:GLN:N	2.39	0.56
1:P:348:ASP:OD2	1:P:352:GLN:N	2.39	0.56
1:P:696:ARG:HH21	1:P:698:ASN:HD21	1.54	0.56
1:R:348:ASP:OD2	1:R:352:GLN:N	2.39	0.56
1:R:696:ARG:HH21	1:R:698:ASN:HD21	1.53	0.56
1:S:348:ASP:OD2	1:S:352:GLN:N	2.39	0.56
1:W:440:LEU:HD11	1:Y:279:SER:HB2	1.87	0.56
1:Z:696:ARG:HH21	1:Z:698:ASN:HD21	1.54	0.56
1:7:439:PRO:O	1:7:470:PRO:HG3	2.05	0.56
1:5:358:GLY:O	1:7:479:ASN:ND2	2.37	0.56
1:8:348:ASP:OD2	1:8:352:GLN:N	2.39	0.56
1:K:358:GLY:O	1:8:479:ASN:ND2	2.37	0.56
1:A:479:ASN:ND2	1:8:358:GLY:O	147.67	0.56
1:C:348:ASP:OD2	1:C:352:GLN:N	2.39	0.56
1:I:348:ASP:OD2	1:I:352:GLN:N	2.39	0.56
1:D:440:LEU:HD11	1:L:279:SER:HB2	131.51	0.56
1:T:315:ASN:OD1	1:T:316:PHE:N	2.39	0.56
1:V:407:ARG:HD2	1:1:225:SER:CA	152.80	0.56
1:X:348:ASP:OD2	1:X:352:GLN:N	2.39	0.56
1:X:439:PRO:O	1:X:470:PRO:HG3	2.05	0.56
1:Y:251:PRO:HG3	1:Y:374:MET:HE3	1.88	0.56
1:1:440:LEU:HD11	1:2:279:SER:HB2	1.87	0.55
1:2:333:LYS:NZ	1:3:659:ASP:OD2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:SER:HB2	1:I:440:LEU:HD11	1.87	0.55
1:B:315:ASN:OD1	1:B:316:PHE:N	2.39	0.55
1:E:315:ASN:OD1	1:E:316:PHE:N	2.39	0.55
1:H:315:ASN:OD1	1:H:316:PHE:N	2.39	0.55
1:I:225:SER:CA	1:T:407:ARG:HD2	164.06	0.55
1:M:358:GLY:O	1:O:479:ASN:ND2	87.33	0.55
1:S:315:ASN:OD1	1:S:316:PHE:N	2.39	0.55
1:U:315:ASN:OD1	1:U:316:PHE:N	2.39	0.55
1:U:440:LEU:HD11	1:V:279:SER:HB2	42.58	0.55
1:V:315:ASN:OD1	1:V:316:PHE:N	2.39	0.55
1:W:348:ASP:OD2	1:W:352:GLN:N	2.39	0.55
1:X:315:ASN:OD1	1:X:316:PHE:N	2.39	0.55
1:Y:348:ASP:OD2	1:Y:352:GLN:N	2.39	0.55
1:Y:696:ARG:HH21	1:Y:698:ASN:HD21	1.54	0.55
1:6:696:ARG:HH21	1:6:698:ASN:HD21	1.53	0.55
1:7:315:ASN:OD1	1:7:316:PHE:N	2.39	0.55
1:7:348:ASP:OD2	1:7:352:GLN:N	2.39	0.55
1:A:348:ASP:OD2	1:A:352:GLN:N	2.39	0.55
1:B:564:SER:OG	1:B:566:GLU:HG2	2.07	0.55
1:C:315:ASN:OD1	1:C:316:PHE:N	2.39	0.55
1:E:348:ASP:OD2	1:E:352:GLN:N	2.39	0.55
1:I:315:ASN:OD1	1:I:316:PHE:N	2.39	0.55
1:K:315:ASN:OD1	1:K:316:PHE:N	2.39	0.55
1:J:440:LEU:HD11	1:L:279:SER:HB2	1.87	0.55
1:M:290:PHE:O	1:M:293:HIS:N	2.39	0.55
1:Q:440:LEU:HD11	1:R:279:SER:HB2	42.59	0.55
1:V:348:ASP:OD2	1:V:352:GLN:N	2.39	0.55
1:W:315:ASN:OD1	1:W:316:PHE:N	2.39	0.55
1:X:564:SER:OG	1:X:566:GLU:HG2	2.07	0.55
1:Q:702:GLN:N	1:X:704:THR:OG1	110.28	0.55
1:Z:358:GLY:O	1:3:479:ASN:ND2	2.37	0.55
1:2:564:SER:OG	1:2:566:GLU:HG2	2.06	0.55
1:3:696:ARG:HH21	1:3:698:ASN:HD21	1.54	0.55
1:A:564:SER:OG	1:A:566:GLU:HG2	2.07	0.55
1:B:407:ARG:HD2	1:C:225:SER:CA	2.33	0.55
1:C:439:PRO:O	1:C:470:PRO:HG3	2.05	0.55
1:C:564:SER:OG	1:C:566:GLU:HG2	2.07	0.55
1:D:564:SER:OG	1:D:566:GLU:HG2	2.07	0.55
1:G:564:SER:OG	1:G:566:GLU:HG2	2.07	0.55
1:L:564:SER:OG	1:L:566:GLU:HG2	2.07	0.55
1:N:564:SER:OG	1:N:566:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:696:ARG:HH21	1:O:698:ASN:HD21	1.53	0.55
1:P:564:SER:OG	1:P:566:GLU:HG2	2.07	0.55
1:Q:348:ASP:OD2	1:Q:352:GLN:N	2.39	0.55
1:X:324:LYS:NZ	1:X:337:ASN:OD1	2.36	0.55
1:5:696:ARG:HH21	1:5:698:ASN:HD21	1.53	0.55
1:O:225:SER:CA	1:7:407:ARG:HD2	151.65	0.55
1:B:279:SER:HB2	1:C:440:LEU:HD11	63.35	0.55
1:B:407:ARG:HD2	1:L:225:SER:CA	74.33	0.55
1:D:479:ASN:ND2	1:N:358:GLY:O	2.37	0.55
1:F:696:ARG:HH21	1:F:698:ASN:HD21	1.53	0.55
1:G:279:SER:HB2	1:H:440:LEU:HD11	42.60	0.55
1:J:290:PHE:O	1:J:293:HIS:N	2.39	0.55
1:J:564:SER:OG	1:J:566:GLU:HG2	2.07	0.55
1:C:279:SER:HB2	1:M:440:LEU:HD11	1.87	0.55
1:Q:315:ASN:OD1	1:Q:316:PHE:N	2.39	0.55
1:R:315:ASN:OD1	1:R:316:PHE:N	2.39	0.55
1:X:696:ARG:NE	1:X:698:ASN:OD1	2.36	0.55
1:Y:564:SER:OG	1:Y:566:GLU:HG2	2.07	0.55
1:5:348:ASP:OD2	1:5:352:GLN:N	2.39	0.55
1:8:696:ARG:HH21	1:8:698:ASN:HD21	1.54	0.55
1:D:290:PHE:O	1:D:293:HIS:N	2.39	0.55
1:D:659:ASP:OD2	1:S:333:LYS:NZ	113.89	0.55
1:E:358:GLY:O	1:F:479:ASN:ND2	2.37	0.55
1:F:348:ASP:OD2	1:F:352:GLN:N	2.39	0.55
1:F:564:SER:OG	1:F:566:GLU:HG2	2.07	0.55
1:I:279:SER:HB2	1:K:440:LEU:HD11	67.07	0.55
1:K:564:SER:OG	1:K:566:GLU:HG2	2.07	0.55
1:B:279:SER:HB2	1:L:440:LEU:HD11	1.87	0.55
1:N:440:LEU:HD11	1:P:279:SER:HB2	1.87	0.55
1:P:382:THR:HG22	1:P:383:LEU:H	1.72	0.55
1:W:440:LEU:HD11	1:X:279:SER:HB2	42.58	0.55
1:X:440:LEU:HD11	1:Y:279:SER:HB2	63.35	0.55
1:Y:315:ASN:OD1	1:Y:316:PHE:N	2.39	0.55
1:Y:382:THR:HG22	1:Y:383:LEU:H	1.72	0.55
1:2:290:PHE:O	1:2:293:HIS:N	2.39	0.55
1:6:382:THR:HG22	1:6:383:LEU:H	1.72	0.55
1:8:382:THR:HG22	1:8:383:LEU:H	1.72	0.55
1:K:279:SER:HB2	1:8:440:LEU:HD11	1.87	0.55
1:A:382:THR:HG22	1:A:383:LEU:H	1.72	0.55
1:C:290:PHE:O	1:C:293:HIS:N	2.39	0.55
1:E:564:SER:OG	1:E:566:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:THR:HG22	1:F:383:LEU:H	1.72	0.55
1:G:290:PHE:O	1:G:293:HIS:N	2.39	0.55
1:H:564:SER:OG	1:H:566:GLU:HG2	2.07	0.55
1:I:290:PHE:O	1:I:293:HIS:N	2.39	0.55
1:I:382:THR:HG22	1:I:383:LEU:H	1.72	0.55
1:I:564:SER:OG	1:I:566:GLU:HG2	2.07	0.55
1:M:315:ASN:OD1	1:M:316:PHE:N	2.39	0.55
1:M:440:LEU:HD11	1:N:279:SER:HB2	63.35	0.55
1:R:564:SER:OG	1:R:566:GLU:HG2	2.07	0.55
1:V:659:ASP:OD2	1:W:333:LYS:NZ	2.32	0.55
1:W:564:SER:OG	1:W:566:GLU:HG2	2.07	0.55
1:Z:564:SER:OG	1:Z:566:GLU:HG2	2.07	0.55
1:A:440:LEU:HD11	1:8:279:SER:HB2	169.67	0.55
1:B:696:ARG:NE	1:B:698:ASN:OD1	2.36	0.55
1:D:382:THR:HG22	1:D:383:LEU:H	1.72	0.55
1:E:696:ARG:NE	1:E:698:ASN:OD1	2.36	0.55
1:K:696:ARG:HH21	1:K:698:ASN:HD21	1.54	0.55
1:L:315:ASN:OD1	1:L:316:PHE:N	2.39	0.55
1:L:329:ASN:O	1:L:332:THR:OG1	2.21	0.55
1:B:479:ASN:ND2	1:M:358:GLY:O	114.23	0.55
1:M:382:THR:HG22	1:M:383:LEU:H	1.72	0.55
1:O:382:THR:HG22	1:O:383:LEU:H	1.72	0.55
1:S:564:SER:OG	1:S:566:GLU:HG2	2.07	0.55
1:U:564:SER:OG	1:U:566:GLU:HG2	2.07	0.55
1:V:382:THR:HG22	1:V:383:LEU:H	1.72	0.55
1:W:358:GLY:O	1:Y:479:ASN:ND2	37.43	0.55
1:X:382:THR:HG22	1:X:383:LEU:H	1.72	0.55
1:Z:348:ASP:OD2	1:Z:352:GLN:N	2.39	0.55
1:3:564:SER:OG	1:3:566:GLU:HG2	2.07	0.55
1:4:564:SER:OG	1:4:566:GLU:HG2	2.07	0.55
1:5:382:THR:HG22	1:5:383:LEU:H	1.72	0.55
1:6:348:ASP:OD2	1:6:352:GLN:N	2.39	0.55
1:6:479:ASN:ND2	1:7:358:GLY:O	2.37	0.55
1:A:736:ARG:HH21	1:G:626:HIS:CD2	2.25	0.55
1:D:279:SER:HB2	1:P:440:LEU:HD11	1.87	0.55
1:D:315:ASN:OD1	1:D:316:PHE:N	2.39	0.55
1:G:382:THR:HG22	1:G:383:LEU:H	1.72	0.55
1:H:348:ASP:OD2	1:H:352:GLN:N	2.39	0.55
1:H:696:ARG:HH21	1:H:698:ASN:HD21	1.54	0.55
1:J:382:THR:HG22	1:J:383:LEU:H	1.72	0.55
1:L:382:THR:HG22	1:L:383:LEU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:564:SER:OG	1:M:566:GLU:HG2	2.07	0.55
1:R:382:THR:HG22	1:R:383:LEU:H	1.72	0.55
1:R:531:ASP:OD1	1:R:569:LYS:NZ	2.28	0.55
1:S:290:PHE:O	1:S:293:HIS:N	2.39	0.55
1:S:696:ARG:HH21	1:S:698:ASN:HD21	1.54	0.55
1:D:279:SER:HB2	1:T:440:LEU:HD11	120.59	0.55
1:T:564:SER:OG	1:T:566:GLU:HG2	2.06	0.55
1:V:279:SER:HB2	1:X:440:LEU:HD11	1.87	0.55
1:V:564:SER:OG	1:V:566:GLU:HG2	2.07	0.55
1:Z:659:ASP:OD2	1:4:333:LYS:NZ	113.14	0.55
1:4:315:ASN:OD1	1:4:316:PHE:N	2.39	0.55
1:4:696:ARG:HH21	1:4:698:ASN:HD21	1.53	0.55
1:7:704:THR:OG1	1:8:702:GLN:N	2.37	0.55
1:A:290:PHE:O	1:A:293:HIS:N	2.39	0.55
1:A:315:ASN:OD1	1:A:316:PHE:N	2.39	0.55
1:E:382:THR:HG22	1:E:383:LEU:H	1.72	0.55
1:J:696:ARG:NE	1:J:698:ASN:OD1	2.36	0.55
1:K:382:THR:HG22	1:K:383:LEU:H	1.72	0.55
1:N:290:PHE:O	1:N:293:HIS:N	2.39	0.55
1:O:564:SER:OG	1:O:566:GLU:HG2	2.07	0.55
1:Q:279:SER:HB2	1:S:440:LEU:HD11	105.07	0.55
1:Q:382:THR:HG22	1:Q:383:LEU:H	1.72	0.55
1:S:479:ASN:ND2	1:U:358:GLY:O	2.37	0.55
1:T:382:THR:HG22	1:T:383:LEU:H	1.72	0.55
1:W:696:ARG:NE	1:W:698:ASN:OD1	2.36	0.55
1:Z:382:THR:HG22	1:Z:383:LEU:H	1.72	0.55
1:7:382:THR:HG22	1:7:383:LEU:H	1.72	0.55
1:8:315:ASN:OD1	1:8:316:PHE:N	2.39	0.55
1:B:696:ARG:HH21	1:B:698:ASN:HD21	1.53	0.55
1:C:382:THR:HG22	1:C:383:LEU:H	1.72	0.55
1:E:704:THR:OG1	1:P:702:GLN:N	2.37	0.55
1:K:340:THR:HB	1:K:407:ARG:HH21	1.73	0.55
1:A:358:GLY:O	1:K:479:ASN:ND2	114.97	0.55
1:L:290:PHE:O	1:L:293:HIS:N	2.39	0.55
1:N:315:ASN:OD1	1:N:316:PHE:N	2.39	0.55
1:N:382:THR:HG22	1:N:383:LEU:H	1.72	0.55
1:P:315:ASN:OD1	1:P:316:PHE:N	2.39	0.55
1:U:290:PHE:O	1:U:293:HIS:N	2.39	0.55
1:U:696:ARG:HH21	1:U:698:ASN:HD21	1.53	0.55
1:X:382:THR:HG21	1:X:394:SER:H	1.72	0.55
1:Z:315:ASN:OD1	1:Z:316:PHE:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:279:SER:HB2	1:4:440:LEU:HD11	1.87	0.54
1:5:315:ASN:OD1	1:5:316:PHE:N	2.39	0.54
1:6:315:ASN:OD1	1:6:316:PHE:N	2.39	0.54
1:7:382:THR:HG21	1:7:394:SER:H	1.72	0.54
1:7:564:SER:OG	1:7:566:GLU:HG2	2.07	0.54
1:7:696:ARG:NE	1:7:698:ASN:OD1	2.36	0.54
1:B:479:ASN:ND2	1:J:358:GLY:O	2.37	0.54
1:D:382:THR:HG21	1:D:394:SER:H	1.73	0.54
1:G:315:ASN:OD1	1:G:316:PHE:N	2.39	0.54
1:H:290:PHE:O	1:H:293:HIS:N	2.39	0.54
1:K:382:THR:HG21	1:K:394:SER:H	1.73	0.54
1:N:307:TRP:CE2	1:N:692:GLU:HG2	2.43	0.54
1:P:696:ARG:NE	1:P:698:ASN:OD1	2.36	0.54
1:R:307:TRP:CE2	1:R:692:GLU:HG2	2.43	0.54
1:S:382:THR:HG22	1:S:383:LEU:H	1.72	0.54
1:U:382:THR:HG22	1:U:383:LEU:H	1.72	0.54
1:Z:290:PHE:O	1:Z:293:HIS:N	2.39	0.54
1:Z:382:THR:HG21	1:Z:394:SER:H	1.72	0.54
1:4:307:TRP:CE2	1:4:692:GLU:HG2	2.43	0.54
1:6:564:SER:OG	1:6:566:GLU:HG2	2.07	0.54
1:B:307:TRP:CE2	1:B:692:GLU:HG2	2.43	0.54
1:E:382:THR:HG21	1:E:394:SER:H	1.73	0.54
1:G:382:THR:HG21	1:G:394:SER:H	1.73	0.54
1:H:340:THR:HB	1:H:407:ARG:HH21	1.73	0.54
1:L:307:TRP:CE2	1:L:692:GLU:HG2	2.43	0.54
1:N:440:LEU:HD11	1:O:279:SER:HB2	42.58	0.54
1:P:382:THR:HG21	1:P:394:SER:H	1.73	0.54
1:T:307:TRP:CE2	1:T:692:GLU:HG2	2.43	0.54
1:U:307:TRP:CE2	1:U:692:GLU:HG2	2.43	0.54
1:V:696:ARG:HH21	1:V:698:ASN:HD21	1.53	0.54
1:W:307:TRP:CE2	1:W:692:GLU:HG2	2.43	0.54
1:Z:307:TRP:CE2	1:Z:692:GLU:HG2	2.43	0.54
1:1:307:TRP:CE2	1:1:692:GLU:HG2	2.43	0.54
1:1:564:SER:OG	1:1:566:GLU:HG2	2.07	0.54
1:2:340:THR:HB	1:2:407:ARG:HH21	1.73	0.54
1:4:254:ASN:O	1:4:255:ASN:C	2.42	0.54
1:7:290:PHE:O	1:7:293:HIS:N	2.39	0.54
1:C:307:TRP:CE2	1:C:692:GLU:HG2	2.43	0.54
1:D:340:THR:HB	1:D:407:ARG:HH21	1.73	0.54
1:E:290:PHE:O	1:E:293:HIS:N	2.39	0.54
1:E:358:GLY:O	1:V:479:ASN:ND2	143.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:TRP:CE2	1:E:692:GLU:HG2	2.43	0.54
1:G:307:TRP:CE2	1:G:692:GLU:HG2	2.43	0.54
1:H:382:THR:HG22	1:H:383:LEU:H	1.72	0.54
1:H:440:LEU:HD11	1:W:279:SER:HB2	1.88	0.54
1:I:307:TRP:CE2	1:I:692:GLU:HG2	2.43	0.54
1:J:307:TRP:CE2	1:J:692:GLU:HG2	2.43	0.54
1:L:260:GLN:NE2	1:L:276:PHE:HE1	2.06	0.54
1:L:382:THR:HG21	1:L:394:SER:H	1.73	0.54
1:L:659:ASP:OD2	1:N:333:LYS:NZ	141.45	0.54
1:O:704:THR:OG1	1:6:702:GLN:N	156.89	0.54
1:P:290:PHE:O	1:P:293:HIS:N	2.39	0.54
1:Q:260:GLN:NE2	1:Q:276:PHE:HE1	2.06	0.54
1:Q:564:SER:OG	1:Q:566:GLU:HG2	2.07	0.54
1:V:307:TRP:CE2	1:V:692:GLU:HG2	2.43	0.54
1:W:382:THR:HG21	1:W:394:SER:H	1.72	0.54
1:Q:333:LYS:NZ	1:Y:659:ASP:OD2	182.15	0.54
1:Z:260:GLN:NE2	1:Z:276:PHE:HE1	2.06	0.54
1:Z:440:LEU:HD11	1:4:279:SER:HB2	1.88	0.54
1:1:298:ASP:OD1	1:1:301:ARG:NH1	2.41	0.54
1:3:340:THR:HB	1:3:407:ARG:HH21	1.73	0.54
1:4:382:THR:HG22	1:4:383:LEU:H	1.72	0.54
1:8:564:SER:OG	1:8:566:GLU:HG2	2.07	0.54
1:8:696:ARG:NE	1:8:698:ASN:OD1	2.36	0.54
1:C:382:THR:HG21	1:C:394:SER:H	1.73	0.54
1:D:298:ASP:OD1	1:D:301:ARG:NH1	2.41	0.54
1:G:260:GLN:NE2	1:G:276:PHE:HE1	2.06	0.54
1:G:298:ASP:OD1	1:G:301:ARG:NH1	2.41	0.54
1:I:298:ASP:OD1	1:I:301:ARG:NH1	2.41	0.54
1:J:340:THR:HB	1:J:407:ARG:HH21	1.73	0.54
1:L:298:ASP:OD1	1:L:301:ARG:NH1	2.41	0.54
1:K:225:SER:CA	1:L:407:ARG:HD2	2.33	0.54
1:M:307:TRP:CE2	1:M:692:GLU:HG2	2.43	0.54
1:N:382:THR:HG21	1:N:394:SER:H	1.73	0.54
1:O:315:ASN:OD1	1:O:316:PHE:N	2.39	0.54
1:O:382:THR:HG21	1:O:394:SER:H	1.73	0.54
1:P:260:GLN:NE2	1:P:276:PHE:HE1	2.06	0.54
1:P:298:ASP:OD1	1:P:301:ARG:NH1	2.41	0.54
1:Q:307:TRP:CE2	1:Q:692:GLU:HG2	2.43	0.54
1:R:382:THR:HG21	1:R:394:SER:H	1.73	0.54
1:S:260:GLN:NE2	1:S:276:PHE:HE1	2.06	0.54
1:T:382:THR:HG21	1:T:394:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:340:THR:HB	1:T:407:ARG:HH21	1.73	0.54
1:U:260:GLN:NE2	1:U:276:PHE:HE1	2.06	0.54
1:X:307:TRP:CE2	1:X:692:GLU:HG2	2.43	0.54
1:Z:298:ASP:OD1	1:Z:301:ARG:NH1	2.41	0.54
1:2:315:ASN:OD1	1:2:316:PHE:N	2.39	0.54
1:3:382:THR:HG22	1:3:383:LEU:H	1.72	0.54
1:5:564:SER:OG	1:5:566:GLU:HG2	2.07	0.54
1:6:298:ASP:OD1	1:6:301:ARG:NH1	2.41	0.54
1:6:340:THR:HB	1:6:407:ARG:HH21	1.73	0.54
1:A:382:THR:HG21	1:A:394:SER:H	1.73	0.54
1:C:298:ASP:OD1	1:C:301:ARG:NH1	2.41	0.54
1:C:407:ARG:HD2	1:D:225:SER:CA	2.33	0.54
1:E:260:GLN:NE2	1:E:276:PHE:HE1	2.06	0.54
1:F:298:ASP:OD1	1:F:301:ARG:NH1	2.41	0.54
1:H:298:ASP:OD1	1:H:301:ARG:NH1	2.41	0.54
1:H:382:THR:HG21	1:H:394:SER:H	1.73	0.54
1:M:260:GLN:NE2	1:M:276:PHE:HE1	2.06	0.54
1:O:340:THR:HB	1:O:407:ARG:HH21	1.73	0.54
1:P:307:TRP:CE2	1:P:692:GLU:HG2	2.43	0.54
1:Q:696:ARG:NE	1:Q:698:ASN:OD1	2.36	0.54
1:R:340:THR:HB	1:R:407:ARG:HH21	1.73	0.54
1:T:298:ASP:OD1	1:T:301:ARG:NH1	2.41	0.54
1:U:298:ASP:OD1	1:U:301:ARG:NH1	2.41	0.54
1:U:340:THR:HB	1:U:407:ARG:HH21	1.73	0.54
1:V:298:ASP:OD1	1:V:301:ARG:NH1	2.41	0.54
1:V:340:THR:HB	1:V:407:ARG:HH21	1.73	0.54
1:W:260:GLN:NE2	1:W:276:PHE:HE1	2.06	0.54
1:Y:340:THR:HB	1:Y:407:ARG:HH21	1.73	0.54
1:Y:307:TRP:CE2	1:Y:692:GLU:HG2	2.43	0.54
1:1:340:THR:HB	1:1:407:ARG:HH21	1.73	0.54
1:2:298:ASP:OD1	1:2:301:ARG:NH1	2.41	0.54
1:5:307:TRP:O	1:5:426:SER:OG	2.18	0.54
1:5:340:THR:HB	1:5:407:ARG:HH21	1.73	0.54
1:5:407:ARG:HD2	1:8:225:SER:CA	2.34	0.54
1:8:307:TRP:CE2	1:8:692:GLU:HG2	2.43	0.54
1:A:340:THR:HB	1:A:407:ARG:HH21	1.73	0.54
1:F:340:THR:HB	1:F:407:ARG:HH21	1.73	0.54
1:A:393:SER:O	1:I:696:ARG:NH2	2.40	0.54
1:K:260:GLN:NE2	1:K:276:PHE:HE1	2.06	0.54
1:M:340:THR:HB	1:M:407:ARG:HH21	1.73	0.54
1:M:696:ARG:NE	1:M:698:ASN:OD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:298:ASP:OD1	1:S:301:ARG:NH1	2.41	0.54
1:S:382:THR:HG21	1:S:394:SER:H	1.73	0.54
1:V:260:GLN:NE2	1:V:276:PHE:HE1	2.06	0.54
1:U:479:ASN:ND2	1:V:358:GLY:O	53.78	0.54
1:1:382:THR:HG21	1:1:394:SER:H	1.73	0.54
1:3:298:ASP:OD1	1:3:301:ARG:NH1	2.41	0.54
1:4:382:THR:HG21	1:4:394:SER:H	1.73	0.54
1:5:298:ASP:OD1	1:5:301:ARG:NH1	2.41	0.54
1:6:382:THR:HG21	1:6:394:SER:H	1.73	0.54
1:8:260:GLN:NE2	1:8:276:PHE:HE1	2.06	0.54
1:A:307:TRP:CE2	1:A:692:GLU:HG2	2.43	0.54
1:C:659:ASP:OD2	1:S:333:LYS:NZ	118.19	0.54
1:C:696:ARG:NE	1:C:698:ASN:OD1	2.36	0.54
1:H:260:GLN:NE2	1:H:276:PHE:HE1	2.06	0.54
1:H:307:TRP:CE2	1:H:692:GLU:HG2	2.43	0.54
1:O:298:ASP:OD1	1:O:301:ARG:NH1	2.41	0.54
1:Q:298:ASP:OD1	1:Q:301:ARG:NH1	2.41	0.54
1:Q:340:THR:HB	1:Q:407:ARG:HH21	1.73	0.54
1:R:329:ASN:O	1:R:332:THR:OG1	2.21	0.54
1:S:340:THR:HB	1:S:407:ARG:HH21	1.73	0.54
1:W:382:THR:HG22	1:W:383:LEU:H	1.72	0.54
1:3:315:ASN:OD1	1:3:316:PHE:N	2.39	0.54
1:6:260:GLN:NE2	1:6:276:PHE:HE1	2.06	0.54
1:7:307:TRP:CE2	1:7:692:GLU:HG2	2.43	0.54
1:B:382:THR:HG22	1:B:383:LEU:H	1.72	0.54
1:D:307:TRP:CE2	1:D:692:GLU:HG2	2.43	0.54
1:D:702:GLN:H	1:N:704:THR:HG1	64.38	0.54
1:F:382:THR:HG21	1:F:394:SER:H	1.73	0.54
1:F:307:TRP:CE2	1:F:692:GLU:HG2	2.43	0.54
1:I:382:THR:HG21	1:I:394:SER:H	1.73	0.54
1:P:333:LYS:NZ	1:Q:659:ASP:OD2	2.32	0.54
1:S:307:TRP:CE2	1:S:692:GLU:HG2	2.43	0.54
1:2:382:THR:HG21	1:2:394:SER:H	1.73	0.54
1:3:382:THR:HG21	1:3:394:SER:H	1.73	0.54
1:4:260:GLN:NE2	1:4:276:PHE:HE1	2.06	0.54
1:5:696:ARG:NE	1:5:698:ASN:OD1	2.36	0.54
1:6:307:TRP:CE2	1:6:692:GLU:HG2	2.43	0.54
1:F:260:GLN:NE2	1:F:276:PHE:HE1	2.06	0.54
1:J:260:GLN:NE2	1:J:276:PHE:HE1	2.06	0.54
1:J:382:THR:HG21	1:J:394:SER:H	1.73	0.54
1:K:298:ASP:OD1	1:K:301:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:298:ASP:OD1	1:M:301:ARG:NH1	2.41	0.54
1:N:260:GLN:NE2	1:N:276:PHE:HE1	2.06	0.54
1:P:340:THR:HB	1:P:407:ARG:HH21	1.73	0.54
1:W:696:ARG:NH2	1:X:393:SER:O	54.87	0.54
1:W:479:ASN:ND2	1:Y:358:GLY:O	2.37	0.54
1:Z:340:THR:HB	1:Z:407:ARG:HH21	1.73	0.54
1:1:290:PHE:O	1:1:293:HIS:N	2.39	0.54
1:5:307:TRP:CE2	1:5:692:GLU:HG2	2.43	0.54
1:D:260:GLN:NE2	1:D:276:PHE:HE1	2.06	0.54
1:A:702:GLN:N	1:F:704:THR:OG1	2.35	0.54
1:G:340:THR:HB	1:G:407:ARG:HH21	1.73	0.54
1:I:329:ASN:O	1:I:332:THR:OG1	2.21	0.54
1:J:298:ASP:OD1	1:J:301:ARG:NH1	2.41	0.54
1:K:307:TRP:CE2	1:K:692:GLU:HG2	2.43	0.54
1:Q:382:THR:HG21	1:Q:394:SER:H	1.73	0.54
1:Q:479:ASN:ND2	1:R:358:GLY:O	53.78	0.54
1:R:298:ASP:OD1	1:R:301:ARG:NH1	2.41	0.54
1:X:260:GLN:NE2	1:X:276:PHE:HE1	2.06	0.54
1:1:382:THR:HG22	1:1:383:LEU:H	1.72	0.53
1:8:298:ASP:OD1	1:8:301:ARG:NH1	2.41	0.53
1:A:260:GLN:NE2	1:A:276:PHE:HE1	2.06	0.53
1:B:382:THR:HG21	1:B:394:SER:H	1.73	0.53
1:D:329:ASN:O	1:D:332:THR:OG1	2.21	0.53
1:H:700:GLU:HB2	1:H:702:GLN:HE21	1.74	0.53
1:I:696:ARG:NH2	1:J:393:SER:O	27.63	0.53
1:T:290:PHE:O	1:T:293:HIS:N	2.39	0.53
1:T:329:ASN:O	1:T:332:THR:OG1	2.21	0.53
1:U:382:THR:HG21	1:U:394:SER:H	1.73	0.53
1:V:700:GLU:HB2	1:V:702:GLN:HE21	1.74	0.53
1:Y:298:ASP:OD1	1:Y:301:ARG:NH1	2.41	0.53
1:5:382:THR:HG21	1:5:394:SER:H	1.73	0.53
1:7:340:THR:HB	1:7:407:ARG:HH21	1.73	0.53
1:A:305:ASN:OD1	1:F:305:ASN:ND2	2.41	0.53
1:C:700:GLU:HB2	1:C:702:GLN:HE21	1.74	0.53
1:E:298:ASP:OD1	1:E:301:ARG:NH1	2.41	0.53
1:L:700:GLU:HB2	1:L:702:GLN:HE21	1.74	0.53
1:D:702:GLN:N	1:N:704:THR:OG1	63.14	0.53
1:O:307:TRP:CE2	1:O:692:GLU:HG2	2.43	0.53
1:S:700:GLU:HB2	1:S:702:GLN:HE21	1.74	0.53
1:U:700:GLU:HB2	1:U:702:GLN:HE21	1.74	0.53
1:W:298:ASP:OD1	1:W:301:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:340:THR:HB	1:W:407:ARG:HH21	1.73	0.53
1:X:298:ASP:OD1	1:X:301:ARG:NH1	2.41	0.53
1:X:340:THR:HB	1:X:407:ARG:HH21	1.73	0.53
1:X:696:ARG:NH2	1:Y:393:SER:O	27.63	0.53
1:2:307:TRP:CE2	1:2:692:GLU:HG2	2.43	0.53
1:4:298:ASP:OD1	1:4:301:ARG:NH1	2.41	0.53
1:2:702:GLN:N	1:4:704:THR:OG1	2.36	0.53
1:8:340:THR:HB	1:8:407:ARG:HH21	1.73	0.53
1:8:382:THR:HG21	1:8:394:SER:H	1.73	0.53
1:8:700:GLU:HB2	1:8:702:GLN:HE21	1.74	0.53
1:B:659:ASP:OD2	1:C:333:LYS:NZ	2.31	0.53
1:C:329:ASN:O	1:C:332:THR:OG1	2.21	0.53
1:C:340:THR:HB	1:C:407:ARG:HH21	1.73	0.53
1:E:340:THR:HB	1:E:407:ARG:HH21	1.73	0.53
1:E:696:ARG:NH2	1:X:393:SER:O	168.89	0.53
1:G:700:GLU:HB2	1:G:702:GLN:HE21	1.74	0.53
1:E:333:LYS:NZ	1:H:659:ASP:OD2	141.44	0.53
1:I:700:GLU:HB2	1:I:702:GLN:HE21	1.74	0.53
1:L:340:THR:HB	1:L:407:ARG:HH21	1.73	0.53
1:M:382:THR:HG21	1:M:394:SER:H	1.73	0.53
1:P:700:GLU:HB2	1:P:702:GLN:HE21	1.74	0.53
1:V:393:SER:O	1:X:696:ARG:NH2	2.42	0.53
1:Y:329:ASN:O	1:Y:332:THR:OG1	2.21	0.53
1:Y:382:THR:HG21	1:Y:394:SER:H	1.73	0.53
1:6:700:GLU:HB2	1:6:702:GLN:HE21	1.74	0.53
1:A:298:ASP:OD1	1:A:301:ARG:NH1	2.41	0.53
1:A:700:GLU:HB2	1:A:702:GLN:HE21	1.74	0.53
1:C:260:GLN:NE2	1:C:276:PHE:HE1	2.06	0.53
1:C:659:ASP:OD2	1:D:333:LYS:NZ	2.31	0.53
1:F:700:GLU:HB2	1:F:702:GLN:HE21	1.74	0.53
1:H:704:THR:OG1	1:K:702:GLN:N	104.37	0.53
1:I:340:THR:HB	1:I:407:ARG:HH21	1.73	0.53
1:N:298:ASP:OD1	1:N:301:ARG:NH1	2.41	0.53
1:O:260:GLN:NE2	1:O:276:PHE:HE1	2.06	0.53
1:Q:700:GLU:HB2	1:Q:702:GLN:HE21	1.74	0.53
1:U:696:ARG:NE	1:U:698:ASN:OD1	2.36	0.53
1:V:382:THR:HG21	1:V:394:SER:H	1.73	0.53
1:Y:260:GLN:NE2	1:Y:276:PHE:HE1	2.06	0.53
1:2:382:THR:HG22	1:2:383:LEU:H	1.72	0.53
1:5:700:GLU:HB2	1:5:702:GLN:HE21	1.74	0.53
1:A:696:ARG:NE	1:A:698:ASN:OD1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:THR:HB	1:B:407:ARG:HH21	1.73	0.53
1:B:696:ARG:NH2	1:J:393:SER:O	2.42	0.53
1:D:393:SER:O	1:T:696:ARG:NH2	114.66	0.53
1:B:696:ARG:NH2	1:M:393:SER:O	129.14	0.53
1:R:260:GLN:NE2	1:R:276:PHE:HE1	2.06	0.53
1:R:700:GLU:HB2	1:R:702:GLN:HE21	1.74	0.53
1:U:696:ARG:NH2	1:V:393:SER:O	54.87	0.53
1:E:393:SER:O	1:V:696:ARG:NH2	127.07	0.53
1:7:260:GLN:NE2	1:7:276:PHE:HE1	2.06	0.53
1:B:700:GLU:HB2	1:B:702:GLN:HE21	1.74	0.53
1:I:260:GLN:NE2	1:I:276:PHE:HE1	2.06	0.53
1:N:340:THR:HB	1:N:407:ARG:HH21	1.73	0.53
1:N:531:ASP:OD1	1:N:569:LYS:NZ	2.28	0.53
1:O:329:ASN:O	1:O:332:THR:OG1	2.21	0.53
1:O:696:ARG:NH2	1:P:393:SER:O	27.63	0.53
1:O:700:GLU:HB2	1:O:702:GLN:HE21	1.74	0.53
1:R:290:PHE:O	1:R:293:HIS:N	2.39	0.53
1:R:393:SER:O	1:U:696:ARG:NH2	2.42	0.53
1:S:696:ARG:NH2	1:U:393:SER:O	2.42	0.53
1:T:393:SER:O	1:V:696:ARG:NH2	89.97	0.53
1:1:260:GLN:NE2	1:1:276:PHE:HE1	2.06	0.53
1:3:260:GLN:NE2	1:3:276:PHE:HE1	2.06	0.53
1:4:290:PHE:O	1:4:293:HIS:N	2.39	0.53
1:4:340:THR:HB	1:4:407:ARG:HH21	1.73	0.53
1:3:393:SER:O	1:4:696:ARG:NH2	2.42	0.53
1:5:260:GLN:NE2	1:5:276:PHE:HE1	2.06	0.53
1:7:298:ASP:OD1	1:7:301:ARG:NH1	2.41	0.53
1:B:290:PHE:O	1:B:293:HIS:N	2.39	0.53
1:D:696:ARG:NH2	1:N:393:SER:O	2.42	0.53
1:H:348:ASP:OD1	1:H:351:TYR:N	2.42	0.53
1:K:348:ASP:OD1	1:K:351:TYR:N	2.42	0.53
1:K:333:LYS:NZ	1:L:659:ASP:OD2	2.32	0.53
1:E:696:ARG:NH2	1:Q:393:SER:O	2.42	0.53
1:T:260:GLN:NE2	1:T:276:PHE:HE1	2.06	0.53
1:T:700:GLU:HB2	1:T:702:GLN:HE21	1.74	0.53
1:V:348:ASP:OD1	1:V:351:TYR:N	2.42	0.53
1:W:348:ASP:OD1	1:W:351:TYR:N	2.42	0.53
1:X:700:GLU:HB2	1:X:702:GLN:HE21	1.74	0.53
1:1:700:GLU:HB2	1:1:702:GLN:HE21	1.74	0.53
1:2:260:GLN:NE2	1:2:276:PHE:HE1	2.06	0.53
1:A:696:ARG:NH2	1:8:393:SER:O	158.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:702:GLN:N	1:8:704:THR:OG1	2.37	0.53
1:A:348:ASP:OD1	1:A:351:TYR:N	2.42	0.53
1:B:260:GLN:NE2	1:B:276:PHE:HE1	2.06	0.53
1:C:348:ASP:OD1	1:C:351:TYR:N	2.42	0.53
1:D:348:ASP:OD1	1:D:351:TYR:N	2.42	0.53
1:F:348:ASP:OD1	1:F:351:TYR:N	2.42	0.53
1:F:393:SER:O	1:G:696:ARG:NH2	102.62	0.53
1:J:696:ARG:NH2	1:L:393:SER:O	2.42	0.53
1:L:348:ASP:OD1	1:L:351:TYR:N	2.42	0.53
1:C:393:SER:O	1:M:696:ARG:NH2	2.42	0.53
1:N:348:ASP:OD1	1:N:351:TYR:N	2.42	0.53
1:N:696:ARG:NH2	1:O:393:SER:O	54.87	0.53
1:E:702:GLN:N	1:P:704:THR:OG1	2.37	0.53
1:Q:348:ASP:OD1	1:Q:351:TYR:N	2.42	0.53
1:R:696:ARG:NH2	1:S:393:SER:O	2.42	0.53
1:S:348:ASP:OD1	1:S:351:TYR:N	2.42	0.53
1:U:348:ASP:OD1	1:U:351:TYR:N	2.42	0.53
1:U:702:GLN:H	1:V:704:THR:HG1	1.57	0.53
1:Y:290:PHE:O	1:Y:293:HIS:N	2.39	0.53
1:Z:348:ASP:OD1	1:Z:351:TYR:N	2.42	0.53
1:3:307:TRP:CE2	1:3:692:GLU:HG2	2.43	0.53
1:6:348:ASP:OD1	1:6:351:TYR:N	2.42	0.53
1:A:329:ASN:O	1:A:332:THR:OG1	2.21	0.53
1:F:290:PHE:O	1:F:293:HIS:N	2.39	0.53
1:F:696:ARG:NH2	1:H:393:SER:O	126.22	0.53
1:I:348:ASP:OD1	1:I:351:TYR:N	2.42	0.53
1:J:348:ASP:OD1	1:J:351:TYR:N	2.42	0.53
1:O:348:ASP:OD1	1:O:351:TYR:N	2.42	0.53
1:G:333:LYS:NZ	1:W:659:ASP:OD2	2.33	0.53
1:V:333:LYS:NZ	1:W:659:ASP:OD2	32.91	0.53
1:Y:348:ASP:OD1	1:Y:351:TYR:N	2.42	0.53
1:1:348:ASP:OD1	1:1:351:TYR:N	2.42	0.53
1:2:700:GLU:HB2	1:2:702:GLN:HE21	1.74	0.53
1:A:393:SER:O	1:K:696:ARG:NH2	82.11	0.53
1:B:298:ASP:OD1	1:B:301:ARG:NH1	2.41	0.53
1:D:704:THR:OG1	1:M:702:GLN:N	2.37	0.53
1:G:393:SER:O	1:H:696:ARG:NH2	54.88	0.53
1:J:700:GLU:HB2	1:J:702:GLN:HE21	1.74	0.53
1:M:348:ASP:OD1	1:M:351:TYR:N	2.42	0.53
1:T:348:ASP:OD1	1:T:351:TYR:N	2.42	0.53
1:2:348:ASP:OD1	1:2:351:TYR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:348:ASP:OD1	1:3:351:TYR:N	2.42	0.52
1:5:393:SER:O	1:7:696:ARG:NH2	2.42	0.52
1:D:700:GLU:HB2	1:D:702:GLN:HE21	1.74	0.52
1:I:393:SER:O	1:K:696:ARG:NH2	89.97	0.52
1:N:696:ARG:NH2	1:P:393:SER:O	2.42	0.52
1:N:702:GLN:N	1:O:704:THR:OG1	2.36	0.52
1:H:696:ARG:NH2	1:W:393:SER:O	2.42	0.52
1:W:700:GLU:HB2	1:W:702:GLN:HE21	1.74	0.52
1:7:700:GLU:HB2	1:7:702:GLN:HE21	1.74	0.52
1:O:696:ARG:NE	1:O:698:ASN:OD1	2.36	0.52
1:S:240:VAL:HG13	1:S:687:TRP:HB2	1.92	0.52
1:H:393:SER:O	1:Y:696:ARG:NH2	2.42	0.52
1:W:393:SER:O	1:Y:696:ARG:NH2	58.92	0.52
1:1:696:ARG:NH2	1:2:393:SER:O	2.42	0.52
1:3:700:GLU:HB2	1:3:702:GLN:HE21	1.74	0.52
1:5:696:ARG:NH2	1:6:393:SER:O	2.42	0.52
1:7:348:ASP:OD1	1:7:351:TYR:N	2.42	0.52
1:8:240:VAL:HG13	1:8:687:TRP:HB2	1.92	0.52
1:A:696:ARG:NH2	1:G:393:SER:O	2.43	0.52
1:E:700:GLU:HB2	1:E:702:GLN:HE21	1.74	0.52
1:E:393:SER:O	1:F:696:ARG:NH2	2.42	0.52
1:J:696:ARG:NH2	1:K:393:SER:O	54.87	0.52
1:J:702:GLN:N	1:K:704:THR:OG1	2.37	0.52
1:M:393:SER:O	1:O:696:ARG:NH2	89.96	0.52
1:P:240:VAL:HG13	1:P:687:TRP:HB2	1.92	0.52
1:R:348:ASP:OD1	1:R:351:TYR:N	2.42	0.52
1:S:696:ARG:NE	1:S:698:ASN:OD1	2.36	0.52
1:X:348:ASP:OD1	1:X:351:TYR:N	2.42	0.52
1:Z:696:ARG:NH2	1:1:393:SER:O	105.47	0.52
1:Z:696:ARG:NH2	1:4:393:SER:O	2.42	0.52
1:A:704:THR:OG1	1:F:702:GLN:N	2.38	0.52
1:D:393:SER:O	1:P:696:ARG:NH2	2.42	0.52
1:E:348:ASP:OD1	1:E:351:TYR:N	2.42	0.52
1:O:290:PHE:O	1:O:293:HIS:N	2.39	0.52
1:P:348:ASP:OD1	1:P:351:TYR:N	2.42	0.52
1:Q:531:ASP:OD1	1:Q:569:LYS:NZ	2.28	0.52
1:U:240:VAL:HG13	1:U:687:TRP:HB2	1.92	0.52
1:V:702:GLN:H	1:Y:704:THR:HG1	126.84	0.52
1:Y:700:GLU:HB2	1:Y:702:GLN:HE21	1.74	0.52
1:Z:329:ASN:O	1:Z:332:THR:OG1	2.21	0.52
1:A:333:LYS:NZ	1:Z:659:ASP:OD2	118.69	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:702:GLN:N	1:Z:704:THR:OG1	2.37	0.52
1:3:696:ARG:NE	1:3:698:ASN:OD1	2.36	0.52
1:8:348:ASP:OD1	1:8:351:TYR:N	2.42	0.52
1:K:393:SER:O	1:8:696:ARG:NH2	2.42	0.52
1:G:348:ASP:OD1	1:G:351:TYR:N	2.42	0.52
1:G:240:VAL:HG13	1:G:687:TRP:HB2	1.92	0.52
1:I:240:VAL:HG13	1:I:687:TRP:HB2	1.92	0.52
1:K:240:VAL:HG13	1:K:687:TRP:HB2	1.92	0.52
1:D:696:ARG:NH2	1:L:393:SER:O	126.22	0.52
1:N:700:GLU:HB2	1:N:702:GLN:HE21	1.74	0.52
1:Q:393:SER:O	1:S:696:ARG:NH2	102.63	0.52
1:T:240:VAL:HG13	1:T:687:TRP:HB2	1.92	0.52
1:D:240:VAL:HG13	1:D:687:TRP:HB2	1.92	0.52
1:F:393:SER:O	1:Q:696:ARG:NH2	2.42	0.52
1:K:700:GLU:HB2	1:K:702:GLN:HE21	1.74	0.52
1:M:704:THR:OG1	1:R:702:GLN:N	127.96	0.52
1:Q:696:ARG:NH2	1:R:393:SER:O	54.88	0.52
1:R:240:VAL:HG13	1:R:687:TRP:HB2	1.92	0.52
1:V:240:VAL:HG13	1:V:687:TRP:HB2	1.92	0.52
1:B:348:ASP:OD1	1:B:351:TYR:N	2.42	0.52
1:C:393:SER:O	1:P:696:ARG:NH2	56.84	0.52
1:E:240:VAL:HG13	1:E:687:TRP:HB2	1.92	0.52
1:A:305:ASN:ND2	1:F:305:ASN:OD1	2.42	0.52
1:M:696:ARG:NH2	1:N:393:SER:O	27.63	0.52
1:W:696:ARG:NH2	1:Y:393:SER:O	2.42	0.52
1:1:696:ARG:NE	1:1:698:ASN:OD1	2.36	0.52
1:3:290:PHE:O	1:3:293:HIS:N	2.39	0.52
1:A:702:GLN:N	1:3:704:THR:OG1	151.86	0.52
1:6:696:ARG:NH2	1:7:393:SER:O	2.42	0.52
1:E:354:PRO:HB3	1:V:431:GLN:NE2	134.30	0.52
1:F:240:VAL:HG13	1:F:687:TRP:HB2	1.92	0.52
1:J:240:VAL:HG13	1:J:687:TRP:HB2	1.92	0.52
1:J:704:THR:HG1	1:K:702:GLN:H	1.57	0.52
1:Q:290:PHE:O	1:Q:293:HIS:N	2.39	0.52
1:V:290:PHE:O	1:V:293:HIS:N	2.39	0.52
1:V:704:THR:OG1	1:Y:702:GLN:N	125.25	0.52
1:W:290:PHE:O	1:W:293:HIS:N	2.39	0.52
1:W:240:VAL:HG13	1:W:687:TRP:HB2	1.92	0.52
1:Y:240:VAL:HG13	1:Y:687:TRP:HB2	1.92	0.52
1:A:305:ASN:ND2	1:3:305:ASN:OD1	135.69	0.52
1:4:700:GLU:HB2	1:4:702:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG13	1:B:687:TRP:HB2	1.92	0.52
1:C:696:ARG:NH2	1:O:393:SER:O	167.80	0.52
1:N:305:ASN:ND2	1:O:305:ASN:OD1	2.43	0.52
1:Q:240:VAL:HG13	1:Q:687:TRP:HB2	1.92	0.52
1:S:702:GLN:N	1:T:704:THR:OG1	2.36	0.52
1:W:354:PRO:HB3	1:Y:431:GLN:NE2	47.67	0.52
1:J:702:GLN:N	1:W:704:THR:OG1	155.27	0.52
1:Z:393:SER:O	1:3:696:ARG:NH2	2.42	0.52
1:Z:700:GLU:HB2	1:Z:702:GLN:HE21	1.74	0.52
1:5:240:VAL:HG13	1:5:687:TRP:HB2	1.92	0.52
1:6:240:VAL:HG13	1:6:687:TRP:HB2	1.92	0.52
1:D:696:ARG:NE	1:D:698:ASN:OD1	2.36	0.52
1:A:333:LYS:NZ	1:E:659:ASP:OD2	2.32	0.52
1:H:333:LYS:NZ	1:I:659:ASP:OD2	2.32	0.52
1:K:696:ARG:NE	1:K:698:ASN:OD1	2.36	0.52
1:M:700:GLU:HB2	1:M:702:GLN:HE21	1.74	0.52
1:T:696:ARG:NH2	1:U:393:SER:O	27.64	0.52
1:Z:354:PRO:HB3	1:2:431:GLN:NE2	83.11	0.52
1:5:290:PHE:O	1:5:293:HIS:N	2.39	0.51
1:B:393:SER:O	1:C:696:ARG:NH2	27.64	0.51
1:C:240:VAL:HG13	1:C:687:TRP:HB2	1.92	0.51
1:E:305:ASN:OD1	1:F:305:ASN:ND2	59.12	0.51
1:H:240:VAL:HG13	1:H:687:TRP:HB2	1.92	0.51
1:T:305:ASN:OD1	1:5:305:ASN:ND2	184.87	0.51
1:J:305:ASN:ND2	1:W:305:ASN:OD1	135.50	0.51
1:7:240:VAL:HG13	1:7:687:TRP:HB2	1.92	0.51
1:A:240:VAL:HG13	1:A:687:TRP:HB2	1.92	0.51
1:D:702:GLN:H	1:M:704:THR:HG1	1.57	0.51
1:L:696:ARG:NH2	1:T:393:SER:O	205.15	0.51
1:U:704:THR:OG1	1:V:702:GLN:N	2.37	0.51
1:X:240:VAL:HG13	1:X:687:TRP:HB2	1.92	0.51
1:2:240:VAL:HG13	1:2:687:TRP:HB2	1.92	0.51
1:T:305:ASN:ND2	1:5:305:ASN:OD1	184.17	0.51
1:5:348:ASP:OD1	1:5:351:TYR:N	2.42	0.51
1:B:393:SER:O	1:L:696:ARG:NH2	2.42	0.51
1:F:354:PRO:HB3	1:G:431:GLN:NE2	93.51	0.51
1:K:290:PHE:O	1:K:293:HIS:N	2.39	0.51
1:N:240:VAL:HG13	1:N:687:TRP:HB2	1.92	0.51
1:Q:305:ASN:ND2	1:R:305:ASN:OD1	2.44	0.51
1:Q:305:ASN:OD1	1:R:305:ASN:ND2	2.44	0.51
1:U:702:GLN:N	1:V:704:THR:OG1	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:240:VAL:HG13	1:Z:687:TRP:HB2	1.92	0.51
1:4:348:ASP:OD1	1:4:351:TYR:N	2.42	0.51
1:O:305:ASN:OD1	1:6:305:ASN:ND2	137.32	0.51
1:B:305:ASN:ND2	1:C:305:ASN:OD1	59.88	0.51
1:B:305:ASN:OD1	1:C:305:ASN:ND2	59.92	0.51
1:A:481:LEU:CD1	1:G:636:LEU:HD11	2.41	0.51
1:G:696:ARG:NH2	1:I:393:SER:O	2.43	0.51
1:M:531:ASP:OD1	1:M:569:LYS:NZ	2.28	0.51
1:A:659:ASP:OD2	1:B:333:LYS:NZ	2.33	0.51
1:D:426:SER:HB2	1:D:731:THR:O	2.11	0.51
1:F:659:ASP:OD2	1:Z:333:LYS:NZ	139.20	0.51
1:F:426:SER:HB2	1:F:731:THR:O	2.11	0.51
1:H:426:SER:HB2	1:H:731:THR:O	2.11	0.51
1:I:431:GLN:NE2	1:J:354:PRO:HB3	47.76	0.51
1:J:426:SER:HB2	1:J:731:THR:O	2.11	0.51
1:J:481:LEU:CD1	1:K:636:LEU:HD11	64.72	0.51
1:D:431:GLN:NE2	1:L:354:PRO:HB3	123.21	0.51
1:M:240:VAL:HG13	1:M:687:TRP:HB2	1.92	0.51
1:N:305:ASN:OD1	1:O:305:ASN:ND2	2.43	0.51
1:Q:426:SER:HB2	1:Q:731:THR:O	2.11	0.51
1:R:426:SER:HB2	1:R:731:THR:O	2.11	0.51
1:T:431:GLN:NE2	1:U:354:PRO:HB3	47.77	0.51
1:V:702:GLN:N	1:Y:704:THR:OG1	125.25	0.51
1:U:702:GLN:N	1:1:704:THR:OG1	176.98	0.51
1:2:426:SER:HB2	1:2:731:THR:O	2.11	0.51
1:G:426:SER:HB2	1:G:731:THR:O	2.11	0.51
1:B:305:ASN:OD1	1:I:305:ASN:ND2	2.44	0.51
1:B:305:ASN:ND2	1:I:305:ASN:OD1	2.44	0.51
1:K:426:SER:HB2	1:K:731:THR:O	2.11	0.51
1:L:240:VAL:HG13	1:L:687:TRP:HB2	1.92	0.51
1:T:426:SER:HB2	1:T:731:THR:O	2.11	0.51
1:W:426:SER:HB2	1:W:731:THR:O	2.11	0.51
1:O:702:GLN:N	1:6:704:THR:OG1	149.31	0.51
1:C:305:ASN:ND2	1:L:305:ASN:OD1	2.44	0.51
1:I:305:ASN:ND2	1:L:305:ASN:OD1	60.05	0.51
1:I:426:SER:HB2	1:I:731:THR:O	2.11	0.51
1:C:305:ASN:OD1	1:L:305:ASN:ND2	2.44	0.51
1:Q:329:ASN:O	1:Q:332:THR:OG1	2.21	0.51
1:R:431:GLN:NE2	1:S:354:PRO:HB3	2.24	0.51
1:Q:305:ASN:OD1	1:X:305:ASN:ND2	97.22	0.51
1:E:481:LEU:CD1	1:X:636:LEU:HD11	137.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:481:LEU:CD1	1:Y:636:LEU:HD11	72.94	0.51
1:2:305:ASN:OD1	1:4:305:ASN:ND2	2.43	0.51
1:A:305:ASN:OD1	1:3:305:ASN:ND2	137.22	0.51
1:7:305:ASN:OD1	1:8:305:ASN:ND2	2.43	0.51
1:A:426:SER:HB2	1:A:731:THR:O	2.11	0.51
1:E:704:THR:OG1	1:F:702:GLN:N	63.14	0.51
1:O:426:SER:HB2	1:O:731:THR:O	2.11	0.51
1:U:426:SER:HB2	1:U:731:THR:O	2.11	0.51
1:V:426:SER:HB2	1:V:731:THR:O	2.11	0.51
1:1:240:VAL:HG13	1:1:687:TRP:HB2	1.92	0.51
1:2:305:ASN:ND2	1:4:305:ASN:OD1	2.43	0.51
1:O:305:ASN:ND2	1:6:305:ASN:OD1	138.88	0.51
1:D:636:LEU:HD11	1:P:481:LEU:CD1	2.41	0.51
1:G:305:ASN:ND2	1:Z:305:ASN:OD1	62.97	0.51
1:G:305:ASN:OD1	1:H:305:ASN:ND2	2.43	0.51
1:G:481:LEU:CD1	1:I:636:LEU:HD11	2.41	0.51
1:J:531:ASP:OD1	1:J:569:LYS:NZ	2.28	0.51
1:J:704:THR:OG1	1:K:702:GLN:N	2.37	0.51
1:M:305:ASN:ND2	1:R:305:ASN:OD1	115.77	0.51
1:D:305:ASN:OD1	1:N:305:ASN:ND2	56.94	0.51
1:O:240:VAL:HG13	1:O:687:TRP:HB2	1.92	0.51
1:P:426:SER:HB2	1:P:731:THR:O	2.11	0.51
1:M:305:ASN:OD1	1:R:305:ASN:ND2	115.77	0.51
1:V:636:LEU:HD11	1:X:481:LEU:CD1	2.41	0.51
1:W:704:THR:OG1	1:X:702:GLN:N	2.37	0.51
1:W:305:ASN:OD1	1:X:305:ASN:ND2	2.44	0.51
1:E:431:GLN:NE2	1:X:354:PRO:HB3	153.61	0.51
1:1:426:SER:HB2	1:1:731:THR:O	2.11	0.51
1:1:481:LEU:CD1	1:2:636:LEU:HD11	2.41	0.51
1:6:290:PHE:O	1:6:293:HIS:N	2.39	0.51
1:6:426:SER:HB2	1:6:731:THR:O	2.11	0.51
1:8:426:SER:HB2	1:8:731:THR:O	2.11	0.51
1:K:636:LEU:HD11	1:8:481:LEU:CD1	2.41	0.51
1:B:704:THR:OG1	1:C:702:GLN:N	71.00	0.51
1:E:329:ASN:O	1:E:332:THR:OG1	2.21	0.51
1:D:305:ASN:OD1	1:M:305:ASN:ND2	2.43	0.51
1:D:702:GLN:N	1:M:704:THR:OG1	2.37	0.51
1:E:305:ASN:OD1	1:P:305:ASN:ND2	2.43	0.51
1:S:481:LEU:CD1	1:U:636:LEU:HD11	2.41	0.51
1:S:305:ASN:ND2	1:T:305:ASN:OD1	2.44	0.51
1:U:305:ASN:ND2	1:1:305:ASN:OD1	156.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:305:ASN:ND2	1:X:305:ASN:OD1	2.43	0.51
1:Y:305:ASN:OD1	1:Z:305:ASN:ND2	2.44	0.51
1:3:240:VAL:HG13	1:3:687:TRP:HB2	1.92	0.50
1:T:702:GLN:N	1:5:704:THR:OG1	204.19	0.50
1:6:696:ARG:NE	1:6:698:ASN:OD1	2.36	0.50
1:B:481:LEU:CD1	1:M:636:LEU:HD11	103.23	0.50
1:C:426:SER:HB2	1:C:731:THR:O	2.11	0.50
1:G:354:PRO:HB3	1:H:431:GLN:NE2	49.98	0.50
1:F:481:LEU:CD1	1:H:636:LEU:HD11	128.51	0.50
1:I:704:THR:OG1	1:L:702:GLN:N	62.33	0.50
1:J:305:ASN:ND2	1:K:305:ASN:OD1	2.43	0.50
1:B:481:LEU:CD1	1:J:636:LEU:HD11	2.41	0.50
1:C:431:GLN:NE2	1:O:354:PRO:HB3	152.72	0.50
1:N:481:LEU:CD1	1:P:636:LEU:HD11	2.41	0.50
1:O:481:LEU:CD1	1:P:636:LEU:HD11	72.93	0.50
1:P:704:THR:OG1	1:S:702:GLN:N	105.24	0.50
1:Q:305:ASN:ND2	1:X:305:ASN:OD1	97.18	0.50
1:F:636:LEU:HD11	1:Q:481:LEU:CD1	2.41	0.50
1:Q:636:LEU:HD11	1:S:481:LEU:CD1	82.60	0.50
1:Q:704:THR:OG1	1:X:702:GLN:N	106.60	0.50
1:V:305:ASN:ND2	1:Y:305:ASN:OD1	112.31	0.50
1:W:329:ASN:O	1:W:332:THR:OG1	2.21	0.50
1:W:431:GLN:NE2	1:X:354:PRO:HB3	49.97	0.50
1:G:305:ASN:OD1	1:Z:305:ASN:ND2	60.78	0.50
1:Z:426:SER:HB2	1:Z:731:THR:O	2.11	0.50
1:4:426:SER:HB2	1:4:731:THR:O	2.11	0.50
1:7:305:ASN:ND2	1:8:305:ASN:OD1	2.43	0.50
1:B:636:LEU:HD11	1:C:481:LEU:CD1	72.94	0.50
1:G:696:ARG:NE	1:G:698:ASN:OD1	2.36	0.50
1:B:636:LEU:HD11	1:L:481:LEU:CD1	2.42	0.50
1:L:426:SER:HB2	1:L:731:THR:O	2.11	0.50
1:D:305:ASN:ND2	1:N:305:ASN:OD1	59.12	0.50
1:Q:354:PRO:HB3	1:S:431:GLN:NE2	93.52	0.50
1:S:305:ASN:OD1	1:T:305:ASN:ND2	2.44	0.50
1:S:426:SER:HB2	1:S:731:THR:O	2.11	0.50
1:D:636:LEU:HD11	1:T:481:LEU:CD1	128.43	0.50
1:R:636:LEU:HD11	1:U:481:LEU:CD1	2.41	0.50
1:U:704:THR:OG1	1:1:702:GLN:N	171.09	0.50
1:Y:305:ASN:ND2	1:Z:305:ASN:OD1	2.44	0.50
1:U:305:ASN:OD1	1:1:305:ASN:ND2	156.92	0.50
1:Z:636:LEU:HD11	1:2:481:LEU:CD1	87.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:240:VAL:HG13	1:4:687:TRP:HB2	1.92	0.50
1:W:481:LEU:CD1	1:X:636:LEU:HD11	64.72	0.50
1:Z:393:SER:O	1:2:696:ARG:NH2	78.03	0.50
1:3:354:PRO:HB3	1:4:431:GLN:NE2	2.23	0.50
1:3:426:SER:HB2	1:3:731:THR:O	2.11	0.50
1:7:329:ASN:O	1:7:332:THR:OG1	2.21	0.50
1:A:481:LEU:CD1	1:8:636:LEU:HD11	144.82	0.50
1:B:704:THR:OG1	1:I:702:GLN:N	2.36	0.50
1:E:426:SER:HB2	1:E:731:THR:O	2.11	0.50
1:N:426:SER:HB2	1:N:731:THR:O	2.11	0.50
1:E:305:ASN:ND2	1:P:305:ASN:OD1	2.43	0.50
1:L:481:LEU:CD1	1:T:636:LEU:HD11	203.67	0.50
1:X:290:PHE:O	1:X:293:HIS:N	2.39	0.50
1:G:702:GLN:N	1:Z:704:THR:OG1	65.38	0.50
1:7:426:SER:HB2	1:7:731:THR:O	2.11	0.50
1:C:481:LEU:CD1	1:O:636:LEU:HD11	136.02	0.50
1:E:481:LEU:CD1	1:Q:636:LEU:HD11	2.41	0.50
1:G:704:THR:OG1	1:H:702:GLN:N	2.37	0.50
1:H:481:LEU:CD1	1:W:636:LEU:HD11	2.42	0.50
1:J:659:ASP:OD2	1:L:333:LYS:NZ	113.13	0.50
1:I:305:ASN:OD1	1:L:305:ASN:ND2	60.15	0.50
1:C:636:LEU:HD11	1:M:481:LEU:CD1	2.41	0.50
1:M:426:SER:HB2	1:M:731:THR:O	2.11	0.50
1:N:431:GLN:NE2	1:O:354:PRO:HB3	49.97	0.50
1:C:636:LEU:HD11	1:P:481:LEU:CD1	67.41	0.50
1:Q:481:LEU:CD1	1:R:636:LEU:HD11	64.73	0.50
1:T:636:LEU:HD11	1:V:481:LEU:CD1	106.37	0.50
1:U:305:ASN:ND2	1:V:305:ASN:OD1	2.43	0.50
1:W:636:LEU:HD11	1:Y:481:LEU:CD1	23.85	0.50
1:Y:426:SER:HB2	1:Y:731:THR:O	2.11	0.50
1:5:426:SER:HB2	1:5:731:THR:O	2.11	0.50
1:B:426:SER:HB2	1:B:731:THR:O	2.11	0.50
1:C:704:THR:OG1	1:L:702:GLN:N	2.37	0.50
1:G:531:ASP:OD1	1:G:569:LYS:NZ	2.28	0.50
1:I:354:PRO:HB3	1:K:431:GLN:NE2	81.41	0.50
1:D:305:ASN:ND2	1:M:305:ASN:OD1	2.43	0.50
1:M:354:PRO:HB3	1:O:431:GLN:NE2	81.41	0.50
1:D:481:LEU:CD1	1:N:636:LEU:HD11	2.41	0.50
1:M:481:LEU:CD1	1:N:636:LEU:HD11	72.94	0.50
1:V:254:ASN:OD1	1:V:259:LYS:HD2	2.12	0.50
1:E:636:LEU:HD11	1:V:481:LEU:CD1	140.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:GLN:NE2	1:W:354:PRO:HB3	2.24	0.50
1:W:481:LEU:CD1	1:Y:636:LEU:HD11	2.41	0.50
1:5:481:LEU:CD1	1:6:636:LEU:HD11	2.42	0.50
1:7:254:ASN:OD1	1:7:259:LYS:HD2	2.12	0.50
1:8:290:PHE:O	1:8:293:HIS:N	2.39	0.50
1:E:254:ASN:OD1	1:E:259:LYS:HD2	2.12	0.50
1:G:704:THR:OG1	1:Z:702:GLN:N	70.26	0.50
1:K:254:ASN:OD1	1:K:259:LYS:HD2	2.12	0.50
1:J:305:ASN:OD1	1:K:305:ASN:ND2	2.43	0.50
1:D:481:LEU:CD1	1:L:636:LEU:HD11	128.51	0.50
1:J:481:LEU:CD1	1:L:636:LEU:HD11	2.41	0.50
1:U:254:ASN:OD1	1:U:259:LYS:HD2	2.12	0.50
1:U:481:LEU:CD1	1:V:636:LEU:HD11	64.72	0.50
1:Z:636:LEU:HD11	1:3:481:LEU:CD1	2.41	0.50
1:2:254:ASN:OD1	1:2:259:LYS:HD2	2.12	0.50
1:5:636:LEU:HD11	1:7:481:LEU:CD1	2.41	0.50
1:D:254:ASN:OD1	1:D:259:LYS:HD2	2.12	0.50
1:G:254:ASN:OD1	1:G:259:LYS:HD2	2.12	0.50
1:G:305:ASN:ND2	1:H:305:ASN:OD1	2.43	0.50
1:B:702:GLN:N	1:I:704:THR:OG1	2.36	0.50
1:J:305:ASN:OD1	1:W:305:ASN:ND2	137.05	0.50
1:A:636:LEU:HD11	1:K:481:LEU:CD1	123.13	0.50
1:N:329:ASN:O	1:N:332:THR:OG1	2.21	0.50
1:M:636:LEU:HD11	1:O:481:LEU:CD1	106.36	0.50
1:O:431:GLN:NE2	1:P:354:PRO:HB3	47.76	0.50
1:Q:704:THR:OG1	1:R:702:GLN:N	2.37	0.50
1:P:305:ASN:OD1	1:S:305:ASN:ND2	96.87	0.50
1:P:305:ASN:ND2	1:S:305:ASN:OD1	96.88	0.50
1:T:481:LEU:CD1	1:U:636:LEU:HD11	72.94	0.50
1:3:254:ASN:OD1	1:3:259:LYS:HD2	2.12	0.50
1:4:329:ASN:O	1:4:332:THR:OG1	2.21	0.50
1:E:531:ASP:OD1	1:E:569:LYS:NZ	2.28	0.50
1:E:305:ASN:ND2	1:F:305:ASN:OD1	56.93	0.50
1:A:431:GLN:NE2	1:G:354:PRO:HB3	2.23	0.50
1:J:254:ASN:OD1	1:J:259:LYS:HD2	2.12	0.50
1:C:702:GLN:N	1:L:704:THR:OG1	2.37	0.50
1:M:254:ASN:OD1	1:M:259:LYS:HD2	2.12	0.50
1:P:254:ASN:OD1	1:P:259:LYS:HD2	2.12	0.50
1:W:531:ASP:OD1	1:W:569:LYS:NZ	2.28	0.50
1:X:426:SER:HB2	1:X:731:THR:O	2.11	0.50
1:Y:254:ASN:OD1	1:Y:259:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:254:ASN:OD1	1:Z:259:LYS:HD2	2.12	0.50
1:Z:354:PRO:HB3	1:3:431:GLN:NE2	2.23	0.50
1:4:254:ASN:OD1	1:4:259:LYS:HD2	2.12	0.49
1:6:481:LEU:CD1	1:7:636:LEU:HD11	2.42	0.49
1:A:636:LEU:HD11	1:I:481:LEU:CD1	2.42	0.49
1:B:702:GLN:N	1:C:704:THR:OG1	61.56	0.49
1:F:254:ASN:OD1	1:F:259:LYS:HD2	2.12	0.49
1:G:636:LEU:HD11	1:H:481:LEU:CD1	64.72	0.49
1:I:254:ASN:OD1	1:I:259:LYS:HD2	2.12	0.49
1:I:636:LEU:HD11	1:K:481:LEU:CD1	106.36	0.49
1:I:702:GLN:N	1:L:704:THR:OG1	71.94	0.49
1:D:431:GLN:NE2	1:N:354:PRO:HB3	2.23	0.49
1:R:481:LEU:CD1	1:S:636:LEU:HD11	2.42	0.49
1:S:704:THR:OG1	1:T:702:GLN:N	2.37	0.49
1:L:431:GLN:NE2	1:T:354:PRO:HB3	196.01	0.49
1:X:254:ASN:OD1	1:X:259:LYS:HD2	2.12	0.49
1:Z:431:GLN:NE2	1:1:354:PRO:HB3	95.82	0.49
1:A:704:THR:OG1	1:3:702:GLN:N	152.66	0.49
1:C:254:ASN:OD1	1:C:259:LYS:HD2	2.12	0.49
1:E:636:LEU:HD11	1:F:481:LEU:CD1	2.41	0.49
1:I:696:ARG:NE	1:I:698:ASN:OD1	2.36	0.49
1:L:254:ASN:OD1	1:L:259:LYS:HD2	2.12	0.49
1:N:254:ASN:OD1	1:N:259:LYS:HD2	2.12	0.49
1:O:254:ASN:OD1	1:O:259:LYS:HD2	2.12	0.49
1:U:305:ASN:OD1	1:V:305:ASN:ND2	2.43	0.49
1:W:254:ASN:OD1	1:W:259:LYS:HD2	2.12	0.49
1:Z:481:LEU:CD1	1:1:636:LEU:HD11	86.46	0.49
1:5:254:ASN:OD1	1:5:259:LYS:HD2	2.12	0.49
1:6:431:GLN:NE2	1:7:354:PRO:HB3	2.23	0.49
1:8:254:ASN:OD1	1:8:259:LYS:HD2	2.12	0.49
1:A:354:PRO:HB3	1:K:431:GLN:NE2	95.90	0.49
1:B:254:ASN:OD1	1:B:259:LYS:HD2	2.12	0.49
1:F:636:LEU:HD11	1:G:481:LEU:CD1	82.60	0.49
1:V:656:VAL:HG11	1:1:324:LYS:HE3	172.89	0.49
1:V:305:ASN:OD1	1:Y:305:ASN:ND2	112.31	0.49
1:Z:481:LEU:CD1	1:4:636:LEU:HD11	2.42	0.49
1:6:254:ASN:OD1	1:6:259:LYS:HD2	2.12	0.49
1:A:354:PRO:HB3	1:I:431:GLN:NE2	2.25	0.49
1:Q:254:ASN:OD1	1:Q:259:LYS:HD2	2.12	0.49
1:S:254:ASN:OD1	1:S:259:LYS:HD2	2.12	0.49
1:T:324:LYS:HE3	1:U:656:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:431:GLN:NE2	1:Y:354:PRO:HB3	47.76	0.49
1:5:328:GLN:NE2	1:5:333:LYS:HG3	2.23	0.49
1:A:254:ASN:OD1	1:A:259:LYS:HD2	2.12	0.49
1:H:254:ASN:OD1	1:H:259:LYS:HD2	2.12	0.49
1:H:305:ASN:ND2	1:K:305:ASN:OD1	95.97	0.49
1:D:324:LYS:HE3	1:O:656:VAL:HG11	115.62	0.49
1:H:636:LEU:HD11	1:Y:481:LEU:CD1	2.42	0.49
1:1:254:ASN:OD1	1:1:259:LYS:HD2	2.12	0.49
1:1:431:GLN:NE2	1:2:354:PRO:HB3	2.22	0.49
1:M:324:LYS:HE3	1:N:656:VAL:HG11	1.95	0.49
1:N:704:THR:OG1	1:O:702:GLN:N	2.37	0.49
1:O:324:LYS:HE3	1:7:656:VAL:HG11	174.81	0.49
1:A:656:VAL:HG11	1:J:324:LYS:HE3	91.78	0.49
1:E:354:PRO:HB3	1:F:431:GLN:NE2	2.23	0.49
1:J:431:GLN:NE2	1:K:354:PRO:HB3	49.98	0.49
1:T:254:ASN:OD1	1:T:259:LYS:HD2	2.12	0.49
1:A:360:ALA:HB1	1:I:444:TYR:CZ	2.48	0.49
1:H:305:ASN:OD1	1:K:305:ASN:ND2	99.51	0.49
1:H:702:GLN:N	1:K:704:THR:OG1	112.19	0.49
1:V:324:LYS:HE3	1:W:656:VAL:HG11	27.18	0.49
1:Z:444:TYR:CZ	1:1:360:ALA:HB1	85.58	0.49
1:Z:444:TYR:CZ	1:4:360:ALA:HB1	2.48	0.49
1:D:287:PHE:CE1	1:D:621:TRP:HH2	2.31	0.49
1:E:324:LYS:HE3	1:H:656:VAL:HG11	128.95	0.49
1:I:481:LEU:CD1	1:J:636:LEU:HD11	72.93	0.49
1:K:656:VAL:HG11	1:W:324:LYS:HE3	181.71	0.49
1:2:287:PHE:CE1	1:2:621:TRP:HH2	2.31	0.49
1:3:287:PHE:CE1	1:3:621:TRP:HH2	2.31	0.49
1:5:360:ALA:HB1	1:7:444:TYR:CZ	2.48	0.49
1:A:656:VAL:HG11	1:B:324:LYS:HE3	1.95	0.49
1:A:444:TYR:CZ	1:G:360:ALA:HB1	2.48	0.49
1:H:696:ARG:NE	1:H:698:ASN:OD1	2.36	0.49
1:G:702:GLN:N	1:H:704:THR:OG1	2.36	0.49
1:L:406:LEU:N	1:L:406:LEU:CD1	2.76	0.49
1:B:431:GLN:NE2	1:M:354:PRO:HB3	121.72	0.49
1:N:481:LEU:CD1	1:O:636:LEU:HD11	64.72	0.49
1:E:425:SER:OG	1:Q:628:ASP:OD2	2.30	0.49
1:R:254:ASN:OD1	1:R:259:LYS:HD2	2.12	0.49
1:R:287:PHE:CE1	1:R:621:TRP:HH2	2.31	0.49
1:R:354:PRO:HB3	1:U:431:GLN:NE2	2.23	0.49
1:P:702:GLN:N	1:S:704:THR:OG1	108.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:287:PHE:CE1	1:T:621:TRP:HH2	2.31	0.49
1:T:328:GLN:NE2	1:T:333:LYS:HG3	2.23	0.49
1:U:287:PHE:CE1	1:U:621:TRP:HH2	2.31	0.49
1:V:354:PRO:HB3	1:X:431:GLN:NE2	2.24	0.49
1:X:287:PHE:CE1	1:X:621:TRP:HH2	2.31	0.49
1:2:382:THR:HG22	1:2:383:LEU:N	2.28	0.48
1:3:324:LYS:HE3	1:8:656:VAL:HG11	1.95	0.48
1:5:406:LEU:CD1	1:5:406:LEU:N	2.76	0.48
1:5:287:PHE:CE1	1:5:621:TRP:HH2	2.31	0.48
1:6:406:LEU:CD1	1:6:406:LEU:N	2.76	0.48
1:B:324:LYS:HE3	1:O:656:VAL:HG11	132.44	0.48
1:C:324:LYS:HE3	1:M:656:VAL:HG11	101.24	0.48
1:D:382:THR:HG22	1:D:383:LEU:N	2.29	0.48
1:D:656:VAL:HG11	1:S:324:LYS:HE3	106.08	0.48
1:F:382:THR:HG22	1:F:383:LEU:N	2.29	0.48
1:I:382:THR:HG22	1:I:383:LEU:N	2.28	0.48
1:L:444:TYR:CZ	1:T:360:ALA:HB1	193.20	0.48
1:M:406:LEU:N	1:M:406:LEU:CD1	2.76	0.48
1:O:287:PHE:CE1	1:O:621:TRP:HH2	2.31	0.48
1:C:444:TYR:CZ	1:O:360:ALA:HB1	142.29	0.48
1:P:382:THR:HG22	1:P:383:LEU:N	2.29	0.48
1:Q:406:LEU:CD1	1:Q:406:LEU:N	2.76	0.48
1:S:382:THR:HG22	1:S:383:LEU:N	2.28	0.48
1:T:354:PRO:HB3	1:V:431:GLN:NE2	81.41	0.48
1:R:656:VAL:HG11	1:V:324:LYS:HE3	1.95	0.48
1:T:360:ALA:HB1	1:V:444:TYR:CZ	83.12	0.48
1:V:287:PHE:CE1	1:V:621:TRP:HH2	2.31	0.48
1:Z:406:LEU:CD1	1:Z:406:LEU:N	2.76	0.48
1:P:656:VAL:HG11	1:6:324:LYS:HE3	175.30	0.48
1:C:382:THR:HG22	1:C:383:LEU:N	2.28	0.48
1:D:406:LEU:N	1:D:406:LEU:CD1	2.76	0.48
1:F:406:LEU:N	1:F:406:LEU:CD1	2.76	0.48
1:F:656:VAL:HG11	1:Z:324:LYS:HE3	121.83	0.48
1:G:382:THR:HG22	1:G:383:LEU:N	2.28	0.48
1:H:324:LYS:HE3	1:I:656:VAL:HG11	1.95	0.48
1:H:360:ALA:HB1	1:Y:444:TYR:CZ	2.48	0.48
1:J:382:THR:HG22	1:J:383:LEU:N	2.28	0.48
1:G:656:VAL:HG11	1:K:324:LYS:HE3	168.06	0.48
1:K:406:LEU:CD1	1:K:406:LEU:N	2.76	0.48
1:L:287:PHE:CE1	1:L:621:TRP:HH2	2.31	0.48
1:M:444:TYR:CZ	1:N:360:ALA:HB1	82.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:406:LEU:N	1:O:406:LEU:CD1	2.76	0.48
1:Q:444:TYR:CZ	1:R:360:ALA:HB1	52.80	0.48
1:R:382:THR:HG22	1:R:383:LEU:N	2.28	0.48
1:Q:702:GLN:N	1:R:704:THR:OG1	2.37	0.48
1:S:328:GLN:NE2	1:S:333:LYS:HG3	2.23	0.48
1:U:406:LEU:CD1	1:U:406:LEU:N	2.76	0.48
1:R:360:ALA:HB1	1:U:444:TYR:CZ	2.49	0.48
1:V:406:LEU:CD1	1:V:406:LEU:N	2.76	0.48
1:W:444:TYR:CZ	1:Y:360:ALA:HB1	2.48	0.48
1:Y:382:THR:HG22	1:Y:383:LEU:N	2.29	0.48
1:6:444:TYR:CZ	1:7:360:ALA:HB1	2.49	0.48
1:7:382:THR:HG22	1:7:383:LEU:N	2.29	0.48
1:C:360:ALA:HB1	1:P:444:TYR:CZ	49.06	0.48
1:C:656:VAL:HG11	1:D:324:LYS:HE3	1.95	0.48
1:E:382:THR:HG22	1:E:383:LEU:N	2.29	0.48
1:E:287:PHE:CE1	1:E:621:TRP:HH2	2.31	0.48
1:F:287:PHE:CE1	1:F:621:TRP:HH2	2.31	0.48
1:G:329:ASN:O	1:G:332:THR:OG1	2.21	0.48
1:B:431:GLN:NE2	1:J:354:PRO:HB3	2.23	0.48
1:J:406:LEU:N	1:J:406:LEU:CD1	2.76	0.48
1:J:444:TYR:CZ	1:L:360:ALA:HB1	2.49	0.48
1:J:287:PHE:CE1	1:J:621:TRP:HH2	2.31	0.48
1:O:324:LYS:HE3	1:P:656:VAL:HG11	1.95	0.48
1:E:444:TYR:CZ	1:Q:360:ALA:HB1	2.49	0.48
1:Q:287:PHE:CE1	1:Q:621:TRP:HH2	2.31	0.48
1:R:444:TYR:CZ	1:S:360:ALA:HB1	2.48	0.48
1:D:360:ALA:HB1	1:T:444:TYR:CZ	122.61	0.48
1:E:656:VAL:HG11	1:U:324:LYS:HE3	165.10	0.48
1:U:382:THR:HG22	1:U:383:LEU:N	2.29	0.48
1:W:287:PHE:CE1	1:W:621:TRP:HH2	2.31	0.48
1:W:328:GLN:NE2	1:W:333:LYS:HG3	2.23	0.48
1:W:444:TYR:CZ	1:X:360:ALA:HB1	52.79	0.48
1:E:444:TYR:CZ	1:X:360:ALA:HB1	140.83	0.48
1:Q:324:LYS:HE3	1:Y:656:VAL:HG11	165.91	0.48
1:Z:287:PHE:CE1	1:Z:621:TRP:HH2	2.31	0.48
1:Z:382:THR:HG22	1:Z:383:LEU:N	2.28	0.48
1:1:444:TYR:CZ	1:2:360:ALA:HB1	2.49	0.48
1:Z:360:ALA:HB1	1:2:444:TYR:CZ	96.94	0.48
1:3:406:LEU:N	1:3:406:LEU:CD1	2.76	0.48
1:4:406:LEU:CD1	1:4:406:LEU:N	2.76	0.48
1:3:636:LEU:HD11	1:4:481:LEU:CD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:287:PHE:CE1	1:8:621:TRP:HH2	2.31	0.48
1:A:287:PHE:CE1	1:A:621:TRP:HH2	2.31	0.48
1:C:360:ALA:HB1	1:M:444:TYR:CZ	2.49	0.48
1:D:444:TYR:CZ	1:L:360:ALA:HB1	129.57	0.48
1:E:328:GLN:NE2	1:E:333:LYS:HG3	2.23	0.48
1:E:360:ALA:HB1	1:V:444:TYR:CZ	156.34	0.48
1:E:360:ALA:HB1	1:F:444:TYR:CZ	2.49	0.48
1:G:287:PHE:CE1	1:G:621:TRP:HH2	2.31	0.48
1:H:329:ASN:O	1:H:332:THR:OG1	2.21	0.48
1:F:431:GLN:NE2	1:H:354:PRO:HB3	123.21	0.48
1:H:382:THR:HG22	1:H:383:LEU:N	2.28	0.48
1:H:656:VAL:HG11	1:Z:324:LYS:HE3	1.95	0.48
1:I:324:LYS:HE3	1:J:656:VAL:HG11	1.95	0.48
1:I:324:LYS:HE3	1:T:656:VAL:HG11	187.37	0.48
1:I:406:LEU:CD1	1:I:406:LEU:N	2.76	0.48
1:K:324:LYS:HE3	1:L:656:VAL:HG11	1.95	0.48
1:M:382:THR:HG22	1:M:383:LEU:N	2.29	0.48
1:N:406:LEU:CD1	1:N:406:LEU:N	2.76	0.48
1:N:287:PHE:CE1	1:N:621:TRP:HH2	2.31	0.48
1:N:431:GLN:NE2	1:P:354:PRO:HB3	2.23	0.48
1:V:656:VAL:HG11	1:W:324:LYS:HE3	1.95	0.48
1:W:382:THR:HG22	1:W:383:LEU:N	2.29	0.48
1:X:346:PHE:HB3	1:X:403:SER:HA	1.96	0.48
1:W:360:ALA:HB1	1:Y:444:TYR:CZ	47.33	0.48
1:3:360:ALA:HB1	1:4:444:TYR:CZ	2.48	0.48
1:Z:360:ALA:HB1	1:3:444:TYR:CZ	2.48	0.48
1:4:287:PHE:CE1	1:4:621:TRP:HH2	2.31	0.48
1:5:254:ASN:ND2	1:5:377:GLN:NE2	2.62	0.48
1:A:324:LYS:HE3	1:Z:656:VAL:HG11	116.08	0.48
1:A:346:PHE:HB3	1:A:403:SER:HA	1.96	0.48
1:A:406:LEU:N	1:A:406:LEU:CD1	2.76	0.48
1:B:360:ALA:HB1	1:C:444:TYR:CZ	82.49	0.48
1:F:324:LYS:HE3	1:G:656:VAL:HG11	1.96	0.48
1:E:702:GLN:N	1:F:704:THR:OG1	67.89	0.48
1:G:254:ASN:ND2	1:G:377:GLN:NE2	2.62	0.48
1:H:254:ASN:ND2	1:H:377:GLN:NE2	2.62	0.48
1:H:346:PHE:HB3	1:H:403:SER:HA	1.96	0.48
1:I:578:GLN:OE1	1:I:597:ASN:ND2	2.47	0.48
1:I:287:PHE:CE1	1:I:621:TRP:HH2	2.31	0.48
1:K:382:THR:HG22	1:K:383:LEU:N	2.29	0.48
1:L:610:GLN:HE21	1:T:627:THR:CG2	194.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:346:PHE:HB3	1:O:403:SER:HA	1.96	0.48
1:P:254:ASN:ND2	1:P:377:GLN:NE2	2.62	0.48
1:P:287:PHE:CE1	1:P:621:TRP:HH2	2.31	0.48
1:Q:328:GLN:NE2	1:Q:333:LYS:HG3	2.23	0.48
1:E:431:GLN:NE2	1:Q:354:PRO:HB3	2.23	0.48
1:R:578:GLN:OE1	1:R:597:ASN:ND2	2.47	0.48
1:S:406:LEU:CD1	1:S:406:LEU:N	2.76	0.48
1:T:578:GLN:OE1	1:T:597:ASN:ND2	2.47	0.48
1:U:578:GLN:OE1	1:U:597:ASN:ND2	2.47	0.48
1:V:578:GLN:OE1	1:V:597:ASN:ND2	2.47	0.48
1:T:656:VAL:HG11	1:Y:324:LYS:HE3	129.02	0.48
1:Y:578:GLN:OE1	1:Y:597:ASN:ND2	2.47	0.48
1:2:578:GLN:OE1	1:2:597:ASN:ND2	2.47	0.48
1:2:704:THR:OG1	1:4:702:GLN:N	2.37	0.48
1:4:382:THR:HG22	1:4:383:LEU:N	2.29	0.48
1:U:656:VAL:HG11	1:5:324:LYS:HE3	189.66	0.48
1:B:254:ASN:ND2	1:B:377:GLN:NE2	2.62	0.48
1:B:360:ALA:HB1	1:L:444:TYR:CZ	2.48	0.48
1:C:578:GLN:OE1	1:C:597:ASN:ND2	2.47	0.48
1:C:656:VAL:HG11	1:S:324:LYS:HE3	115.43	0.48
1:G:324:LYS:HE3	1:1:656:VAL:HG11	175.32	0.48
1:G:406:LEU:N	1:G:406:LEU:CD1	2.76	0.48
1:H:406:LEU:N	1:H:406:LEU:CD1	2.76	0.48
1:B:444:TYR:CZ	1:J:360:ALA:HB1	2.48	0.48
1:K:254:ASN:ND2	1:K:377:GLN:NE2	2.62	0.48
1:I:360:ALA:HB1	1:K:444:TYR:CZ	83.11	0.48
1:J:656:VAL:HG11	1:L:324:LYS:HE3	101.23	0.48
1:M:324:LYS:HE3	1:S:656:VAL:HG11	118.39	0.48
1:M:287:PHE:CE1	1:M:621:TRP:HH2	2.31	0.48
1:M:656:VAL:HG11	1:N:324:LYS:HE3	27.17	0.48
1:N:382:THR:HG22	1:N:383:LEU:N	2.29	0.48
1:O:254:ASN:ND2	1:O:377:GLN:NE2	2.62	0.48
1:M:360:ALA:HB1	1:O:444:TYR:CZ	83.11	0.48
1:O:444:TYR:CZ	1:P:360:ALA:HB1	82.49	0.48
1:O:532:ASP:OD1	1:P:385:ASN:ND2	33.31	0.48
1:Q:254:ASN:ND2	1:Q:377:GLN:NE2	2.62	0.48
1:R:254:ASN:ND2	1:R:377:GLN:NE2	2.62	0.48
1:R:457:THR:HG23	1:R:458:GLN:HG3	1.96	0.48
1:U:328:GLN:NE2	1:U:333:LYS:HG3	2.23	0.48
1:U:346:PHE:HB3	1:U:403:SER:HA	1.96	0.48
1:V:382:THR:HG22	1:V:383:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:457:THR:HG23	1:Y:458:GLN:HG3	1.96	0.48
1:1:457:THR:HG23	1:1:458:GLN:HG3	1.96	0.48
1:U:324:LYS:HE3	1:2:656:VAL:HG11	177.45	0.48
1:4:578:GLN:OE1	1:4:597:ASN:ND2	2.47	0.48
1:6:287:PHE:CE1	1:6:621:TRP:HH2	2.31	0.48
1:A:431:GLN:NE2	1:8:354:PRO:HB3	151.92	0.48
1:A:444:TYR:CZ	1:8:360:ALA:HB1	155.70	0.48
1:8:578:GLN:OE1	1:8:597:ASN:ND2	2.47	0.48
1:A:254:ASN:ND2	1:A:377:GLN:NE2	2.62	0.48
1:A:324:LYS:HE3	1:E:656:VAL:HG11	1.96	0.48
1:A:360:ALA:HB1	1:K:444:TYR:CZ	121.28	0.48
1:B:444:TYR:CZ	1:M:360:ALA:HB1	126.10	0.48
1:D:578:GLN:OE1	1:D:597:ASN:ND2	2.47	0.48
1:E:254:ASN:ND2	1:E:377:GLN:NE2	2.62	0.48
1:F:578:GLN:OE1	1:F:597:ASN:ND2	2.47	0.48
1:G:457:THR:HG23	1:G:458:GLN:HG3	1.96	0.48
1:G:360:ALA:HB1	1:H:444:TYR:CZ	52.80	0.48
1:I:457:THR:HG23	1:I:458:GLN:HG3	1.96	0.48
1:J:324:LYS:HE3	1:X:656:VAL:HG11	132.44	0.48
1:J:457:THR:HG23	1:J:458:GLN:HG3	1.96	0.48
1:J:578:GLN:OE1	1:J:597:ASN:ND2	2.47	0.48
1:K:287:PHE:CE1	1:K:621:TRP:HH2	2.31	0.48
1:L:382:THR:HG22	1:L:383:LEU:N	2.28	0.48
1:M:346:PHE:HB3	1:M:403:SER:HA	1.96	0.48
1:M:457:THR:HG23	1:M:458:GLN:HG3	1.96	0.48
1:N:578:GLN:OE1	1:N:597:ASN:ND2	2.47	0.48
1:N:444:TYR:CZ	1:O:360:ALA:HB1	52.79	0.48
1:P:578:GLN:OE1	1:P:597:ASN:ND2	2.47	0.48
1:S:346:PHE:HB3	1:S:403:SER:HA	1.96	0.48
1:T:254:ASN:ND2	1:T:377:GLN:NE2	2.62	0.48
1:T:382:THR:HG22	1:T:383:LEU:N	2.29	0.48
1:T:457:THR:HG23	1:T:458:GLN:HG3	1.96	0.48
1:T:704:THR:OG1	1:5:702:GLN:N	205.72	0.48
1:V:346:PHE:HB3	1:V:403:SER:HA	1.96	0.48
1:W:254:ASN:ND2	1:W:377:GLN:NE2	2.62	0.48
1:Y:406:LEU:CD1	1:Y:406:LEU:N	2.76	0.48
1:Z:254:ASN:ND2	1:Z:377:GLN:NE2	2.62	0.48
1:1:287:PHE:CE1	1:1:621:TRP:HH2	2.31	0.48
1:1:382:THR:HG22	1:1:383:LEU:N	2.29	0.48
1:4:254:ASN:ND2	1:4:377:GLN:NE2	2.62	0.48
1:5:444:TYR:CZ	1:6:360:ALA:HB1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:578:GLN:OE1	1:5:597:ASN:ND2	2.47	0.48
1:A:382:THR:HG22	1:A:383:LEU:N	2.29	0.48
1:B:656:VAL:HG11	1:L:324:LYS:HE3	85.48	0.48
1:B:656:VAL:HG11	1:C:324:LYS:HE3	1.95	0.48
1:C:287:PHE:CE1	1:C:621:TRP:HH2	2.31	0.48
1:E:578:GLN:OE1	1:E:597:ASN:ND2	2.47	0.48
1:H:287:PHE:CE1	1:H:621:TRP:HH2	2.31	0.48
1:K:346:PHE:HB3	1:K:403:SER:HA	1.96	0.48
1:N:254:ASN:ND2	1:N:377:GLN:NE2	2.62	0.48
1:O:382:THR:HG22	1:O:383:LEU:N	2.28	0.48
1:Q:324:LYS:HE3	1:S:656:VAL:HG11	1.95	0.48
1:V:457:THR:HG23	1:V:458:GLN:HG3	1.96	0.48
1:5:354:PRO:HB3	1:7:431:GLN:NE2	2.24	0.48
1:5:382:THR:HG22	1:5:383:LEU:N	2.28	0.48
1:6:382:THR:HG22	1:6:383:LEU:N	2.28	0.48
1:D:354:PRO:HB3	1:T:431:GLN:NE2	116.03	0.48
1:D:360:ALA:HB1	1:P:444:TYR:CZ	2.49	0.48
1:D:346:PHE:HB3	1:D:403:SER:HA	1.96	0.48
1:D:704:THR:OG1	1:N:702:GLN:N	67.89	0.48
1:E:406:LEU:CD1	1:E:406:LEU:N	2.76	0.48
1:G:346:PHE:HB3	1:G:403:SER:HA	1.96	0.48
1:I:346:PHE:HB3	1:I:403:SER:HA	1.96	0.48
1:J:254:ASN:ND2	1:J:377:GLN:NE2	2.62	0.48
1:K:360:ALA:HB1	1:8:444:TYR:CZ	2.49	0.48
1:K:340:THR:HB	1:K:407:ARG:NH2	2.29	0.48
1:L:254:ASN:ND2	1:L:377:GLN:NE2	2.62	0.48
1:M:254:ASN:ND2	1:M:377:GLN:NE2	2.62	0.48
1:P:346:PHE:HB3	1:P:403:SER:HA	1.96	0.48
1:P:406:LEU:N	1:P:406:LEU:CD1	2.76	0.48
1:Q:382:THR:HG22	1:Q:383:LEU:N	2.29	0.48
1:Q:578:GLN:OE1	1:Q:597:ASN:ND2	2.47	0.48
1:S:254:ASN:ND2	1:S:377:GLN:NE2	2.62	0.48
1:S:329:ASN:O	1:S:332:THR:OG1	2.21	0.48
1:S:340:THR:HB	1:S:407:ARG:NH2	2.29	0.48
1:W:578:GLN:OE1	1:W:597:ASN:ND2	2.47	0.48
1:X:610:GLN:HE21	1:Y:627:THR:CG2	45.56	0.48
1:Z:346:PHE:HB3	1:Z:403:SER:HA	1.96	0.48
1:Z:610:GLN:HE21	1:1:627:THR:CG2	88.94	0.48
1:1:532:ASP:OD1	1:2:385:ASN:ND2	2.47	0.48
1:4:457:THR:HG23	1:4:458:GLN:HG3	1.96	0.48
1:5:346:PHE:HB3	1:5:403:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:340:THR:HB	1:5:407:ARG:NH2	2.29	0.48
1:7:346:PHE:HB3	1:7:403:SER:HA	1.96	0.48
1:7:340:THR:HB	1:7:407:ARG:NH2	2.29	0.48
1:7:578:GLN:OE1	1:7:597:ASN:ND2	2.47	0.48
1:8:406:LEU:CD1	1:8:406:LEU:N	2.76	0.48
1:8:340:THR:HB	1:8:407:ARG:NH2	2.29	0.48
1:A:578:GLN:OE1	1:A:597:ASN:ND2	2.47	0.48
1:B:578:GLN:OE1	1:B:597:ASN:ND2	2.47	0.48
1:B:623:LYS:HB2	1:B:645:PRO:HG3	1.97	0.48
1:C:254:ASN:ND2	1:C:377:GLN:NE2	2.62	0.48
1:D:656:VAL:HG11	1:E:324:LYS:HE3	1.95	0.48
1:F:254:ASN:ND2	1:F:377:GLN:NE2	2.62	0.48
1:F:385:ASN:ND2	1:Q:532:ASP:OD1	2.47	0.48
1:G:444:TYR:CZ	1:I:360:ALA:HB1	2.49	0.48
1:G:578:GLN:OE1	1:G:597:ASN:ND2	2.47	0.48
1:H:340:THR:HB	1:H:407:ARG:NH2	2.29	0.48
1:I:254:ASN:ND2	1:I:377:GLN:NE2	2.62	0.48
1:J:346:PHE:HB3	1:J:403:SER:HA	1.96	0.48
1:J:704:THR:OG1	1:W:702:GLN:N	147.69	0.48
1:L:328:GLN:NE2	1:L:333:LYS:HG3	2.23	0.48
1:L:346:PHE:HB3	1:L:403:SER:HA	1.96	0.48
1:M:578:GLN:OE1	1:M:597:ASN:ND2	2.47	0.48
1:D:444:TYR:CZ	1:N:360:ALA:HB1	2.49	0.48
1:N:444:TYR:CZ	1:P:360:ALA:HB1	2.49	0.48
1:O:578:GLN:OE1	1:O:597:ASN:ND2	2.47	0.48
1:Q:346:PHE:HB3	1:Q:403:SER:HA	1.96	0.48
1:Q:340:THR:HB	1:Q:407:ARG:NH2	2.29	0.48
1:Q:610:GLN:HE21	1:R:627:THR:CG2	61.64	0.48
1:R:406:LEU:N	1:R:406:LEU:CD1	2.76	0.48
1:S:457:THR:HG23	1:S:458:GLN:HG3	1.96	0.48
1:T:346:PHE:HB3	1:T:403:SER:HA	1.96	0.48
1:T:406:LEU:CD1	1:T:406:LEU:N	2.76	0.48
1:U:254:ASN:ND2	1:U:377:GLN:NE2	2.62	0.48
1:X:382:THR:HG22	1:X:383:LEU:N	2.29	0.48
1:X:340:THR:HB	1:X:407:ARG:NH2	2.29	0.48
1:X:578:GLN:OE1	1:X:597:ASN:ND2	2.47	0.48
1:F:324:LYS:HE3	1:X:656:VAL:HG11	119.96	0.48
1:Z:340:THR:HB	1:Z:407:ARG:NH2	2.29	0.48
1:1:406:LEU:CD1	1:1:406:LEU:N	2.76	0.47
1:3:254:ASN:ND2	1:3:377:GLN:NE2	2.62	0.47
1:3:382:THR:HG22	1:3:383:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:340:THR:HB	1:3:407:ARG:NH2	2.29	0.47
1:5:457:THR:HG23	1:5:458:GLN:HG3	1.96	0.47
1:8:346:PHE:HB3	1:8:403:SER:HA	1.96	0.47
1:A:328:GLN:NE2	1:A:333:LYS:HG3	2.23	0.47
1:A:385:ASN:ND2	1:K:532:ASP:OD1	99.91	0.47
1:A:617:GLN:OE1	1:A:617:GLN:N	2.47	0.47
1:B:346:PHE:HB3	1:B:403:SER:HA	1.96	0.47
1:B:340:THR:HB	1:B:407:ARG:NH2	2.29	0.47
1:B:287:PHE:CE1	1:B:621:TRP:HH2	2.31	0.47
1:C:385:ASN:ND2	1:M:532:ASP:OD1	2.47	0.47
1:D:532:ASP:OD1	1:N:385:ASN:ND2	2.47	0.47
1:E:346:PHE:HB3	1:E:403:SER:HA	1.96	0.47
1:E:340:THR:HB	1:E:407:ARG:NH2	2.29	0.47
1:E:623:LYS:HB2	1:E:645:PRO:HG3	1.96	0.47
1:F:340:THR:HB	1:F:407:ARG:NH2	2.29	0.47
1:H:457:THR:HG23	1:H:458:GLN:HG3	1.96	0.47
1:J:532:ASP:OD1	1:L:385:ASN:ND2	2.47	0.47
1:K:656:VAL:HG11	1:7:324:LYS:HE3	1.95	0.47
1:J:431:GLN:NE2	1:L:354:PRO:HB3	2.23	0.47
1:L:340:THR:HB	1:L:407:ARG:NH2	2.29	0.47
1:L:578:GLN:OE1	1:L:597:ASN:ND2	2.47	0.47
1:N:457:THR:HG23	1:N:458:GLN:HG3	1.96	0.47
1:N:610:GLN:HE21	1:P:627:THR:CG2	2.25	0.47
1:N:617:GLN:N	1:N:617:GLN:OE1	2.47	0.47
1:P:340:THR:HB	1:P:407:ARG:NH2	2.29	0.47
1:Q:457:THR:HG23	1:Q:458:GLN:HG3	1.96	0.47
1:Q:431:GLN:NE2	1:R:354:PRO:HB3	49.98	0.47
1:R:346:PHE:HB3	1:R:403:SER:HA	1.96	0.47
1:R:617:GLN:OE1	1:R:617:GLN:N	2.47	0.47
1:M:702:GLN:N	1:R:704:THR:OG1	127.96	0.47
1:S:623:LYS:HB2	1:S:645:PRO:HG3	1.96	0.47
1:T:617:GLN:OE1	1:T:617:GLN:N	2.47	0.47
1:U:623:LYS:HB2	1:U:645:PRO:HG3	1.96	0.47
1:W:340:THR:HB	1:W:407:ARG:NH2	2.29	0.47
1:W:406:LEU:N	1:W:406:LEU:CD1	2.76	0.47
1:E:532:ASP:OD1	1:X:385:ASN:ND2	182.31	0.47
1:Z:578:GLN:OE1	1:Z:597:ASN:ND2	2.47	0.47
1:Z:623:LYS:HB2	1:Z:645:PRO:HG3	1.96	0.47
1:1:346:PHE:HB3	1:1:403:SER:HA	1.96	0.47
1:2:324:LYS:HE3	1:3:656:VAL:HG11	1.96	0.47
1:3:531:ASP:OD1	1:3:569:LYS:NZ	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:578:GLN:OE1	1:3:597:ASN:ND2	2.47	0.47
1:4:340:THR:HB	1:4:407:ARG:NH2	2.29	0.47
1:6:340:THR:HB	1:6:407:ARG:NH2	2.29	0.47
1:7:623:LYS:HB2	1:7:645:PRO:HG3	1.97	0.47
1:5:656:VAL:HG11	1:8:324:LYS:HE3	1.95	0.47
1:8:382:THR:HG22	1:8:383:LEU:N	2.29	0.47
1:C:340:THR:HB	1:C:407:ARG:NH2	2.29	0.47
1:G:340:THR:HB	1:G:407:ARG:NH2	2.29	0.47
1:J:340:THR:HB	1:J:407:ARG:NH2	2.29	0.47
1:M:340:THR:HB	1:M:407:ARG:NH2	2.29	0.47
1:M:623:LYS:HB2	1:M:645:PRO:HG3	1.96	0.47
1:N:532:ASP:OD1	1:P:385:ASN:ND2	2.47	0.47
1:S:617:GLN:OE1	1:S:617:GLN:N	2.47	0.47
1:S:287:PHE:CE1	1:S:621:TRP:HH2	2.31	0.47
1:T:324:LYS:HE3	1:6:656:VAL:HG11	182.42	0.47
1:U:444:TYR:CZ	1:V:360:ALA:HB1	52.79	0.47
1:V:623:LYS:HB2	1:V:645:PRO:HG3	1.96	0.47
1:H:444:TYR:CZ	1:W:360:ALA:HB1	2.48	0.47
1:W:346:PHE:HB3	1:W:403:SER:HA	1.96	0.47
1:X:312:LYS:O	1:X:418:PHE:N	2.43	0.47
1:V:627:THR:CG2	1:X:610:GLN:HE21	2.25	0.47
1:Y:287:PHE:CE1	1:Y:621:TRP:HH2	2.31	0.47
1:Z:328:GLN:NE2	1:Z:333:LYS:HG3	2.23	0.47
1:Z:385:ASN:ND2	1:2:532:ASP:OD1	84.21	0.47
1:2:346:PHE:HB3	1:2:403:SER:HA	1.96	0.47
1:5:532:ASP:OD1	1:6:385:ASN:ND2	2.48	0.47
1:6:531:ASP:OD1	1:6:569:LYS:NZ	2.28	0.47
1:B:457:THR:HG23	1:B:458:GLN:HG3	1.96	0.47
1:C:354:PRO:HB3	1:M:431:GLN:NE2	2.23	0.47
1:D:457:THR:HG23	1:D:458:GLN:HG3	1.96	0.47
1:G:617:GLN:N	1:G:617:GLN:OE1	2.47	0.47
1:H:578:GLN:OE1	1:H:597:ASN:ND2	2.47	0.47
1:I:340:THR:HB	1:I:407:ARG:NH2	2.29	0.47
1:I:623:LYS:HB2	1:I:645:PRO:HG3	1.96	0.47
1:J:312:LYS:O	1:J:418:PHE:N	2.43	0.47
1:M:659:ASP:OD2	1:N:333:LYS:NZ	32.90	0.47
1:N:340:THR:HB	1:N:407:ARG:NH2	2.29	0.47
1:O:531:ASP:OD1	1:O:569:LYS:NZ	2.28	0.47
1:O:617:GLN:OE1	1:O:617:GLN:N	2.47	0.47
1:P:324:LYS:HE3	1:Q:656:VAL:HG11	1.95	0.47
1:P:457:THR:HG23	1:P:458:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:617:GLN:N	1:P:617:GLN:OE1	2.47	0.47
1:Q:617:GLN:N	1:Q:617:GLN:OE1	2.47	0.47
1:Q:623:LYS:HB2	1:Q:645:PRO:HG3	1.96	0.47
1:T:444:TYR:CZ	1:U:360:ALA:HB1	82.49	0.47
1:U:617:GLN:N	1:U:617:GLN:OE1	2.47	0.47
1:V:340:THR:HB	1:V:407:ARG:NH2	2.29	0.47
1:W:610:GLN:HE21	1:Y:627:THR:CG2	2.25	0.47
1:X:254:ASN:ND2	1:X:377:GLN:NE2	2.62	0.47
1:W:532:ASP:OD1	1:X:385:ASN:ND2	68.31	0.47
1:X:406:LEU:N	1:X:406:LEU:CD1	2.76	0.47
1:W:431:GLN:NE2	1:Y:354:PRO:HB3	2.23	0.47
1:Y:623:LYS:HB2	1:Y:645:PRO:HG3	1.97	0.47
1:1:578:GLN:OE1	1:1:597:ASN:ND2	2.47	0.47
1:3:346:PHE:HB3	1:3:403:SER:HA	1.96	0.47
1:5:623:LYS:HB2	1:5:645:PRO:HG3	1.96	0.47
1:6:254:ASN:ND2	1:6:377:GLN:NE2	2.62	0.47
1:7:406:LEU:N	1:7:406:LEU:CD1	2.76	0.47
1:A:224:SER:O	1:E:407:ARG:HD2	2.14	0.47
1:A:464:LEU:HD23	1:G:554:ASN:HB3	1.96	0.47
1:A:532:ASP:OD1	1:8:385:ASN:ND2	169.45	0.47
1:A:610:GLN:HE21	1:8:627:THR:CG2	135.99	0.47
1:A:623:LYS:HB2	1:A:645:PRO:HG3	1.96	0.47
1:B:617:GLN:N	1:B:617:GLN:OE1	2.47	0.47
1:F:360:ALA:HB1	1:Q:444:TYR:CZ	2.48	0.47
1:H:617:GLN:N	1:H:617:GLN:OE1	2.47	0.47
1:K:578:GLN:OE1	1:K:597:ASN:ND2	2.47	0.47
1:M:312:LYS:O	1:M:418:PHE:N	2.44	0.47
1:O:340:THR:HB	1:O:407:ARG:NH2	2.29	0.47
1:P:531:ASP:OD1	1:P:569:LYS:NZ	2.28	0.47
1:Q:360:ALA:HB1	1:S:444:TYR:CZ	89.40	0.47
1:U:340:THR:HB	1:U:407:ARG:NH2	2.29	0.47
1:W:617:GLN:OE1	1:W:617:GLN:N	2.47	0.47
1:G:324:LYS:HE3	1:W:656:VAL:HG11	1.96	0.47
1:X:444:TYR:CZ	1:Y:360:ALA:HB1	82.49	0.47
1:Y:704:THR:OG1	1:Z:702:GLN:N	2.37	0.47
1:1:254:ASN:ND2	1:1:377:GLN:NE2	2.62	0.47
1:2:457:THR:HG23	1:2:458:GLN:HG3	1.96	0.47
1:Z:656:VAL:HG11	1:4:324:LYS:HE3	101.24	0.47
1:7:287:PHE:CE1	1:7:621:TRP:HH2	2.31	0.47
1:C:346:PHE:HB3	1:C:403:SER:HA	1.96	0.47
1:D:532:ASP:OD1	1:L:385:ASN:ND2	142.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:610:GLN:HE21	1:X:627:THR:CG2	142.16	0.47
1:F:444:TYR:CZ	1:H:360:ALA:HB1	129.57	0.47
1:F:656:VAL:HG11	1:R:324:LYS:HE3	1.95	0.47
1:G:623:LYS:HB2	1:G:645:PRO:HG3	1.96	0.47
1:K:457:THR:HG23	1:K:458:GLN:HG3	1.96	0.47
1:O:328:GLN:NE2	1:O:333:LYS:HG3	2.23	0.47
1:P:623:LYS:HB2	1:P:645:PRO:HG3	1.96	0.47
1:S:578:GLN:OE1	1:S:597:ASN:ND2	2.47	0.47
1:E:385:ASN:ND2	1:V:532:ASP:OD1	136.69	0.47
1:W:623:LYS:HB2	1:W:645:PRO:HG3	1.97	0.47
1:V:360:ALA:HB1	1:X:444:TYR:CZ	2.49	0.47
1:6:578:GLN:OE1	1:6:597:ASN:ND2	2.47	0.47
1:7:328:GLN:NE2	1:7:333:LYS:HG3	2.23	0.47
1:8:457:THR:HG23	1:8:458:GLN:HG3	1.96	0.47
1:A:532:ASP:OD1	1:G:385:ASN:ND2	2.48	0.47
1:B:406:LEU:CD1	1:B:406:LEU:N	2.76	0.47
1:E:312:LYS:O	1:E:418:PHE:N	2.44	0.47
1:G:224:SER:O	1:I:407:ARG:HD2	152.40	0.47
1:G:431:GLN:NE2	1:I:354:PRO:HB3	2.23	0.47
1:I:444:TYR:CZ	1:J:360:ALA:HB1	82.49	0.47
1:L:623:LYS:HB2	1:L:645:PRO:HG3	1.97	0.47
1:N:623:LYS:HB2	1:N:645:PRO:HG3	1.97	0.47
1:S:444:TYR:CZ	1:U:360:ALA:HB1	2.49	0.47
1:W:457:THR:HG23	1:W:458:GLN:HG3	1.96	0.47
1:W:610:GLN:HE21	1:X:627:THR:CG2	61.64	0.47
1:Z:439:PRO:HB3	1:4:381:LEU:HD21	1.97	0.47
1:Z:627:THR:CG2	1:2:610:GLN:HE21	71.89	0.47
1:Z:385:ASN:ND2	1:3:532:ASP:OD1	2.47	0.47
1:Y:324:LYS:HE3	1:4:656:VAL:HG11	1.95	0.47
1:7:254:ASN:ND2	1:7:377:GLN:NE2	2.62	0.47
1:8:254:ASN:ND2	1:8:377:GLN:NE2	2.62	0.47
1:8:623:LYS:HB2	1:8:645:PRO:HG3	1.97	0.47
1:B:312:LYS:O	1:B:418:PHE:N	2.44	0.47
1:C:617:GLN:OE1	1:C:617:GLN:N	2.47	0.47
1:D:224:SER:O	1:O:407:ARG:HD2	101.13	0.47
1:D:254:ASN:ND2	1:D:377:GLN:NE2	2.62	0.47
1:F:360:ALA:HB1	1:G:444:TYR:CZ	89.40	0.47
1:I:617:GLN:OE1	1:I:617:GLN:N	2.47	0.47
1:J:532:ASP:OD1	1:K:385:ASN:ND2	68.31	0.47
1:M:385:ASN:ND2	1:O:532:ASP:OD1	111.39	0.47
1:L:656:VAL:HG11	1:N:324:LYS:HE3	128.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:346:PHE:HB3	1:N:403:SER:HA	1.96	0.47
1:S:429:HIS:CG	1:S:738:LEU:HD12	2.50	0.47
1:U:429:HIS:CG	1:U:738:LEU:HD12	2.50	0.47
1:G:224:SER:O	1:W:407:ARG:HD2	2.15	0.47
1:X:623:LYS:HB2	1:X:645:PRO:HG3	1.96	0.47
1:Y:254:ASN:ND2	1:Y:377:GLN:NE2	2.62	0.47
1:Z:457:THR:HG23	1:Z:458:GLN:HG3	1.96	0.47
1:2:254:ASN:ND2	1:2:377:GLN:NE2	2.62	0.47
1:3:623:LYS:HB2	1:3:645:PRO:HG3	1.97	0.47
1:Y:224:SER:O	1:4:407:ARG:HD2	2.15	0.47
1:6:623:LYS:HB2	1:6:645:PRO:HG3	1.96	0.47
1:8:617:GLN:OE1	1:8:617:GLN:N	2.47	0.47
1:A:340:THR:HB	1:A:407:ARG:NH2	2.29	0.47
1:B:354:PRO:HB3	1:C:431:GLN:NE2	47.77	0.47
1:B:354:PRO:HB3	1:L:431:GLN:NE2	2.23	0.47
1:B:382:THR:HG22	1:B:383:LEU:N	2.28	0.47
1:C:457:THR:HG23	1:C:458:GLN:HG3	1.96	0.47
1:C:532:ASP:OD1	1:O:385:ASN:ND2	181.58	0.47
1:D:407:ARG:HD2	1:S:224:SER:O	93.94	0.47
1:F:346:PHE:HB3	1:F:403:SER:HA	1.96	0.47
1:F:528:THR:H	1:F:565:GLU:HB2	1.80	0.47
1:F:623:LYS:HB2	1:F:645:PRO:HG3	1.96	0.47
1:F:429:HIS:CG	1:F:738:LEU:HD12	2.50	0.47
1:H:429:HIS:CG	1:H:738:LEU:HD12	2.50	0.47
1:H:623:LYS:HB2	1:H:645:PRO:HG3	1.97	0.47
1:L:457:THR:HG23	1:L:458:GLN:HG3	1.96	0.47
1:P:429:HIS:CG	1:P:738:LEU:HD12	2.50	0.47
1:N:656:VAL:HG11	1:R:324:LYS:HE3	168.05	0.47
1:R:656:VAL:HG11	1:X:324:LYS:HE3	93.73	0.47
1:Q:627:THR:CG2	1:S:610:GLN:HE21	86.13	0.47
1:T:429:HIS:CG	1:T:738:LEU:HD12	2.50	0.47
1:E:407:ARG:HD2	1:U:224:SER:O	145.37	0.47
1:U:528:THR:H	1:U:565:GLU:HB2	1.80	0.47
1:V:528:THR:H	1:V:565:GLU:HB2	1.80	0.47
1:W:312:LYS:O	1:W:418:PHE:N	2.44	0.47
1:X:457:THR:HG23	1:X:458:GLN:HG3	1.96	0.47
1:Y:346:PHE:HB3	1:Y:403:SER:HA	1.96	0.47
1:Y:528:THR:H	1:Y:565:GLU:HB2	1.80	0.47
1:1:623:LYS:HB2	1:1:645:PRO:HG3	1.96	0.47
1:2:406:LEU:CD1	1:2:406:LEU:N	2.76	0.47
1:4:312:LYS:O	1:4:418:PHE:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:346:PHE:HB3	1:4:403:SER:HA	1.96	0.47
1:5:429:HIS:CG	1:5:738:LEU:HD12	2.50	0.47
1:6:346:PHE:HB3	1:6:403:SER:HA	1.96	0.47
1:6:528:THR:H	1:6:565:GLU:HB2	1.80	0.47
1:8:429:HIS:CG	1:8:738:LEU:HD12	2.50	0.47
1:8:531:ASP:OD1	1:8:569:LYS:NZ	2.28	0.47
1:A:457:THR:HG23	1:A:458:GLN:HG3	1.96	0.47
1:H:381:LEU:HD21	1:Y:439:PRO:HB3	1.97	0.47
1:J:429:HIS:CG	1:J:738:LEU:HD12	2.50	0.47
1:K:385:ASN:ND2	1:8:532:ASP:OD1	2.48	0.47
1:M:224:SER:O	1:N:407:ARG:HD2	2.15	0.47
1:B:532:ASP:OD1	1:M:385:ASN:ND2	132.25	0.47
1:M:439:PRO:HB3	1:N:381:LEU:HD21	57.41	0.47
1:O:457:THR:HG23	1:O:458:GLN:HG3	1.96	0.47
1:O:623:LYS:HB2	1:O:645:PRO:HG3	1.97	0.47
1:D:385:ASN:ND2	1:P:532:ASP:OD1	2.48	0.47
1:R:429:HIS:CG	1:R:738:LEU:HD12	2.50	0.47
1:S:532:ASP:OD1	1:U:385:ASN:ND2	2.47	0.47
1:D:385:ASN:ND2	1:T:532:ASP:OD1	131.33	0.47
1:U:532:ASP:OD1	1:V:385:ASN:ND2	68.32	0.47
1:V:312:LYS:O	1:V:418:PHE:N	2.44	0.47
1:1:429:HIS:CG	1:1:738:LEU:HD12	2.50	0.47
1:B:532:ASP:OD1	1:J:385:ASN:ND2	2.47	0.47
1:C:429:HIS:CG	1:C:738:LEU:HD12	2.50	0.47
1:B:385:ASN:ND2	1:C:532:ASP:OD1	33.32	0.47
1:E:429:HIS:CG	1:E:738:LEU:HD12	2.50	0.47
1:G:464:LEU:HD23	1:I:554:ASN:HB3	1.97	0.47
1:G:416:TYR:OH	1:G:644:HIS:O	2.33	0.47
1:G:659:ASP:OD2	1:K:333:LYS:NZ	189.63	0.47
1:I:429:HIS:CG	1:I:738:LEU:HD12	2.50	0.47
1:J:224:SER:O	1:X:407:ARG:HD2	112.02	0.47
1:J:407:ARG:HD2	1:L:224:SER:O	89.56	0.47
1:J:444:TYR:CZ	1:K:360:ALA:HB1	52.80	0.47
1:L:532:ASP:OD1	1:T:385:ASN:ND2	230.83	0.47
1:B:627:THR:CG2	1:L:610:GLN:HE21	2.25	0.47
1:L:617:GLN:N	1:L:617:GLN:OE1	2.47	0.47
1:L:429:HIS:CG	1:L:738:LEU:HD12	2.50	0.47
1:M:429:HIS:CG	1:M:738:LEU:HD12	2.50	0.47
1:N:407:ARG:HD2	1:R:224:SER:O	146.05	0.47
1:P:328:GLN:NE2	1:P:333:LYS:HG3	2.23	0.47
1:Q:528:THR:H	1:Q:565:GLU:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:429:HIS:CG	1:Q:738:LEU:HD12	2.50	0.47
1:T:439:PRO:HB3	1:U:381:LEU:HD21	57.41	0.47
1:V:329:ASN:O	1:V:332:THR:OG1	2.21	0.47
1:W:429:HIS:CG	1:W:738:LEU:HD12	2.50	0.47
1:Z:429:HIS:CG	1:Z:738:LEU:HD12	2.50	0.47
1:A:407:ARG:HD2	1:B:224:SER:O	2.15	0.47
1:C:328:GLN:NE2	1:C:333:LYS:HG3	2.23	0.47
1:C:354:PRO:HB3	1:P:431:GLN:NE2	50.94	0.47
1:B:627:THR:CG2	1:C:610:GLN:HE21	45.57	0.47
1:C:623:LYS:HB2	1:C:645:PRO:HG3	1.97	0.47
1:D:384:ASN:ND2	1:D:386:GLY:O	2.49	0.47
1:F:457:THR:HG23	1:F:458:GLN:HG3	1.96	0.47
1:F:532:ASP:OD1	1:H:385:ASN:ND2	142.72	0.47
1:F:617:GLN:N	1:F:617:GLN:OE1	2.47	0.47
1:G:312:LYS:O	1:G:418:PHE:N	2.44	0.47
1:H:528:THR:H	1:H:565:GLU:HB2	1.80	0.47
1:I:333:LYS:NZ	1:J:659:ASP:OD2	2.32	0.47
1:K:617:GLN:N	1:K:617:GLN:OE1	2.47	0.47
1:B:385:ASN:ND2	1:L:532:ASP:OD1	2.47	0.47
1:N:328:GLN:NE2	1:N:333:LYS:HG3	2.23	0.47
1:Q:224:SER:O	1:S:407:ARG:HD2	2.15	0.47
1:R:623:LYS:HB2	1:R:645:PRO:HG3	1.97	0.47
1:R:439:PRO:HB3	1:S:381:LEU:HD21	1.97	0.47
1:S:528:THR:H	1:S:565:GLU:HB2	1.80	0.47
1:L:439:PRO:HB3	1:T:381:LEU:HD21	209.70	0.47
1:T:528:THR:H	1:T:565:GLU:HB2	1.80	0.47
1:U:329:ASN:O	1:U:332:THR:OG1	2.21	0.47
1:V:254:ASN:ND2	1:V:377:GLN:NE2	2.62	0.47
1:W:384:ASN:ND2	1:W:386:GLY:O	2.49	0.47
1:W:528:THR:H	1:W:565:GLU:HB2	1.80	0.47
1:Y:508:ALA:HB1	1:Y:519:LEU:HD13	1.97	0.47
1:Z:384:ASN:ND2	1:Z:386:GLY:O	2.49	0.47
1:Z:617:GLN:OE1	1:Z:617:GLN:N	2.47	0.47
1:1:528:THR:H	1:1:565:GLU:HB2	1.80	0.46
1:4:528:THR:H	1:4:565:GLU:HB2	1.80	0.46
1:6:617:GLN:N	1:6:617:GLN:OE1	2.47	0.46
1:8:328:GLN:NE2	1:8:333:LYS:HG3	2.23	0.46
1:C:406:LEU:CD1	1:C:406:LEU:N	2.76	0.46
1:D:617:GLN:N	1:D:617:GLN:OE1	2.47	0.46
1:F:384:ASN:ND2	1:F:386:GLY:O	2.49	0.46
1:G:528:THR:H	1:G:565:GLU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:532:ASP:OD1	1:I:385:ASN:ND2	2.47	0.46
1:I:224:SER:O	1:J:407:ARG:HD2	2.15	0.46
1:I:224:SER:O	1:T:407:ARG:HD2	163.39	0.46
1:I:312:LYS:O	1:I:418:PHE:N	2.44	0.46
1:I:528:THR:H	1:I:565:GLU:HB2	1.80	0.46
1:J:384:ASN:ND2	1:J:386:GLY:O	2.49	0.46
1:J:617:GLN:OE1	1:J:617:GLN:N	2.47	0.46
1:K:381:LEU:HD21	1:8:439:PRO:HB3	1.97	0.46
1:K:384:ASN:ND2	1:K:386:GLY:O	2.49	0.46
1:I:381:LEU:HD21	1:K:439:PRO:HB3	81.22	0.46
1:K:528:THR:H	1:K:565:GLU:HB2	1.80	0.46
1:L:384:ASN:ND2	1:L:386:GLY:O	2.49	0.46
1:M:384:ASN:ND2	1:M:386:GLY:O	2.49	0.46
1:N:312:LYS:O	1:N:418:PHE:N	2.44	0.46
1:N:429:HIS:CG	1:N:738:LEU:HD12	2.50	0.46
1:Q:384:ASN:ND2	1:Q:386:GLY:O	2.49	0.46
1:R:384:ASN:ND2	1:R:386:GLY:O	2.49	0.46
1:T:384:ASN:ND2	1:T:386:GLY:O	2.49	0.46
1:T:340:THR:HB	1:T:407:ARG:NH2	2.29	0.46
1:T:623:LYS:HB2	1:T:645:PRO:HG3	1.97	0.46
1:U:457:THR:HG23	1:U:458:GLN:HG3	1.96	0.46
1:V:429:HIS:CG	1:V:738:LEU:HD12	2.50	0.46
1:V:508:ALA:HB1	1:V:519:LEU:HD13	1.98	0.46
1:Y:312:LYS:O	1:Y:418:PHE:N	2.44	0.46
1:Y:617:GLN:OE1	1:Y:617:GLN:N	2.47	0.46
1:2:384:ASN:ND2	1:2:386:GLY:O	2.49	0.46
1:2:623:LYS:HB2	1:2:645:PRO:HG3	1.97	0.46
1:3:528:THR:H	1:3:565:GLU:HB2	1.80	0.46
1:4:429:HIS:CG	1:4:738:LEU:HD12	2.50	0.46
1:5:508:ALA:HB1	1:5:519:LEU:HD13	1.97	0.46
1:8:384:ASN:ND2	1:8:386:GLY:O	2.49	0.46
1:A:407:ARG:HD2	1:J:224:SER:O	83.66	0.46
1:A:429:HIS:CG	1:A:738:LEU:HD12	2.50	0.46
1:B:381:LEU:HD21	1:C:439:PRO:HB3	57.42	0.46
1:B:429:HIS:CG	1:B:738:LEU:HD12	2.50	0.46
1:C:224:SER:O	1:M:407:ARG:HD2	89.56	0.46
1:D:623:LYS:HB2	1:D:645:PRO:HG3	1.96	0.46
1:J:623:LYS:HB2	1:J:645:PRO:HG3	1.96	0.46
1:K:429:HIS:CG	1:K:738:LEU:HD12	2.50	0.46
1:B:381:LEU:HD21	1:L:439:PRO:HB3	1.97	0.46
1:L:508:ALA:HB1	1:L:519:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:528:THR:H	1:N:565:GLU:HB2	1.80	0.46
1:O:429:HIS:CG	1:O:738:LEU:HD12	2.50	0.46
1:P:224:SER:O	1:Q:407:ARG:HD2	2.15	0.46
1:P:384:ASN:ND2	1:P:386:GLY:O	2.49	0.46
1:P:528:THR:H	1:P:565:GLU:HB2	1.80	0.46
1:Q:439:PRO:HB3	1:R:381:LEU:HD21	50.84	0.46
1:R:508:ALA:HB1	1:R:519:LEU:HD13	1.97	0.46
1:U:508:ALA:HB1	1:U:519:LEU:HD13	1.97	0.46
1:R:627:THR:CG2	1:U:610:GLN:HE21	2.25	0.46
1:V:384:ASN:ND2	1:V:386:GLY:O	2.49	0.46
1:V:617:GLN:N	1:V:617:GLN:OE1	2.47	0.46
1:W:381:LEU:HD21	1:Y:439:PRO:HB3	55.02	0.46
1:X:224:SER:O	1:Y:407:ARG:HD2	2.15	0.46
1:X:324:LYS:HE3	1:Y:656:VAL:HG11	1.95	0.46
1:F:224:SER:O	1:X:407:ARG:HD2	101.61	0.46
1:1:340:THR:HB	1:1:407:ARG:NH2	2.29	0.46
1:3:429:HIS:CG	1:3:738:LEU:HD12	2.50	0.46
1:3:457:THR:HG23	1:3:458:GLN:HG3	1.96	0.46
1:4:384:ASN:ND2	1:4:386:GLY:O	2.49	0.46
1:5:384:ASN:ND2	1:5:386:GLY:O	2.49	0.46
1:6:457:THR:HG23	1:6:458:GLN:HG3	1.96	0.46
1:7:429:HIS:CG	1:7:738:LEU:HD12	2.50	0.46
1:B:508:ALA:HB1	1:B:519:LEU:HD13	1.98	0.46
1:D:407:ARG:HD2	1:E:224:SER:O	2.15	0.46
1:G:429:HIS:CG	1:G:738:LEU:HD12	2.50	0.46
1:H:384:ASN:ND2	1:H:386:GLY:O	2.49	0.46
1:H:610:GLN:HE21	1:W:627:THR:CG2	2.25	0.46
1:J:508:ALA:HB1	1:J:519:LEU:HD13	1.97	0.46
1:O:528:THR:H	1:O:565:GLU:HB2	1.80	0.46
1:R:340:THR:HB	1:R:407:ARG:NH2	2.29	0.46
1:R:528:THR:H	1:R:565:GLU:HB2	1.80	0.46
1:S:384:ASN:ND2	1:S:386:GLY:O	2.49	0.46
1:U:384:ASN:ND2	1:U:386:GLY:O	2.49	0.46
1:X:416:TYR:OH	1:X:644:HIS:O	2.33	0.46
1:Y:384:ASN:ND2	1:Y:386:GLY:O	2.49	0.46
1:Y:340:THR:HB	1:Y:407:ARG:NH2	2.29	0.46
1:Z:381:LEU:HD21	1:3:439:PRO:HB3	1.97	0.46
1:Z:439:PRO:HB3	1:1:381:LEU:HD21	101.42	0.46
1:Z:508:ALA:HB1	1:Z:519:LEU:HD13	1.98	0.46
1:Z:532:ASP:OD1	1:1:385:ASN:ND2	113.41	0.46
1:5:617:GLN:N	1:5:617:GLN:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:627:THR:CG2	1:7:610:GLN:HE21	2.25	0.46
1:8:416:TYR:OH	1:8:644:HIS:O	2.33	0.46
1:A:439:PRO:HB3	1:G:381:LEU:HD21	1.98	0.46
1:D:381:LEU:HD21	1:P:439:PRO:HB3	1.98	0.46
1:D:340:THR:HB	1:D:407:ARG:NH2	2.29	0.46
1:E:508:ALA:HB1	1:E:519:LEU:HD13	1.97	0.46
1:F:508:ALA:HB1	1:F:519:LEU:HD13	1.98	0.46
1:A:583:ALA:O	1:G:487:ARG:HD2	2.16	0.46
1:G:508:ALA:HB1	1:G:519:LEU:HD13	1.98	0.46
1:I:385:ASN:ND2	1:K:532:ASP:OD1	111.39	0.46
1:K:623:LYS:HB2	1:K:645:PRO:HG3	1.97	0.46
1:J:439:PRO:HB3	1:L:381:LEU:HD21	1.98	0.46
1:M:328:GLN:NE2	1:M:333:LYS:HG3	2.23	0.46
1:M:508:ALA:HB1	1:M:519:LEU:HD13	1.97	0.46
1:N:384:ASN:ND2	1:N:386:GLY:O	2.49	0.46
1:C:439:PRO:HB3	1:O:381:LEU:HD21	167.12	0.46
1:P:416:TYR:OH	1:P:644:HIS:O	2.33	0.46
1:Q:508:ALA:HB1	1:Q:519:LEU:HD13	1.98	0.46
1:Q:532:ASP:OD1	1:R:385:ASN:ND2	68.32	0.46
1:R:416:TYR:OH	1:R:644:HIS:O	2.33	0.46
1:S:508:ALA:HB1	1:S:519:LEU:HD13	1.97	0.46
1:S:610:GLN:HE21	1:U:627:THR:CG2	2.25	0.46
1:V:224:SER:O	1:W:407:ARG:HD2	21.30	0.46
1:W:508:ALA:HB1	1:W:519:LEU:HD13	1.97	0.46
1:W:532:ASP:OD1	1:Y:385:ASN:ND2	2.48	0.46
1:X:297:ARG:O	1:X:300:GLN:N	2.48	0.46
1:W:439:PRO:HB3	1:Y:381:LEU:HD21	1.98	0.46
1:Y:429:HIS:CG	1:Y:738:LEU:HD12	2.50	0.46
1:2:224:SER:O	1:3:407:ARG:HD2	2.15	0.46
1:2:340:THR:HB	1:2:407:ARG:NH2	2.29	0.46
1:2:528:THR:H	1:2:565:GLU:HB2	1.80	0.46
1:Z:532:ASP:OD1	1:4:385:ASN:ND2	2.47	0.46
1:8:312:LYS:O	1:8:418:PHE:N	2.44	0.46
1:B:224:SER:O	1:O:407:ARG:HD2	112.02	0.46
1:B:528:THR:H	1:B:565:GLU:HB2	1.80	0.46
1:C:384:ASN:ND2	1:C:386:GLY:O	2.49	0.46
1:C:416:TYR:OH	1:C:644:HIS:O	2.33	0.46
1:D:381:LEU:HD21	1:T:439:PRO:HB3	122.63	0.46
1:D:528:THR:H	1:D:565:GLU:HB2	1.80	0.46
1:E:457:THR:HG23	1:E:458:GLN:HG3	1.96	0.46
1:F:354:PRO:HB3	1:Q:431:GLN:NE2	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:PRO:HB3	1:H:381:LEU:HD21	134.51	0.46
1:G:384:ASN:ND2	1:G:386:GLY:O	2.48	0.46
1:H:354:PRO:HB3	1:Y:431:GLN:NE2	2.24	0.46
1:G:385:ASN:ND2	1:H:532:ASP:OD1	68.31	0.46
1:H:416:TYR:OH	1:H:644:HIS:O	2.33	0.46
1:I:384:ASN:ND2	1:I:386:GLY:O	2.49	0.46
1:A:381:LEU:HD21	1:I:439:PRO:HB3	1.98	0.46
1:I:508:ALA:HB1	1:I:519:LEU:HD13	1.98	0.46
1:K:224:SER:O	1:L:407:ARG:HD2	2.15	0.46
1:M:407:ARG:HD2	1:N:224:SER:O	21.30	0.46
1:C:381:LEU:HD21	1:M:439:PRO:HB3	1.98	0.46
1:M:532:ASP:OD1	1:N:385:ASN:ND2	33.31	0.46
1:M:617:GLN:N	1:M:617:GLN:OE1	2.47	0.46
1:C:333:LYS:NZ	1:M:659:ASP:OD2	113.13	0.46
1:O:224:SER:O	1:7:407:ARG:HD2	153.10	0.46
1:S:416:TYR:OH	1:S:644:HIS:O	2.33	0.46
1:T:532:ASP:OD1	1:U:385:ASN:ND2	33.32	0.46
1:T:416:TYR:OH	1:T:644:HIS:O	2.33	0.46
1:U:312:LYS:O	1:U:418:PHE:N	2.44	0.46
1:S:431:GLN:NE2	1:U:354:PRO:HB3	2.23	0.46
1:R:385:ASN:ND2	1:U:532:ASP:OD1	2.48	0.46
1:E:381:LEU:HD21	1:V:439:PRO:HB3	150.75	0.46
1:T:385:ASN:ND2	1:V:532:ASP:OD1	111.39	0.46
1:T:627:THR:CG2	1:V:610:GLN:HE21	101.45	0.46
1:R:407:ARG:HD2	1:X:224:SER:O	84.76	0.46
1:Y:416:TYR:OH	1:Y:644:HIS:O	2.33	0.46
1:U:407:ARG:HD2	1:5:224:SER:O	163.57	0.46
1:5:407:ARG:HD2	1:8:224:SER:O	2.16	0.46
1:K:407:ARG:HD2	1:7:224:SER:O	2.15	0.46
1:5:381:LEU:HD21	1:7:439:PRO:HB3	1.97	0.46
1:C:381:LEU:HD21	1:P:439:PRO:HB3	49.21	0.46
1:E:384:ASN:ND2	1:E:386:GLY:O	2.49	0.46
1:E:439:PRO:HB3	1:X:381:LEU:HD21	165.97	0.46
1:E:617:GLN:OE1	1:E:617:GLN:N	2.47	0.46
1:F:307:TRP:NE1	1:F:692:GLU:HG2	2.31	0.46
1:G:381:LEU:HD21	1:H:439:PRO:HB3	50.84	0.46
1:J:439:PRO:HB3	1:K:381:LEU:HD21	50.83	0.46
1:L:528:THR:H	1:L:565:GLU:HB2	1.80	0.46
1:M:381:LEU:HD21	1:O:439:PRO:HB3	81.22	0.46
1:C:385:ASN:ND2	1:P:532:ASP:OD1	69.76	0.46
1:S:312:LYS:O	1:S:418:PHE:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:381:LEU:HD21	1:S:439:PRO:HB3	104.45	0.46
1:U:610:GLN:HE21	1:V:627:THR:CG2	61.63	0.46
1:W:297:ARG:O	1:W:300:GLN:N	2.48	0.46
1:H:439:PRO:HB3	1:W:381:LEU:HD21	1.98	0.46
1:X:307:TRP:NE1	1:X:692:GLU:HG2	2.31	0.46
1:6:329:ASN:O	1:6:332:THR:OG1	2.21	0.46
1:5:431:GLN:NE2	1:6:354:PRO:HB3	2.24	0.46
1:T:224:SER:O	1:6:407:ARG:HD2	160.23	0.46
1:7:307:TRP:NE1	1:7:692:GLU:HG2	2.31	0.46
1:A:508:ALA:HB1	1:A:519:LEU:HD13	1.97	0.46
1:C:407:ARG:HD2	1:D:224:SER:O	2.15	0.46
1:D:610:GLN:HE21	1:N:627:THR:CG2	2.25	0.46
1:D:429:HIS:CG	1:D:738:LEU:HD12	2.50	0.46
1:E:307:TRP:NE1	1:E:692:GLU:HG2	2.31	0.46
1:G:328:GLN:NE2	1:G:333:LYS:HG3	2.23	0.46
1:G:407:ARG:HD2	1:K:224:SER:O	146.06	0.46
1:F:385:ASN:ND2	1:G:532:ASP:OD1	111.52	0.46
1:I:416:TYR:OH	1:I:644:HIS:O	2.33	0.46
1:J:307:TRP:NE1	1:J:692:GLU:HG2	2.31	0.46
1:J:702:GLN:H	1:W:704:THR:HG1	156.58	0.46
1:M:224:SER:O	1:S:407:ARG:HD2	101.74	0.46
1:P:312:LYS:O	1:P:418:PHE:N	2.44	0.46
1:P:508:ALA:HB1	1:P:519:LEU:HD13	1.97	0.46
1:R:532:ASP:OD1	1:S:385:ASN:ND2	2.48	0.46
1:T:610:GLN:HE21	1:U:627:THR:CG2	45.57	0.46
1:V:407:ARG:HD2	1:1:224:SER:O	152.04	0.46
1:W:439:PRO:HB3	1:X:381:LEU:HD21	50.83	0.46
1:F:407:ARG:HD2	1:Z:224:SER:O	102.82	0.46
1:Z:528:THR:H	1:Z:565:GLU:HB2	1.80	0.46
1:2:429:HIS:CG	1:2:738:LEU:HD12	2.50	0.46
1:3:617:GLN:N	1:3:617:GLN:OE1	2.47	0.46
1:4:508:ALA:HB1	1:4:519:LEU:HD13	1.97	0.46
1:8:508:ALA:HB1	1:8:519:LEU:HD13	1.98	0.46
1:8:528:THR:H	1:8:565:GLU:HB2	1.80	0.46
1:A:312:LYS:O	1:A:418:PHE:N	2.44	0.46
1:A:384:ASN:ND2	1:A:386:GLY:O	2.49	0.46
1:A:528:THR:H	1:A:565:GLU:HB2	1.80	0.46
1:B:384:ASN:ND2	1:B:386:GLY:O	2.49	0.46
1:B:531:ASP:OD1	1:B:569:LYS:NZ	2.28	0.46
1:C:528:THR:H	1:C:565:GLU:HB2	1.80	0.46
1:D:416:TYR:OH	1:D:644:HIS:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:ARG:O	1:G:300:GLN:N	2.48	0.46
1:G:307:TRP:NE1	1:G:692:GLU:HG2	2.31	0.46
1:H:297:ARG:O	1:H:300:GLN:N	2.48	0.46
1:H:307:TRP:NE1	1:H:692:GLU:HG2	2.31	0.46
1:I:307:TRP:NE1	1:I:692:GLU:HG2	2.31	0.46
1:K:297:ARG:O	1:K:300:GLN:N	2.48	0.46
1:K:307:TRP:NE1	1:K:692:GLU:HG2	2.31	0.46
1:O:384:ASN:ND2	1:O:386:GLY:O	2.48	0.46
1:O:439:PRO:HB3	1:P:381:LEU:HD21	57.41	0.46
1:O:508:ALA:HB1	1:O:519:LEU:HD13	1.98	0.46
1:O:416:TYR:OH	1:O:644:HIS:O	2.33	0.46
1:P:307:TRP:NE1	1:P:692:GLU:HG2	2.31	0.46
1:Q:297:ARG:O	1:Q:300:GLN:N	2.48	0.46
1:R:610:GLN:HE21	1:S:627:THR:CG2	2.25	0.46
1:T:224:SER:O	1:U:407:ARG:HD2	2.16	0.46
1:V:307:TRP:NE1	1:V:692:GLU:HG2	2.31	0.46
1:2:617:GLN:N	1:2:617:GLN:OE1	2.47	0.46
1:3:312:LYS:O	1:3:418:PHE:N	2.44	0.46
1:6:384:ASN:ND2	1:6:386:GLY:O	2.49	0.46
1:7:457:THR:HG23	1:7:458:GLN:HG3	1.96	0.46
1:7:528:THR:H	1:7:565:GLU:HB2	1.80	0.46
1:C:407:ARG:HD2	1:S:224:SER:O	102.03	0.46
1:C:554:ASN:HB3	1:P:464:LEU:HD23	58.21	0.46
1:E:224:SER:O	1:H:407:ARG:HD2	111.07	0.46
1:E:528:THR:H	1:E:565:GLU:HB2	1.80	0.46
1:G:583:ALA:O	1:I:487:ARG:HD2	2.16	0.46
1:H:328:GLN:NE2	1:H:333:LYS:HG3	2.23	0.46
1:H:407:ARG:HD2	1:Z:224:SER:O	2.15	0.46
1:J:328:GLN:NE2	1:J:333:LYS:HG3	2.23	0.46
1:L:307:TRP:NE1	1:L:692:GLU:HG2	2.31	0.46
1:N:508:ALA:HB1	1:N:519:LEU:HD13	1.98	0.46
1:O:610:GLN:HE21	1:P:627:THR:CG2	45.56	0.46
1:P:297:ARG:O	1:P:300:GLN:N	2.48	0.46
1:R:238:ASP:OD1	1:R:239:ARG:N	2.49	0.46
1:R:328:GLN:NE2	1:R:333:LYS:HG3	2.23	0.46
1:R:307:TRP:NE1	1:R:692:GLU:HG2	2.31	0.46
1:S:307:TRP:NE1	1:S:692:GLU:HG2	2.31	0.46
1:T:238:ASP:OD1	1:T:239:ARG:N	2.49	0.46
1:U:238:ASP:OD1	1:U:239:ARG:N	2.49	0.46
1:U:307:TRP:NE1	1:U:692:GLU:HG2	2.31	0.46
1:U:431:GLN:NE2	1:V:354:PRO:HB3	49.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:508:ALA:HB1	1:X:519:LEU:HD13	1.97	0.46
1:X:532:ASP:OD1	1:Y:385:ASN:ND2	33.31	0.46
1:Y:307:TRP:NE1	1:Y:692:GLU:HG2	2.31	0.46
1:Y:328:GLN:NE2	1:Y:333:LYS:HG3	2.23	0.46
1:2:416:TYR:OH	1:2:644:HIS:O	2.33	0.46
1:4:328:GLN:NE2	1:4:333:LYS:HG3	2.23	0.46
1:6:429:HIS:CG	1:6:738:LEU:HD12	2.50	0.46
1:7:238:ASP:OD1	1:7:239:ARG:N	2.49	0.46
1:C:299:TRP:CG	1:C:616:LEU:HD13	2.51	0.46
1:D:307:TRP:NE1	1:D:692:GLU:HG2	2.31	0.46
1:E:238:ASP:OD1	1:E:239:ARG:N	2.49	0.46
1:H:224:SER:O	1:I:407:ARG:HD2	2.16	0.46
1:H:508:ALA:HB1	1:H:519:LEU:HD13	1.98	0.46
1:I:299:TRP:CG	1:I:616:LEU:HD13	2.52	0.46
1:I:532:ASP:OD1	1:J:385:ASN:ND2	33.31	0.46
1:J:583:ALA:O	1:K:487:ARG:HD2	80.79	0.46
1:K:354:PRO:HB3	1:8:431:GLN:NE2	2.23	0.46
1:K:407:ARG:HD2	1:W:224:SER:O	158.48	0.46
1:A:381:LEU:HD21	1:K:439:PRO:HB3	103.52	0.46
1:A:627:THR:CG2	1:K:610:GLN:HE21	99.57	0.46
1:M:238:ASP:OD1	1:M:239:ARG:N	2.49	0.46
1:Q:307:TRP:NE1	1:Q:692:GLU:HG2	2.31	0.46
1:E:439:PRO:HB3	1:Q:381:LEU:HD21	1.98	0.46
1:V:238:ASP:OD1	1:V:239:ARG:N	2.49	0.46
1:X:528:THR:H	1:X:565:GLU:HB2	1.80	0.46
1:X:583:ALA:O	1:Y:487:ARG:HD2	94.92	0.46
1:Z:238:ASP:OD1	1:Z:239:ARG:N	2.49	0.46
1:A:224:SER:O	1:Z:407:ARG:HD2	102.82	0.46
1:Z:307:TRP:NE1	1:Z:692:GLU:HG2	2.31	0.46
1:1:439:PRO:HB3	1:2:381:LEU:HD21	1.98	0.45
1:3:508:ALA:HB1	1:3:519:LEU:HD13	1.98	0.45
1:4:307:TRP:NE1	1:4:692:GLU:HG2	2.31	0.45
1:3:381:LEU:HD21	1:4:439:PRO:HB3	1.98	0.45
1:5:385:ASN:ND2	1:7:532:ASP:OD1	2.48	0.45
1:7:384:ASN:ND2	1:7:386:GLY:O	2.49	0.45
1:A:299:TRP:CG	1:A:616:LEU:HD13	2.52	0.45
1:B:238:ASP:OD1	1:B:239:ARG:N	2.49	0.45
1:C:307:TRP:NE1	1:C:692:GLU:HG2	2.31	0.45
1:C:508:ALA:HB1	1:C:519:LEU:HD13	1.97	0.45
1:E:532:ASP:OD1	1:Q:385:ASN:ND2	2.48	0.45
1:F:407:ARG:HD2	1:R:224:SER:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238:ASP:OD1	1:G:239:ARG:N	2.49	0.45
1:G:439:PRO:HB3	1:I:381:LEU:HD21	1.98	0.45
1:L:238:ASP:OD1	1:L:239:ARG:N	2.49	0.45
1:L:312:LYS:O	1:L:418:PHE:N	2.44	0.45
1:L:407:ARG:HD2	1:N:224:SER:O	111.07	0.45
1:M:307:TRP:NE1	1:M:692:GLU:HG2	2.31	0.45
1:N:299:TRP:CG	1:N:616:LEU:HD13	2.52	0.45
1:N:439:PRO:HB3	1:O:381:LEU:HD21	50.83	0.45
1:N:610:GLN:HE21	1:O:627:THR:CG2	61.63	0.45
1:P:238:ASP:OD1	1:P:239:ARG:N	2.49	0.45
1:T:407:ARG:HD2	1:Y:224:SER:O	112.16	0.45
1:R:381:LEU:HD21	1:U:439:PRO:HB3	1.98	0.45
1:U:416:TYR:OH	1:U:644:HIS:O	2.33	0.45
1:T:381:LEU:HD21	1:V:439:PRO:HB3	81.22	0.45
1:W:307:TRP:NE1	1:W:692:GLU:HG2	2.31	0.45
1:X:329:ASN:O	1:X:332:THR:OG1	2.21	0.45
1:1:299:TRP:CG	1:1:616:LEU:HD13	2.52	0.45
1:1:508:ALA:HB1	1:1:519:LEU:HD13	1.98	0.45
1:Z:554:ASN:HB3	1:2:464:LEU:HD23	117.88	0.45
1:2:508:ALA:HB1	1:2:519:LEU:HD13	1.98	0.45
1:3:328:GLN:NE2	1:3:333:LYS:HG3	2.23	0.45
1:3:384:ASN:ND2	1:3:386:GLY:O	2.49	0.45
1:6:299:TRP:CG	1:6:616:LEU:HD13	2.52	0.45
1:A:439:PRO:HB3	1:8:381:LEU:HD21	166.37	0.45
1:B:425:SER:HB2	1:B:427:TYR:CE2	2.52	0.45
1:B:299:TRP:CG	1:B:616:LEU:HD13	2.51	0.45
1:C:238:ASP:OD1	1:C:239:ARG:N	2.49	0.45
1:D:425:SER:HB2	1:D:427:TYR:CE2	2.52	0.45
1:D:508:ALA:HB1	1:D:519:LEU:HD13	1.97	0.45
1:F:238:ASP:OD1	1:F:239:ARG:N	2.49	0.45
1:F:299:TRP:CG	1:F:616:LEU:HD13	2.51	0.45
1:I:328:GLN:NE2	1:I:333:LYS:HG3	2.23	0.45
1:J:238:ASP:OD1	1:J:239:ARG:N	2.49	0.45
1:J:299:TRP:CG	1:J:616:LEU:HD13	2.52	0.45
1:K:328:GLN:NE2	1:K:333:LYS:HG3	2.23	0.45
1:K:425:SER:HB2	1:K:427:TYR:CE2	2.52	0.45
1:M:299:TRP:CG	1:M:616:LEU:HD13	2.52	0.45
1:M:583:ALA:O	1:N:487:ARG:HD2	94.92	0.45
1:N:439:PRO:HB3	1:P:381:LEU:HD21	1.98	0.45
1:O:307:TRP:NE1	1:O:692:GLU:HG2	2.31	0.45
1:Q:425:SER:HB2	1:Q:427:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:407:ARG:HD2	1:V:224:SER:O	2.15	0.45
1:S:297:ARG:O	1:S:300:GLN:N	2.48	0.45
1:T:425:SER:HB2	1:T:427:TYR:CE2	2.52	0.45
1:T:508:ALA:HB1	1:T:519:LEU:HD13	1.97	0.45
1:L:464:LEU:HD23	1:T:554:ASN:HB3	229.34	0.45
1:U:297:ARG:O	1:U:300:GLN:N	2.48	0.45
1:V:487:ARG:HD2	1:X:583:ALA:O	2.17	0.45
1:V:385:ASN:ND2	1:X:532:ASP:OD1	2.48	0.45
1:X:429:HIS:CG	1:X:738:LEU:HD12	2.50	0.45
1:Y:238:ASP:OD1	1:Y:239:ARG:N	2.49	0.45
1:2:297:ARG:O	1:2:300:GLN:N	2.48	0.45
1:3:224:SER:O	1:8:407:ARG:HD2	2.15	0.45
1:3:307:TRP:NE1	1:3:692:GLU:HG2	2.31	0.45
1:Z:407:ARG:HD2	1:4:224:SER:O	89.56	0.45
1:4:297:ARG:O	1:4:300:GLN:N	2.48	0.45
1:4:623:LYS:HB2	1:4:645:PRO:HG3	1.96	0.45
1:5:425:SER:HB2	1:5:427:TYR:CE2	2.52	0.45
1:5:528:THR:H	1:5:565:GLU:HB2	1.80	0.45
1:8:251:PRO:HG3	1:8:374:MET:CE	2.47	0.45
1:B:407:ARG:HD2	1:C:224:SER:O	2.15	0.45
1:B:307:TRP:NE1	1:B:692:GLU:HG2	2.31	0.45
1:F:251:PRO:HG3	1:F:374:MET:CE	2.47	0.45
1:H:385:ASN:ND2	1:Y:532:ASP:OD1	2.47	0.45
1:J:251:PRO:HG3	1:J:374:MET:CE	2.47	0.45
1:K:299:TRP:CG	1:K:616:LEU:HD13	2.52	0.45
1:K:312:LYS:O	1:K:418:PHE:N	2.44	0.45
1:L:416:TYR:OH	1:L:644:HIS:O	2.33	0.45
1:M:528:THR:H	1:M:565:GLU:HB2	1.80	0.45
1:N:297:ARG:O	1:N:300:GLN:N	2.48	0.45
1:N:307:TRP:NE1	1:N:692:GLU:HG2	2.31	0.45
1:O:312:LYS:O	1:O:418:PHE:N	2.44	0.45
1:R:425:SER:HB2	1:R:427:TYR:CE2	2.52	0.45
1:S:299:TRP:CG	1:S:616:LEU:HD13	2.51	0.45
1:S:425:SER:HB2	1:S:427:TYR:CE2	2.52	0.45
1:S:531:ASP:OD1	1:S:569:LYS:NZ	2.28	0.45
1:T:299:TRP:CG	1:T:616:LEU:HD13	2.52	0.45
1:U:299:TRP:CG	1:U:616:LEU:HD13	2.52	0.45
1:U:425:SER:HB2	1:U:427:TYR:CE2	2.52	0.45
1:V:299:TRP:CG	1:V:616:LEU:HD13	2.52	0.45
1:Y:299:TRP:CG	1:Y:616:LEU:HD13	2.51	0.45
1:Q:224:SER:O	1:Y:407:ARG:HD2	145.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:487:ARG:HD2	1:2:583:ALA:O	98.10	0.45
1:1:384:ASN:ND2	1:1:386:GLY:O	2.49	0.45
1:4:299:TRP:CG	1:4:616:LEU:HD13	2.51	0.45
1:6:307:TRP:NE1	1:6:692:GLU:HG2	2.31	0.45
1:D:251:PRO:HG3	1:D:374:MET:CE	2.47	0.45
1:D:297:ARG:O	1:D:300:GLN:N	2.48	0.45
1:D:354:PRO:HB3	1:P:431:GLN:NE2	2.24	0.45
1:E:583:ALA:O	1:Q:487:ARG:HD2	2.17	0.45
1:E:416:TYR:OH	1:E:644:HIS:O	2.33	0.45
1:F:328:GLN:NE2	1:F:333:LYS:HG3	2.23	0.45
1:G:425:SER:HB2	1:G:427:TYR:CE2	2.52	0.45
1:F:381:LEU:HD21	1:G:439:PRO:HB3	104.44	0.45
1:H:312:LYS:O	1:H:418:PHE:N	2.44	0.45
1:I:297:ARG:O	1:I:300:GLN:N	2.48	0.45
1:I:425:SER:HB2	1:I:427:TYR:CE2	2.52	0.45
1:I:439:PRO:HB3	1:J:381:LEU:HD21	57.41	0.45
1:J:528:THR:H	1:J:565:GLU:HB2	1.80	0.45
1:K:251:PRO:HG3	1:K:374:MET:CE	2.47	0.45
1:D:439:PRO:HB3	1:L:381:LEU:HD21	134.51	0.45
1:M:431:GLN:NE2	1:N:354:PRO:HB3	47.76	0.45
1:D:439:PRO:HB3	1:N:381:LEU:HD21	1.98	0.45
1:N:416:TYR:OH	1:N:644:HIS:O	2.33	0.45
1:P:251:PRO:HG3	1:P:374:MET:CE	2.47	0.45
1:O:224:SER:O	1:P:407:ARG:HD2	2.16	0.45
1:Q:401:PHE:HE1	1:S:695:LYS:HB3	92.89	0.45
1:R:299:TRP:CG	1:R:616:LEU:HD13	2.52	0.45
1:U:224:SER:O	1:2:407:ARG:HD2	153.11	0.45
1:R:487:ARG:HD2	1:U:583:ALA:O	2.16	0.45
1:Y:425:SER:HB2	1:Y:427:TYR:CE2	2.52	0.45
1:Z:297:ARG:O	1:Z:300:GLN:N	2.48	0.45
1:1:425:SER:HB2	1:1:427:TYR:CE2	2.52	0.45
1:3:627:THR:CG2	1:4:610:GLN:HE21	2.25	0.45
1:Z:429:HIS:NE2	1:4:627:THR:HG22	2.31	0.45
1:5:307:TRP:NE1	1:5:692:GLU:HG2	2.31	0.45
1:5:439:PRO:HB3	1:6:381:LEU:HD21	1.97	0.45
1:6:439:PRO:HB3	1:7:381:LEU:HD21	1.98	0.45
1:6:508:ALA:HB1	1:6:519:LEU:HD13	1.97	0.45
1:7:416:TYR:OH	1:7:644:HIS:O	2.33	0.45
1:8:299:TRP:CG	1:8:616:LEU:HD13	2.52	0.45
1:8:307:TRP:NE1	1:8:692:GLU:HG2	2.31	0.45
1:A:238:ASP:OD1	1:A:239:ARG:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:ND2	1:I:532:ASP:OD1	2.49	0.45
1:C:312:LYS:O	1:C:418:PHE:N	2.44	0.45
1:D:299:TRP:CG	1:D:616:LEU:HD13	2.52	0.45
1:D:583:ALA:O	1:L:487:ARG:HD2	144.79	0.45
1:E:251:PRO:HG3	1:E:374:MET:CE	2.47	0.45
1:E:381:LEU:HD21	1:F:439:PRO:HB3	1.98	0.45
1:E:557:TYR:HE1	1:E:562:LEU:HD11	1.82	0.45
1:F:487:ARG:HD2	1:Q:583:ALA:O	2.16	0.45
1:E:704:THR:HG1	1:F:702:GLN:H	64.35	0.45
1:H:299:TRP:CG	1:H:616:LEU:HD13	2.52	0.45
1:H:695:LYS:HB3	1:W:401:PHE:HE1	1.82	0.45
1:J:464:LEU:HD23	1:K:554:ASN:HB3	59.84	0.45
1:J:416:TYR:OH	1:J:644:HIS:O	2.33	0.45
1:I:627:THR:HG22	1:K:429:HIS:NE2	99.33	0.45
1:B:407:ARG:HD2	1:L:224:SER:O	76.75	0.45
1:L:251:PRO:HG3	1:L:374:MET:CE	2.47	0.45
1:O:238:ASP:OD1	1:O:239:ARG:N	2.49	0.45
1:O:695:LYS:HB3	1:P:401:PHE:HE1	36.01	0.45
1:R:251:PRO:HG3	1:R:374:MET:CE	2.47	0.45
1:U:429:HIS:NE2	1:V:627:THR:HG22	60.25	0.45
1:V:407:ARG:HD2	1:W:224:SER:O	2.16	0.45
1:V:425:SER:HB2	1:V:427:TYR:CE2	2.52	0.45
1:W:251:PRO:HG3	1:W:374:MET:CE	2.47	0.45
1:W:429:HIS:NE2	1:X:627:THR:HG22	60.25	0.45
1:W:557:TYR:HE1	1:W:562:LEU:HD11	1.82	0.45
1:X:425:SER:HB2	1:X:427:TYR:CE2	2.52	0.45
1:V:381:LEU:HD21	1:X:439:PRO:HB3	1.98	0.45
1:X:617:GLN:OE1	1:X:617:GLN:N	2.47	0.45
1:Y:251:PRO:HG3	1:Y:374:MET:CE	2.47	0.45
1:Z:251:PRO:HG3	1:Z:374:MET:CE	2.47	0.45
1:Z:425:SER:HB2	1:Z:427:TYR:CE2	2.52	0.45
1:1:617:GLN:N	1:1:617:GLN:OE1	2.47	0.45
1:2:307:TRP:NE1	1:2:692:GLU:HG2	2.31	0.45
1:5:299:TRP:CG	1:5:616:LEU:HD13	2.51	0.45
1:6:532:ASP:OD1	1:7:385:ASN:ND2	2.47	0.45
1:7:557:TYR:HE1	1:7:562:LEU:HD11	1.82	0.45
1:E:282:TRP:CD1	1:E:398:LEU:HD12	2.52	0.45
1:H:531:ASP:OD1	1:H:569:LYS:NZ	2.28	0.45
1:I:251:PRO:HG3	1:I:374:MET:CE	2.47	0.45
1:J:429:HIS:NE2	1:L:627:THR:HG22	2.32	0.45
1:L:425:SER:HB2	1:L:427:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:583:ALA:O	1:T:487:ARG:HD2	229.48	0.45
1:M:297:ARG:O	1:M:300:GLN:N	2.48	0.45
1:M:425:SER:HB2	1:M:427:TYR:CE2	2.52	0.45
1:M:416:TYR:OH	1:M:644:HIS:O	2.33	0.45
1:O:299:TRP:CG	1:O:616:LEU:HD13	2.52	0.45
1:O:425:SER:HB2	1:O:427:TYR:CE2	2.52	0.45
1:P:282:TRP:CD1	1:P:398:LEU:HD12	2.52	0.45
1:P:299:TRP:CG	1:P:616:LEU:HD13	2.52	0.45
1:P:407:ARG:HD2	1:6:224:SER:O	152.39	0.45
1:Q:299:TRP:CG	1:Q:616:LEU:HD13	2.52	0.45
1:Q:583:ALA:O	1:R:487:ARG:HD2	80.79	0.45
1:R:557:TYR:HE1	1:R:562:LEU:HD11	1.82	0.45
1:T:251:PRO:HG3	1:T:374:MET:CE	2.47	0.45
1:T:557:TYR:HE1	1:T:562:LEU:HD11	1.82	0.45
1:V:282:TRP:CD1	1:V:398:LEU:HD12	2.52	0.45
1:V:328:GLN:NE2	1:V:333:LYS:HG3	2.23	0.45
1:W:282:TRP:CD1	1:W:398:LEU:HD12	2.52	0.45
1:W:583:ALA:O	1:Y:487:ARG:HD2	2.17	0.45
1:X:238:ASP:OD1	1:X:239:ARG:N	2.49	0.45
1:X:299:TRP:CG	1:X:616:LEU:HD13	2.52	0.45
1:X:282:TRP:NE1	1:X:398:LEU:HB2	2.32	0.45
1:W:695:LYS:HB3	1:X:401:PHE:HE1	42.80	0.45
1:W:702:GLN:N	1:X:704:THR:OG1	2.37	0.45
1:X:439:PRO:HB3	1:Y:381:LEU:HD21	57.41	0.45
1:Y:557:TYR:HE1	1:Y:562:LEU:HD11	1.82	0.45
1:Z:381:LEU:HD21	1:2:439:PRO:HB3	93.17	0.45
1:Z:429:HIS:NE2	1:1:627:THR:HG22	88.03	0.45
1:1:282:TRP:CD1	1:1:398:LEU:HD12	2.52	0.45
1:2:531:ASP:OD1	1:2:569:LYS:NZ	2.28	0.45
1:Z:627:THR:HG22	1:3:429:HIS:NE2	2.32	0.45
1:4:416:TYR:OH	1:4:644:HIS:O	2.33	0.45
1:6:251:PRO:HG3	1:6:374:MET:CE	2.47	0.45
1:6:583:ALA:O	1:7:487:ARG:HD2	2.17	0.45
1:5:487:ARG:HD2	1:7:583:ALA:O	2.17	0.45
1:8:282:TRP:CD1	1:8:398:LEU:HD12	2.52	0.45
1:A:425:SER:HB2	1:A:427:TYR:CE2	2.52	0.45
1:A:627:THR:HG22	1:K:429:HIS:NE2	96.27	0.45
1:B:487:ARG:HD2	1:C:583:ALA:O	94.93	0.45
1:C:627:THR:HG22	1:M:429:HIS:NE2	2.32	0.45
1:D:328:GLN:NE2	1:D:333:LYS:HG3	2.23	0.45
1:E:487:ARG:HD2	1:F:583:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:627:THR:HG22	1:G:429:HIS:NE2	88.92	0.45
1:G:557:TYR:HE1	1:G:562:LEU:HD11	1.82	0.45
1:H:251:PRO:HG3	1:H:374:MET:CE	2.47	0.45
1:H:425:SER:HB2	1:H:427:TYR:CE2	2.52	0.45
1:I:695:LYS:HB3	1:J:401:PHE:HE1	36.01	0.45
1:K:238:ASP:OD1	1:K:239:ARG:N	2.49	0.45
1:K:508:ALA:HB1	1:K:519:LEU:HD13	1.98	0.45
1:L:429:HIS:NE2	1:T:627:THR:HG22	193.57	0.45
1:B:487:ARG:HD2	1:L:583:ALA:O	2.17	0.45
1:N:583:ALA:O	1:P:487:ARG:HD2	2.16	0.45
1:E:464:LEU:HD23	1:Q:554:ASN:HB3	1.99	0.45
1:S:251:PRO:HG3	1:S:374:MET:CE	2.47	0.45
1:S:282:TRP:CD1	1:S:398:LEU:HD12	2.52	0.45
1:T:282:TRP:CD1	1:T:398:LEU:HD12	2.52	0.45
1:U:282:TRP:CD1	1:U:398:LEU:HD12	2.52	0.45
1:V:251:PRO:HG3	1:V:374:MET:CE	2.47	0.45
1:V:416:TYR:OH	1:V:644:HIS:O	2.33	0.45
1:Y:282:TRP:CD1	1:Y:398:LEU:HD12	2.52	0.45
1:W:487:ARG:HD2	1:Y:583:ALA:O	18.56	0.45
1:2:299:TRP:CG	1:2:616:LEU:HD13	2.52	0.45
1:2:282:TRP:CD1	1:2:398:LEU:HD12	2.52	0.45
1:1:695:LYS:HB3	1:2:401:PHE:HE1	1.81	0.45
1:2:557:TYR:HE1	1:2:562:LEU:HD11	1.82	0.45
1:3:238:ASP:OD1	1:3:239:ARG:N	2.49	0.45
1:3:299:TRP:CG	1:3:616:LEU:HD13	2.52	0.45
1:Z:583:ALA:O	1:4:487:ARG:HD2	2.17	0.45
1:7:617:GLN:N	1:7:617:GLN:OE1	2.47	0.45
1:B:328:GLN:NE2	1:B:333:LYS:HG3	2.23	0.45
1:C:425:SER:HB2	1:C:427:TYR:CE2	2.52	0.45
1:C:557:TYR:HE1	1:C:562:LEU:HD11	1.82	0.45
1:D:238:ASP:OD1	1:D:239:ARG:N	2.49	0.45
1:F:282:TRP:CD1	1:F:398:LEU:HD12	2.52	0.45
1:G:251:PRO:HG3	1:G:374:MET:CE	2.47	0.45
1:F:487:ARG:HD2	1:G:583:ALA:O	86.94	0.45
1:I:557:TYR:HE1	1:I:562:LEU:HD11	1.82	0.45
1:B:439:PRO:HB3	1:J:381:LEU:HD21	1.98	0.45
1:J:282:TRP:NE1	1:J:398:LEU:HB2	2.32	0.45
1:B:695:LYS:HB3	1:J:401:PHE:HE1	1.82	0.45
1:J:425:SER:HB2	1:J:427:TYR:CE2	2.52	0.45
1:J:695:LYS:HB3	1:K:401:PHE:HE1	42.80	0.45
1:B:439:PRO:HB3	1:M:381:LEU:HD21	137.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:282:TRP:NE1	1:M:398:LEU:HB2	2.32	0.45
1:O:557:TYR:HE1	1:O:562:LEU:HD11	1.82	0.45
1:Q:385:ASN:ND2	1:S:532:ASP:OD1	111.52	0.45
1:Q:557:TYR:HE1	1:Q:562:LEU:HD11	1.82	0.45
1:Q:416:TYR:OH	1:Q:644:HIS:O	2.33	0.45
1:R:429:HIS:NE2	1:S:627:THR:HG22	2.32	0.45
1:S:282:TRP:NE1	1:S:398:LEU:HB2	2.32	0.45
1:S:464:LEU:HD23	1:U:554:ASN:HB3	1.99	0.45
1:T:464:LEU:HD23	1:U:554:ASN:HB3	100.68	0.45
1:S:583:ALA:O	1:U:487:ARG:HD2	2.17	0.45
1:V:282:TRP:NE1	1:V:398:LEU:HB2	2.32	0.45
1:H:532:ASP:OD1	1:W:385:ASN:ND2	2.48	0.45
1:E:695:LYS:HB3	1:X:401:PHE:HE1	153.20	0.45
1:X:464:LEU:HD23	1:Y:554:ASN:HB3	100.68	0.45
1:E:583:ALA:O	1:X:487:ARG:HD2	142.79	0.45
1:H:554:ASN:HB3	1:Y:464:LEU:HD23	1.99	0.45
1:Z:282:TRP:NE1	1:Z:398:LEU:HB2	2.32	0.45
1:Z:554:ASN:HB3	1:3:464:LEU:HD23	1.99	0.45
1:2:238:ASP:OD1	1:2:239:ARG:N	2.49	0.45
1:3:557:TYR:HE1	1:3:562:LEU:HD11	1.82	0.45
1:5:282:TRP:NE1	1:5:398:LEU:HB2	2.32	0.45
1:6:282:TRP:CD1	1:6:398:LEU:HD12	2.52	0.45
1:K:401:PHE:HE1	1:8:695:LYS:HB3	1.82	0.45
1:A:282:TRP:CD1	1:A:398:LEU:HD12	2.52	0.45
1:A:307:TRP:NE1	1:A:692:GLU:HG2	2.31	0.45
1:A:610:GLN:HE21	1:G:627:THR:CG2	2.26	0.45
1:B:695:LYS:HB3	1:M:401:PHE:HE1	123.78	0.45
1:C:282:TRP:CD1	1:C:398:LEU:HD12	2.52	0.45
1:D:282:TRP:CD1	1:D:398:LEU:HD12	2.52	0.45
1:D:557:TYR:HE1	1:D:562:LEU:HD11	1.82	0.45
1:E:385:ASN:ND2	1:F:532:ASP:OD1	2.47	0.45
1:F:557:TYR:HE1	1:F:562:LEU:HD11	1.82	0.45
1:F:401:PHE:HE1	1:G:695:LYS:HB3	92.88	0.45
1:G:487:ARG:HD2	1:H:583:ALA:O	80.78	0.45
1:I:429:HIS:NE2	1:J:627:THR:HG22	43.24	0.45
1:L:282:TRP:CD1	1:L:398:LEU:HD12	2.52	0.45
1:L:557:TYR:HE1	1:L:562:LEU:HD11	1.82	0.45
1:D:695:LYS:HB3	1:N:401:PHE:HE1	1.82	0.45
1:N:464:LEU:HD23	1:P:554:ASN:HB3	1.99	0.45
1:D:401:PHE:HE1	1:P:695:LYS:HB3	1.82	0.45
1:R:282:TRP:NE1	1:R:398:LEU:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:282:TRP:NE1	1:U:398:LEU:HB2	2.32	0.45
1:T:429:HIS:NE2	1:U:627:THR:HG22	43.24	0.45
1:U:439:PRO:HB3	1:V:381:LEU:HD21	50.83	0.45
1:T:487:ARG:HD2	1:V:583:ALA:O	132.20	0.45
1:Y:282:TRP:NE1	1:Y:398:LEU:HB2	2.32	0.45
1:Z:299:TRP:CG	1:Z:616:LEU:HD13	2.52	0.45
1:Z:557:TYR:HE1	1:Z:562:LEU:HD11	1.82	0.45
1:3:282:TRP:NE1	1:3:398:LEU:HB2	2.32	0.45
1:Z:487:ARG:HD2	1:3:583:ALA:O	2.17	0.45
1:5:416:TYR:OH	1:5:644:HIS:O	2.33	0.45
1:A:251:PRO:HG3	1:A:374:MET:CE	2.47	0.45
1:B:401:PHE:HE1	1:C:695:LYS:HB3	36.01	0.45
1:B:429:HIS:NE2	1:J:627:THR:HG22	2.32	0.45
1:C:464:LEU:HD23	1:O:554:ASN:HB3	169.21	0.45
1:E:282:TRP:NE1	1:E:398:LEU:HB2	2.32	0.45
1:E:487:ARG:HD2	1:V:583:ALA:O	158.99	0.45
1:G:299:TRP:CG	1:G:616:LEU:HD13	2.52	0.45
1:G:282:TRP:NE1	1:G:398:LEU:HB2	2.32	0.45
1:G:282:TRP:CD1	1:G:398:LEU:HD12	2.52	0.45
1:G:554:ASN:HB3	1:H:464:LEU:HD23	59.84	0.45
1:H:282:TRP:CD1	1:H:398:LEU:HD12	2.52	0.45
1:F:695:LYS:HB3	1:H:401:PHE:HE1	113.32	0.45
1:F:583:ALA:O	1:H:487:ARG:HD2	144.79	0.45
1:I:282:TRP:NE1	1:I:398:LEU:HB2	2.32	0.45
1:J:557:TYR:HE1	1:J:562:LEU:HD11	1.82	0.45
1:K:282:TRP:CD1	1:K:398:LEU:HD12	2.52	0.45
1:N:251:PRO:HG3	1:N:374:MET:CE	2.47	0.45
1:N:282:TRP:CD1	1:N:398:LEU:HD12	2.52	0.45
1:O:251:PRO:HG3	1:O:374:MET:CE	2.47	0.45
1:O:282:TRP:NE1	1:O:398:LEU:HB2	2.32	0.45
1:M:627:THR:HG22	1:O:429:HIS:NE2	99.33	0.45
1:O:616:LEU:HD22	1:O:729:ILE:HD12	1.99	0.45
1:Q:282:TRP:NE1	1:Q:398:LEU:HB2	2.32	0.45
1:S:439:PRO:HB3	1:U:381:LEU:HD21	1.98	0.45
1:S:695:LYS:HB3	1:U:401:PHE:HE1	1.82	0.45
1:T:307:TRP:NE1	1:T:692:GLU:HG2	2.31	0.45
1:U:251:PRO:HG3	1:U:374:MET:CE	2.47	0.45
1:W:299:TRP:CG	1:W:616:LEU:HD13	2.51	0.45
1:X:384:ASN:ND2	1:X:386:GLY:O	2.49	0.45
1:X:616:LEU:HD22	1:X:729:ILE:HD12	2.00	0.45
1:Z:695:LYS:HB3	1:1:401:PHE:HE1	95.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:238:ASP:OD1	1:1:239:ARG:N	2.49	0.44
1:2:616:LEU:HD22	1:2:729:ILE:HD12	1.99	0.44
1:5:429:HIS:NE2	1:6:627:THR:HG22	2.32	0.44
1:7:251:PRO:HG3	1:7:374:MET:CE	2.47	0.44
1:7:282:TRP:NE1	1:7:398:LEU:HB2	2.32	0.44
1:5:627:THR:HG22	1:7:429:HIS:NE2	2.32	0.44
1:7:299:TRP:CG	1:7:616:LEU:HD13	2.52	0.44
1:K:554:ASN:HB3	1:8:464:LEU:HD23	1.99	0.44
1:A:583:ALA:O	1:8:487:ARG:HD2	155.37	0.44
1:A:416:TYR:OH	1:A:644:HIS:O	2.33	0.44
1:A:616:LEU:HD22	1:A:729:ILE:HD12	2.00	0.44
1:C:282:TRP:NE1	1:C:398:LEU:HB2	2.32	0.44
1:C:610:GLN:HE21	1:O:627:THR:CG2	141.08	0.44
1:E:299:TRP:CG	1:E:616:LEU:HD13	2.52	0.44
1:F:554:ASN:HB3	1:Q:464:LEU:HD23	1.99	0.44
1:H:487:ARG:HD2	1:Y:583:ALA:O	2.17	0.44
1:F:429:HIS:NE2	1:H:627:THR:HG22	120.05	0.44
1:H:627:THR:HG22	1:Y:429:HIS:NE2	2.32	0.44
1:J:282:TRP:CD1	1:J:398:LEU:HD12	2.52	0.44
1:K:329:ASN:O	1:K:332:THR:OG1	2.21	0.44
1:I:487:ARG:HD2	1:K:583:ALA:O	132.19	0.44
1:K:627:THR:HG22	1:8:429:HIS:NE2	2.32	0.44
1:A:401:PHE:HE1	1:K:695:LYS:HB3	76.34	0.44
1:L:299:TRP:CG	1:L:616:LEU:HD13	2.52	0.44
1:B:401:PHE:HE1	1:L:695:LYS:HB3	1.82	0.44
1:M:282:TRP:CD1	1:M:398:LEU:HD12	2.52	0.44
1:M:429:HIS:NE2	1:N:627:THR:HG22	43.24	0.44
1:M:554:ASN:HB3	1:O:464:LEU:HD23	95.79	0.44
1:M:557:TYR:HE1	1:M:562:LEU:HD11	1.82	0.44
1:B:429:HIS:NE2	1:M:627:THR:HG22	100.22	0.44
1:N:425:SER:HB2	1:N:427:TYR:CE2	2.52	0.44
1:N:532:ASP:OD1	1:O:385:ASN:ND2	68.31	0.44
1:D:429:HIS:NE2	1:N:627:THR:HG22	2.32	0.44
1:O:282:TRP:CD1	1:O:398:LEU:HD12	2.52	0.44
1:C:695:LYS:HB3	1:O:401:PHE:HE1	152.08	0.44
1:M:487:ARG:HD2	1:O:583:ALA:O	132.19	0.44
1:P:282:TRP:NE1	1:P:398:LEU:HB2	2.32	0.44
1:P:425:SER:HB2	1:P:427:TYR:CE2	2.52	0.44
1:D:554:ASN:HB3	1:P:464:LEU:HD23	1.99	0.44
1:P:616:LEU:HD22	1:P:729:ILE:HD12	1.99	0.44
1:Q:251:PRO:HG3	1:Q:374:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:282:TRP:CD1	1:Q:398:LEU:HD12	2.52	0.44
1:F:381:LEU:HD21	1:Q:439:PRO:HB3	1.97	0.44
1:Q:429:HIS:NE2	1:R:627:THR:HG22	60.26	0.44
1:R:616:LEU:HD22	1:R:729:ILE:HD12	2.00	0.44
1:S:557:TYR:HE1	1:S:562:LEU:HD11	1.82	0.44
1:Q:487:ARG:HD2	1:S:583:ALA:O	86.93	0.44
1:T:587:GLN:NE2	1:U:490:ARG:O	105.81	0.44
1:T:583:ALA:O	1:U:487:ARG:HD2	94.92	0.44
1:U:557:TYR:HE1	1:U:562:LEU:HD11	1.82	0.44
1:V:554:ASN:HB3	1:X:464:LEU:HD23	1.99	0.44
1:H:429:HIS:NE2	1:W:627:THR:HG22	2.32	0.44
1:W:616:LEU:HD22	1:W:729:ILE:HD12	2.00	0.44
1:X:282:TRP:CD1	1:X:398:LEU:HD12	2.52	0.44
1:X:695:LYS:HB3	1:Y:401:PHE:HE1	36.01	0.44
1:X:333:LYS:NZ	1:Y:659:ASP:OD2	2.32	0.44
1:Y:616:LEU:HD22	1:Y:729:ILE:HD12	1.99	0.44
1:1:307:TRP:NE1	1:1:692:GLU:HG2	2.31	0.44
1:3:416:TYR:OH	1:3:644:HIS:O	2.33	0.44
1:Z:431:GLN:NE2	1:4:354:PRO:HB3	2.24	0.44
1:4:425:SER:HB2	1:4:427:TYR:CE2	2.52	0.44
1:3:401:PHE:HE1	1:4:695:LYS:HB3	1.82	0.44
1:5:282:TRP:CD1	1:5:398:LEU:HD12	2.52	0.44
1:5:554:ASN:HB3	1:7:464:LEU:HD23	1.99	0.44
1:6:616:LEU:HD22	1:6:729:ILE:HD12	2.00	0.44
1:7:297:ARG:O	1:7:300:GLN:N	2.48	0.44
1:7:508:ALA:HB1	1:7:519:LEU:HD13	1.98	0.44
1:A:695:LYS:HB3	1:8:401:PHE:HE1	146.90	0.44
1:8:425:SER:HB2	1:8:427:TYR:CE2	2.52	0.44
1:C:297:ARG:O	1:C:300:GLN:N	2.48	0.44
1:D:487:ARG:HD2	1:P:583:ALA:O	2.17	0.44
1:D:627:THR:HG22	1:P:429:HIS:NE2	2.32	0.44
1:E:616:LEU:HD22	1:E:729:ILE:HD12	2.00	0.44
1:F:425:SER:HB2	1:F:427:TYR:CE2	2.52	0.44
1:F:490:ARG:O	1:Q:587:GLN:NE2	2.50	0.44
1:F:616:LEU:HD22	1:F:729:ILE:HD12	1.99	0.44
1:G:616:LEU:HD22	1:G:729:ILE:HD12	2.00	0.44
1:H:238:ASP:OD1	1:H:239:ARG:N	2.49	0.44
1:I:554:ASN:HB3	1:K:464:LEU:HD23	95.78	0.44
1:J:587:GLN:NE2	1:K:490:ARG:O	77.16	0.44
1:K:616:LEU:HD22	1:K:729:ILE:HD12	1.99	0.44
1:L:282:TRP:NE1	1:L:398:LEU:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:406:LEU:HD21	1:M:412:PHE:HB2	2.00	0.44
1:C:554:ASN:HB3	1:M:464:LEU:HD23	1.99	0.44
1:M:464:LEU:HD23	1:N:554:ASN:HB3	100.68	0.44
1:N:557:TYR:HE1	1:N:562:LEU:HD11	1.82	0.44
1:Q:554:ASN:HB3	1:S:464:LEU:HD23	104.60	0.44
1:R:587:GLN:NE2	1:S:490:ARG:O	2.51	0.44
1:S:238:ASP:OD1	1:S:239:ARG:N	2.49	0.44
1:S:616:LEU:HD22	1:S:729:ILE:HD12	2.00	0.44
1:U:616:LEU:HD22	1:U:729:ILE:HD12	2.00	0.44
1:U:695:LYS:HB3	1:V:401:PHE:HE1	42.80	0.44
1:W:282:TRP:NE1	1:W:398:LEU:HB2	2.32	0.44
1:V:401:PHE:HE1	1:X:695:LYS:HB3	1.82	0.44
1:W:554:ASN:HB3	1:Y:464:LEU:HD23	59.82	0.44
1:Z:282:TRP:CD1	1:Z:398:LEU:HD12	2.52	0.44
1:3:425:SER:HB2	1:3:427:TYR:CE2	2.52	0.44
1:3:385:ASN:ND2	1:4:532:ASP:OD1	2.47	0.44
1:5:251:PRO:HG3	1:5:374:MET:CE	2.47	0.44
1:6:238:ASP:OD1	1:6:239:ARG:N	2.49	0.44
1:6:406:LEU:HD21	1:6:412:PHE:HB2	2.00	0.44
1:A:587:GLN:NE2	1:G:490:ARG:O	2.50	0.44
1:B:282:TRP:NE1	1:B:398:LEU:HB2	2.32	0.44
1:B:554:ASN:HB3	1:L:464:LEU:HD23	1.99	0.44
1:C:616:LEU:HD22	1:C:729:ILE:HD12	2.00	0.44
1:D:616:LEU:HD22	1:D:729:ILE:HD12	1.99	0.44
1:E:401:PHE:HE1	1:F:695:LYS:HB3	1.82	0.44
1:F:224:SER:O	1:G:407:ARG:HD2	2.17	0.44
1:I:282:TRP:CD1	1:I:398:LEU:HD12	2.52	0.44
1:I:529:HIS:CE1	1:I:534:GLU:HA	2.53	0.44
1:J:464:LEU:HD23	1:L:554:ASN:HB3	2.00	0.44
1:J:529:HIS:CE1	1:J:534:GLU:HA	2.53	0.44
1:J:616:LEU:HD22	1:J:729:ILE:HD12	2.00	0.44
1:K:557:TYR:HE1	1:K:562:LEU:HD11	1.82	0.44
1:D:695:LYS:HB3	1:L:401:PHE:HE1	113.32	0.44
1:N:238:ASP:OD1	1:N:239:ARG:N	2.49	0.44
1:D:583:ALA:O	1:N:487:ARG:HD2	2.17	0.44
1:P:406:LEU:HD21	1:P:412:PHE:HB2	2.00	0.44
1:R:282:TRP:CD1	1:R:398:LEU:HD12	2.52	0.44
1:R:529:HIS:CE1	1:R:534:GLU:HA	2.53	0.44
1:T:282:TRP:NE1	1:T:398:LEU:HB2	2.32	0.44
1:T:490:ARG:O	1:V:587:GLN:NE2	124.94	0.44
1:V:627:THR:HG22	1:X:429:HIS:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:PHE:HE1	1:V:695:LYS:HB3	123.96	0.44
1:X:529:HIS:CE1	1:X:534:GLU:HA	2.53	0.44
1:E:429:HIS:NE2	1:X:627:THR:HG22	142.97	0.44
1:W:627:THR:HG22	1:Y:429:HIS:NE2	30.52	0.44
1:X:587:GLN:NE2	1:Y:490:ARG:O	105.80	0.44
1:W:627:THR:CG2	1:Y:610:GLN:HE21	28.94	0.44
1:Z:406:LEU:HD21	1:Z:412:PHE:HB2	2.00	0.44
1:1:282:TRP:NE1	1:1:398:LEU:HB2	2.32	0.44
1:3:282:TRP:CD1	1:3:398:LEU:HD12	2.52	0.44
1:4:529:HIS:CE1	1:4:534:GLU:HA	2.53	0.44
1:4:617:GLN:N	1:4:617:GLN:OE1	2.47	0.44
1:5:583:ALA:O	1:6:487:ARG:HD2	2.17	0.44
1:8:557:TYR:HE1	1:8:562:LEU:HD11	1.82	0.44
1:A:406:LEU:HD21	1:A:412:PHE:HB2	2.00	0.44
1:C:401:PHE:HE1	1:M:695:LYS:HB3	1.82	0.44
1:B:554:ASN:HB3	1:C:464:LEU:HD23	100.69	0.44
1:D:282:TRP:NE1	1:D:398:LEU:HB2	2.32	0.44
1:E:297:ARG:O	1:E:300:GLN:N	2.48	0.44
1:E:425:SER:HB2	1:E:427:TYR:CE2	2.52	0.44
1:F:406:LEU:HD21	1:F:412:PHE:HB2	2.00	0.44
1:F:529:HIS:CE1	1:F:534:GLU:HA	2.53	0.44
1:G:627:THR:HG22	1:H:429:HIS:NE2	60.26	0.44
1:G:587:GLN:NE2	1:I:490:ARG:O	2.51	0.44
1:I:587:GLN:NE2	1:J:490:ARG:O	105.80	0.44
1:I:583:ALA:O	1:J:487:ARG:HD2	94.92	0.44
1:K:282:TRP:NE1	1:K:398:LEU:HB2	2.32	0.44
1:L:616:LEU:HD22	1:L:729:ILE:HD12	2.00	0.44
1:M:529:HIS:CE1	1:M:534:GLU:HA	2.53	0.44
1:M:610:GLN:HE21	1:N:627:THR:CG2	45.57	0.44
1:N:529:HIS:CE1	1:N:534:GLU:HA	2.53	0.44
1:C:583:ALA:O	1:O:487:ARG:HD2	141.96	0.44
1:O:529:HIS:CE1	1:O:534:GLU:HA	2.53	0.44
1:P:529:HIS:CE1	1:P:534:GLU:HA	2.53	0.44
1:Q:464:LEU:HD23	1:R:554:ASN:HB3	59.84	0.44
1:U:583:ALA:O	1:V:487:ARG:HD2	80.78	0.44
1:W:583:ALA:O	1:X:487:ARG:HD2	80.78	0.44
1:Y:529:HIS:CE1	1:Y:534:GLU:HA	2.53	0.44
1:W:464:LEU:HD23	1:Y:554:ASN:HB3	1.99	0.44
1:Z:529:HIS:CE1	1:Z:534:GLU:HA	2.53	0.44
1:1:329:ASN:O	1:1:332:THR:OG1	2.21	0.44
1:1:529:HIS:CE1	1:1:534:GLU:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:557:TYR:HE1	1:1:562:LEU:HD11	1.82	0.44
1:2:425:SER:HB2	1:2:427:TYR:CE2	2.52	0.44
1:3:529:HIS:CE1	1:3:534:GLU:HA	2.53	0.44
1:4:282:TRP:CD1	1:4:398:LEU:HD12	2.52	0.44
1:4:406:LEU:HD21	1:4:412:PHE:HB2	2.00	0.44
1:6:282:TRP:NE1	1:6:398:LEU:HB2	2.32	0.44
1:5:587:GLN:NE2	1:6:490:ARG:O	2.51	0.44
1:6:695:LYS:HB3	1:7:401:PHE:HE1	1.82	0.44
1:7:425:SER:HB2	1:7:427:TYR:CE2	2.52	0.44
1:8:529:HIS:CE1	1:8:534:GLU:HA	2.53	0.44
1:A:464:LEU:HD23	1:8:554:ASN:HB3	187.60	0.44
1:A:282:TRP:NE1	1:A:398:LEU:HB2	2.32	0.44
1:A:487:ARG:HD2	1:K:583:ALA:O	148.17	0.44
1:A:557:TYR:HE1	1:A:562:LEU:HD11	1.82	0.44
1:B:557:TYR:HE1	1:B:562:LEU:HD11	1.82	0.44
1:C:487:ARG:HD2	1:M:583:ALA:O	2.17	0.44
1:C:529:HIS:CE1	1:C:534:GLU:HA	2.53	0.44
1:C:587:GLN:NE2	1:O:490:ARG:O	147.21	0.44
1:E:263:ASN:HB2	1:E:275:TYR:CE2	2.53	0.44
1:E:429:HIS:NE2	1:Q:627:THR:HG22	2.32	0.44
1:F:587:GLN:NE2	1:H:490:ARG:O	151.06	0.44
1:F:627:THR:HG22	1:Q:429:HIS:NE2	2.32	0.44
1:G:406:LEU:HD21	1:G:412:PHE:HB2	2.00	0.44
1:G:529:HIS:CE1	1:G:534:GLU:HA	2.53	0.44
1:F:490:ARG:O	1:G:587:GLN:NE2	91.35	0.44
1:I:238:ASP:OD1	1:I:239:ARG:N	2.49	0.44
1:J:406:LEU:HD21	1:J:412:PHE:HB2	2.00	0.44
1:K:487:ARG:HD2	1:8:583:ALA:O	2.17	0.44
1:M:251:PRO:HG3	1:M:374:MET:CE	2.47	0.44
1:B:587:GLN:NE2	1:M:490:ARG:O	124.09	0.44
1:M:695:LYS:HB3	1:N:401:PHE:HE1	36.01	0.44
1:M:587:GLN:NE2	1:N:490:ARG:O	105.81	0.44
1:N:583:ALA:O	1:O:487:ARG:HD2	80.78	0.44
1:N:695:LYS:HB3	1:O:401:PHE:HE1	42.80	0.44
1:O:429:HIS:NE2	1:P:627:THR:HG22	43.24	0.44
1:N:695:LYS:HB3	1:P:401:PHE:HE1	1.82	0.44
1:C:627:THR:HG22	1:P:429:HIS:NE2	63.25	0.44
1:R:406:LEU:HD21	1:R:412:PHE:HB2	2.00	0.44
1:R:464:LEU:HD23	1:S:554:ASN:HB3	1.99	0.44
1:R:583:ALA:O	1:S:487:ARG:HD2	2.17	0.44
1:Q:627:THR:HG22	1:S:429:HIS:NE2	88.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:529:HIS:CE1	1:T:534:GLU:HA	2.53	0.44
1:S:429:HIS:NE2	1:U:627:THR:HG22	2.33	0.44
1:V:650:LEU:HA	1:V:650:LEU:HD13	1.87	0.44
1:W:263:ASN:HB2	1:W:275:TYR:CE2	2.53	0.44
1:W:425:SER:HB2	1:W:427:TYR:CE2	2.52	0.44
1:W:695:LYS:HB3	1:Y:401:PHE:HE1	1.82	0.44
1:1:263:ASN:HB2	1:1:275:TYR:CE2	2.53	0.44
1:1:406:LEU:HD21	1:1:412:PHE:HB2	2.00	0.44
1:2:282:TRP:NE1	1:2:398:LEU:HB2	2.32	0.44
1:3:247:THR:HG23	1:3:680:GLN:HE22	1.83	0.44
1:Z:587:GLN:NE2	1:4:490:ARG:O	2.51	0.44
1:6:328:GLN:NE2	1:6:333:LYS:HG3	2.23	0.44
1:6:425:SER:HB2	1:6:427:TYR:CE2	2.52	0.44
1:A:587:GLN:NE2	1:8:490:ARG:O	169.67	0.44
1:A:529:HIS:CE1	1:A:534:GLU:HA	2.53	0.44
1:B:627:THR:HG22	1:L:429:HIS:NE2	2.32	0.44
1:E:529:HIS:CE1	1:E:534:GLU:HA	2.53	0.44
1:E:627:THR:HG22	1:V:429:HIS:NE2	116.60	0.44
1:F:282:TRP:NE1	1:F:398:LEU:HB2	2.32	0.44
1:G:429:HIS:NE2	1:I:627:THR:HG22	2.33	0.44
1:H:529:HIS:CE1	1:H:534:GLU:HA	2.53	0.44
1:H:557:TYR:HE1	1:H:562:LEU:HD11	1.82	0.44
1:K:416:TYR:OH	1:K:644:HIS:O	2.33	0.44
1:L:406:LEU:HD21	1:L:412:PHE:HB2	2.00	0.44
1:L:529:HIS:CE1	1:L:534:GLU:HA	2.53	0.44
1:N:406:LEU:HD21	1:N:412:PHE:HB2	2.00	0.44
1:N:587:GLN:NE2	1:P:490:ARG:O	2.51	0.44
1:O:583:ALA:O	1:P:487:ARG:HD2	94.92	0.44
1:C:429:HIS:NE2	1:O:627:THR:HG22	143.30	0.44
1:C:487:ARG:HD2	1:P:583:ALA:O	83.20	0.44
1:S:529:HIS:CE1	1:S:534:GLU:HA	2.53	0.44
1:L:695:LYS:HB3	1:T:401:PHE:HE1	183.25	0.44
1:T:406:LEU:HD21	1:T:412:PHE:HB2	2.00	0.44
1:U:529:HIS:CE1	1:U:534:GLU:HA	2.53	0.44
1:R:490:ARG:O	1:U:587:GLN:NE2	2.51	0.44
1:E:627:THR:CG2	1:V:610:GLN:HE21	116.95	0.44
1:W:401:PHE:HE1	1:Y:695:LYS:HB3	58.01	0.44
1:W:416:TYR:OH	1:W:644:HIS:O	2.33	0.44
1:Y:406:LEU:HD21	1:Y:412:PHE:HB2	2.00	0.44
1:W:587:GLN:NE2	1:Y:490:ARG:O	2.51	0.44
1:Z:583:ALA:O	1:1:487:ARG:HD2	89.08	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:464:LEU:HD23	1:1:554:ASN:HB3	104.59	0.44
1:2:263:ASN:HB2	1:2:275:TYR:CE2	2.53	0.44
1:3:554:ASN:HB3	1:4:464:LEU:HD23	2.00	0.44
1:3:487:ARG:HD2	1:4:583:ALA:O	2.18	0.44
1:5:238:ASP:OD1	1:5:239:ARG:N	2.49	0.44
1:5:616:LEU:HD22	1:5:729:ILE:HD12	2.00	0.44
1:6:429:HIS:NE2	1:7:627:THR:HG22	2.32	0.44
1:8:263:ASN:HB2	1:8:275:TYR:CE2	2.53	0.44
1:K:490:ARG:O	1:8:587:GLN:NE2	2.51	0.44
1:B:263:ASN:HB2	1:B:275:TYR:CE2	2.53	0.44
1:B:282:TRP:CD1	1:B:398:LEU:HD12	2.52	0.44
1:B:529:HIS:CE1	1:B:534:GLU:HA	2.53	0.44
1:B:583:ALA:O	1:J:487:ARG:HD2	2.17	0.44
1:D:263:ASN:HB2	1:D:275:TYR:CE2	2.53	0.44
1:D:490:ARG:O	1:P:587:GLN:NE2	2.51	0.44
1:D:490:ARG:O	1:T:587:GLN:NE2	149.07	0.44
1:E:464:LEU:HD23	1:X:554:ASN:HB3	169.21	0.44
1:F:464:LEU:HD23	1:H:554:ASN:HB3	153.07	0.44
1:J:297:ARG:O	1:J:300:GLN:N	2.48	0.44
1:J:429:HIS:NE2	1:K:627:THR:HG22	60.25	0.44
1:B:587:GLN:NE2	1:J:490:ARG:O	2.51	0.44
1:J:583:ALA:O	1:L:487:ARG:HD2	2.17	0.44
1:K:529:HIS:CE1	1:K:534:GLU:HA	2.53	0.44
1:J:695:LYS:HB3	1:L:401:PHE:HE1	1.82	0.44
1:M:263:ASN:HB2	1:M:275:TYR:CE2	2.53	0.44
1:B:583:ALA:O	1:M:487:ARG:HD2	104.70	0.44
1:N:282:TRP:NE1	1:N:398:LEU:HB2	2.32	0.44
1:N:464:LEU:HD23	1:O:554:ASN:HB3	59.83	0.44
1:N:650:LEU:HD13	1:N:650:LEU:HA	1.86	0.44
1:O:247:THR:HG23	1:O:680:GLN:HE22	1.83	0.44
1:M:401:PHE:HE1	1:O:695:LYS:HB3	69.79	0.44
1:P:263:ASN:HB2	1:P:275:TYR:CE2	2.53	0.44
1:P:557:TYR:HE1	1:P:562:LEU:HD11	1.82	0.44
1:Q:406:LEU:HD21	1:Q:412:PHE:HB2	2.00	0.44
1:Q:529:HIS:CE1	1:Q:534:GLU:HA	2.53	0.44
1:Q:695:LYS:HB3	1:R:401:PHE:HE1	42.80	0.44
1:Q:616:LEU:HD22	1:Q:729:ILE:HD12	2.00	0.44
1:R:695:LYS:HB3	1:S:401:PHE:HE1	1.82	0.44
1:S:587:GLN:NE2	1:U:490:ARG:O	2.51	0.44
1:T:263:ASN:HB2	1:T:275:TYR:CE2	2.53	0.44
1:D:627:THR:HG22	1:T:429:HIS:NE2	113.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:238:ASP:OD1	1:W:239:ARG:N	2.49	0.44
1:W:406:LEU:HD21	1:W:412:PHE:HB2	2.00	0.44
1:H:583:ALA:O	1:W:487:ARG:HD2	2.18	0.44
1:W:529:HIS:CE1	1:W:534:GLU:HA	2.53	0.44
1:X:557:TYR:HE1	1:X:562:LEU:HD11	1.82	0.44
1:Y:297:ARG:O	1:Y:300:GLN:N	2.48	0.44
1:Z:263:ASN:HB2	1:Z:275:TYR:CE2	2.53	0.44
1:Z:401:PHE:HE1	1:3:695:LYS:HB3	1.82	0.44
1:Z:695:LYS:HB3	1:4:401:PHE:HE1	1.83	0.44
1:1:464:LEU:HD23	1:2:554:ASN:HB3	1.98	0.44
1:3:251:PRO:HG3	1:3:374:MET:CE	2.47	0.44
1:4:247:THR:HG23	1:4:680:GLN:HE22	1.83	0.44
1:5:263:ASN:HB2	1:5:275:TYR:CE2	2.53	0.44
1:5:557:TYR:HE1	1:5:562:LEU:HD11	1.82	0.44
1:7:529:HIS:CE1	1:7:534:GLU:HA	2.53	0.44
1:7:616:LEU:HD22	1:7:729:ILE:HD12	1.99	0.44
1:A:263:ASN:HB2	1:A:275:TYR:CE2	2.53	0.44
1:A:401:PHE:HE1	1:I:695:LYS:HB3	1.83	0.44
1:B:464:LEU:HD23	1:J:554:ASN:HB3	1.99	0.44
1:C:406:LEU:HD21	1:C:412:PHE:HB2	2.00	0.44
1:B:627:THR:HG22	1:C:429:HIS:NE2	43.24	0.44
1:C:650:LEU:HD13	1:C:650:LEU:HA	1.87	0.44
1:D:529:HIS:CE1	1:D:534:GLU:HA	2.53	0.44
1:E:406:LEU:HD21	1:E:412:PHE:HB2	2.00	0.44
1:E:627:THR:HG22	1:F:429:HIS:NE2	2.32	0.44
1:G:263:ASN:HB2	1:G:275:TYR:CE2	2.53	0.44
1:A:481:LEU:HD11	1:G:636:LEU:HD11	2.00	0.44
1:H:282:TRP:NE1	1:H:398:LEU:HB2	2.32	0.44
1:L:247:THR:HG23	1:L:680:GLN:HE22	1.83	0.44
1:L:263:ASN:HB2	1:L:275:TYR:CE2	2.53	0.44
1:B:464:LEU:HD23	1:M:554:ASN:HB3	153.06	0.44
1:N:247:THR:HG23	1:N:680:GLN:HE22	1.83	0.44
1:O:464:LEU:HD23	1:P:554:ASN:HB3	100.68	0.44
1:Q:238:ASP:OD1	1:Q:239:ARG:N	2.49	0.44
1:Q:263:ASN:HB2	1:Q:275:TYR:CE2	2.53	0.44
1:R:554:ASN:HB3	1:U:464:LEU:HD23	1.99	0.44
1:Q:490:ARG:O	1:S:587:GLN:NE2	91.35	0.44
1:T:616:LEU:HD22	1:T:729:ILE:HD12	2.00	0.44
1:V:297:ARG:O	1:V:300:GLN:N	2.48	0.44
1:W:429:HIS:NE2	1:Y:627:THR:HG22	2.32	0.44
1:W:587:GLN:NE2	1:X:490:ARG:O	77.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:587:GLN:NE2	1:X:490:ARG:O	146.88	0.44
1:V:490:ARG:O	1:X:587:GLN:NE2	2.51	0.44
1:Z:627:THR:HG22	1:2:429:HIS:NE2	70.63	0.44
1:1:312:LYS:O	1:1:418:PHE:N	2.44	0.44
1:1:650:LEU:HA	1:1:650:LEU:HD13	1.86	0.44
1:4:238:ASP:OD1	1:4:239:ARG:N	2.49	0.44
1:4:282:TRP:NE1	1:4:398:LEU:HB2	2.32	0.44
1:4:557:TYR:HE1	1:4:562:LEU:HD11	1.82	0.44
1:6:464:LEU:HD23	1:7:554:ASN:HB3	1.99	0.44
1:6:529:HIS:CE1	1:6:534:GLU:HA	2.53	0.44
1:6:557:TYR:HE1	1:6:562:LEU:HD11	1.82	0.44
1:6:650:LEU:HD13	1:6:650:LEU:HA	1.86	0.44
1:7:247:THR:HG23	1:7:680:GLN:HE22	1.83	0.44
1:7:263:ASN:HB2	1:7:275:TYR:CE2	2.53	0.44
1:A:490:ARG:O	1:K:587:GLN:NE2	155.18	0.44
1:A:247:THR:HG23	1:A:680:GLN:HE22	1.83	0.44
1:B:251:PRO:HG3	1:B:374:MET:CE	2.47	0.44
1:D:429:HIS:NE2	1:L:627:THR:HG22	120.05	0.44
1:G:490:ARG:O	1:H:587:GLN:NE2	77.16	0.44
1:I:263:ASN:HB2	1:I:275:TYR:CE2	2.53	0.44
1:L:436:LEU:HD21	1:L:738:LEU:HD22	2.00	0.44
1:C:490:ARG:O	1:M:587:GLN:NE2	2.51	0.44
1:N:263:ASN:HB2	1:N:275:TYR:CE2	2.53	0.44
1:M:490:ARG:O	1:O:587:GLN:NE2	124.94	0.44
1:Q:587:GLN:NE2	1:R:490:ARG:O	77.17	0.44
1:T:247:THR:HG23	1:T:680:GLN:HE22	1.83	0.44
1:T:312:LYS:O	1:T:418:PHE:N	2.44	0.44
1:L:587:GLN:NE2	1:T:490:ARG:O	230.74	0.44
1:T:695:LYS:HB3	1:U:401:PHE:HE1	36.01	0.44
1:U:464:LEU:HD23	1:V:554:ASN:HB3	59.83	0.44
1:E:554:ASN:HB3	1:V:464:LEU:HD23	188.90	0.44
1:U:587:GLN:NE2	1:V:490:ARG:O	77.16	0.44
1:X:263:ASN:HB2	1:X:275:TYR:CE2	2.53	0.44
1:X:406:LEU:HD21	1:X:412:PHE:HB2	2.00	0.44
1:X:429:HIS:NE2	1:Y:627:THR:HG22	43.24	0.44
1:Z:247:THR:HG23	1:Z:680:GLN:HE22	1.83	0.44
1:Z:401:PHE:HE1	1:2:695:LYS:HB3	76.52	0.44
1:Z:610:GLN:HE21	1:4:627:THR:CG2	2.25	0.44
1:Z:416:TYR:OH	1:Z:644:HIS:O	2.33	0.44
1:Z:587:GLN:NE2	1:1:490:ARG:O	90.46	0.43
1:1:587:GLN:NE2	1:2:490:ARG:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:616:LEU:HD22	1:1:729:ILE:HD12	2.00	0.43
1:5:529:HIS:CE1	1:5:534:GLU:HA	2.53	0.43
1:6:263:ASN:HB2	1:6:275:TYR:CE2	2.53	0.43
1:A:650:LEU:HA	1:A:650:LEU:HD13	1.87	0.43
1:B:490:ARG:O	1:L:587:GLN:NE2	2.51	0.43
1:B:490:ARG:O	1:C:587:GLN:NE2	105.81	0.43
1:D:587:GLN:NE2	1:N:490:ARG:O	2.51	0.43
1:E:247:THR:HG23	1:E:680:GLN:HE22	1.83	0.43
1:E:554:ASN:HB3	1:F:464:LEU:HD23	1.99	0.43
1:E:436:LEU:HD21	1:E:738:LEU:HD22	2.01	0.43
1:F:247:THR:HG23	1:F:680:GLN:HE22	1.83	0.43
1:F:263:ASN:HB2	1:F:275:TYR:CE2	2.53	0.43
1:F:297:ARG:O	1:F:300:GLN:N	2.48	0.43
1:G:436:LEU:HD21	1:G:738:LEU:HD22	2.01	0.43
1:H:247:THR:HG23	1:H:680:GLN:HE22	1.83	0.43
1:I:435:ARG:HD3	1:I:435:ARG:HA	1.85	0.43
1:J:247:THR:HG23	1:J:680:GLN:HE22	1.83	0.43
1:K:247:THR:HG23	1:K:680:GLN:HE22	1.83	0.43
1:K:718:ASN:ND2	1:K:722:THR:HB	2.31	0.43
1:D:587:GLN:NE2	1:L:490:ARG:O	151.06	0.43
1:J:587:GLN:NE2	1:L:490:ARG:O	2.51	0.43
1:O:406:LEU:HD21	1:O:412:PHE:HB2	2.00	0.43
1:N:429:HIS:NE2	1:O:627:THR:HG22	60.25	0.43
1:R:247:THR:HG23	1:R:680:GLN:HE22	1.83	0.43
1:R:297:ARG:O	1:R:300:GLN:N	2.48	0.43
1:R:627:THR:HG22	1:U:429:HIS:NE2	2.32	0.43
1:E:490:ARG:O	1:V:587:GLN:NE2	176.96	0.43
1:Y:263:ASN:HB2	1:Y:275:TYR:CE2	2.53	0.43
1:W:385:ASN:ND2	1:Y:532:ASP:OD1	53.73	0.43
1:Z:436:LEU:HD21	1:Z:738:LEU:HD22	2.00	0.43
1:1:247:THR:HG23	1:1:680:GLN:HE22	1.83	0.43
1:3:627:THR:HG22	1:4:429:HIS:NE2	2.32	0.43
1:3:490:ARG:O	1:4:587:GLN:NE2	2.51	0.43
1:4:436:LEU:HD21	1:4:738:LEU:HD22	2.00	0.43
1:7:282:TRP:CD1	1:7:398:LEU:HD12	2.52	0.43
1:8:297:ARG:O	1:8:300:GLN:N	2.48	0.43
1:8:282:TRP:NE1	1:8:398:LEU:HB2	2.32	0.43
1:A:270:THR:HG23	1:A:272:ASP:H	1.84	0.43
1:C:436:LEU:HD21	1:C:738:LEU:HD22	2.00	0.43
1:D:292:CYS:SG	1:D:365:LEU:HB2	2.59	0.43
1:F:416:TYR:OH	1:F:644:HIS:O	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:436:LEU:HD21	1:I:738:LEU:HD22	2.01	0.43
1:J:263:ASN:HB2	1:J:275:TYR:CE2	2.53	0.43
1:K:406:LEU:HD21	1:K:412:PHE:HB2	2.00	0.43
1:M:247:THR:HG23	1:M:680:GLN:HE22	1.83	0.43
1:M:616:LEU:HD22	1:M:729:ILE:HD12	2.00	0.43
1:N:616:LEU:HD22	1:N:729:ILE:HD12	2.00	0.43
1:O:270:THR:HG23	1:O:272:ASP:H	1.84	0.43
1:C:401:PHE:HE1	1:P:695:LYS:HB3	43.72	0.43
1:R:263:ASN:HB2	1:R:275:TYR:CE2	2.53	0.43
1:S:263:ASN:HB2	1:S:275:TYR:CE2	2.53	0.43
1:D:487:ARG:HD2	1:T:583:ALA:O	145.92	0.43
1:V:263:ASN:HB2	1:V:275:TYR:CE2	2.53	0.43
1:V:270:THR:HG23	1:V:272:ASP:H	1.84	0.43
1:V:557:TYR:HE1	1:V:562:LEU:HD11	1.82	0.43
1:W:270:THR:HG23	1:W:272:ASP:H	1.84	0.43
1:H:587:GLN:NE2	1:W:490:ARG:O	2.51	0.43
1:W:436:LEU:HD21	1:W:738:LEU:HD22	2.00	0.43
1:X:247:THR:HG23	1:X:680:GLN:HE22	1.83	0.43
1:X:251:PRO:HG3	1:X:374:MET:CE	2.47	0.43
1:1:436:LEU:HD21	1:1:738:LEU:HD22	2.00	0.43
1:2:292:CYS:SG	1:2:365:LEU:HB2	2.59	0.43
1:6:247:THR:HG23	1:6:680:GLN:HE22	1.83	0.43
1:6:292:CYS:SG	1:6:365:LEU:HB2	2.59	0.43
1:6:297:ARG:O	1:6:300:GLN:N	2.48	0.43
1:5:695:LYS:HB3	1:6:401:PHE:HE1	1.82	0.43
1:8:247:THR:HG23	1:8:680:GLN:HE22	1.83	0.43
1:8:292:CYS:SG	1:8:365:LEU:HB2	2.59	0.43
1:A:292:CYS:SG	1:A:365:LEU:HB2	2.59	0.43
1:A:490:ARG:O	1:I:587:GLN:NE2	2.52	0.43
1:B:270:THR:HG23	1:B:272:ASP:H	1.84	0.43
1:B:292:CYS:SG	1:B:365:LEU:HB2	2.59	0.43
1:B:297:ARG:O	1:B:300:GLN:N	2.48	0.43
1:B:718:ASN:ND2	1:B:722:THR:HB	2.31	0.43
1:C:254:ASN:C	1:C:256:HIS:N	2.72	0.43
1:F:436:LEU:HD21	1:F:738:LEU:HD22	2.01	0.43
1:A:695:LYS:HB3	1:G:401:PHE:HE1	1.83	0.43
1:H:616:LEU:HD22	1:H:729:ILE:HD12	2.00	0.43
1:I:401:PHE:HE1	1:K:695:LYS:HB3	69.79	0.43
1:A:554:ASN:HB3	1:I:464:LEU:HD23	2.00	0.43
1:I:650:LEU:HD13	1:I:650:LEU:HA	1.86	0.43
1:I:616:LEU:HD22	1:I:729:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:292:CYS:SG	1:K:365:LEU:HB2	2.59	0.43
1:N:292:CYS:SG	1:N:365:LEU:HB2	2.59	0.43
1:N:587:GLN:NE2	1:O:490:ARG:O	77.16	0.43
1:N:436:LEU:HD21	1:N:738:LEU:HD22	2.00	0.43
1:O:587:GLN:NE2	1:P:490:ARG:O	105.80	0.43
1:P:292:CYS:SG	1:P:365:LEU:HB2	2.59	0.43
1:Q:270:THR:HG23	1:Q:272:ASP:H	1.84	0.43
1:R:292:CYS:SG	1:R:365:LEU:HB2	2.59	0.43
1:S:718:ASN:ND2	1:S:722:THR:HB	2.31	0.43
1:T:436:LEU:HD21	1:T:738:LEU:HD22	2.00	0.43
1:U:263:ASN:HB2	1:U:275:TYR:CE2	2.53	0.43
1:U:406:LEU:HD21	1:U:412:PHE:HB2	2.00	0.43
1:T:627:THR:HG22	1:V:429:HIS:NE2	99.34	0.43
1:H:464:LEU:HD23	1:W:554:ASN:HB3	2.00	0.43
1:W:490:ARG:O	1:Y:587:GLN:NE2	36.99	0.43
1:Z:490:ARG:O	1:3:587:GLN:NE2	2.51	0.43
1:Z:616:LEU:HD22	1:Z:729:ILE:HD12	2.00	0.43
1:2:718:ASN:ND2	1:2:722:THR:HB	2.31	0.43
1:4:263:ASN:HB2	1:4:275:TYR:CE2	2.53	0.43
1:5:292:CYS:SG	1:5:365:LEU:HB2	2.59	0.43
1:5:464:LEU:HD23	1:6:554:ASN:HB3	2.00	0.43
1:A:429:HIS:NE2	1:8:627:THR:HG22	136.96	0.43
1:D:406:LEU:HD21	1:D:412:PHE:HB2	2.00	0.43
1:D:464:LEU:HD23	1:N:554:ASN:HB3	1.99	0.43
1:F:254:ASN:C	1:F:256:HIS:N	2.72	0.43
1:F:292:CYS:SG	1:F:365:LEU:HB2	2.59	0.43
1:F:554:ASN:HB3	1:G:464:LEU:HD23	104.60	0.43
1:F:650:LEU:HA	1:F:650:LEU:HD13	1.86	0.43
1:G:401:PHE:HE1	1:H:695:LYS:HB3	42.81	0.43
1:I:254:ASN:C	1:I:256:HIS:N	2.72	0.43
1:J:292:CYS:SG	1:J:365:LEU:HB2	2.59	0.43
1:J:436:LEU:HD21	1:J:738:LEU:HD22	2.01	0.43
1:I:490:ARG:O	1:K:587:GLN:NE2	124.94	0.43
1:O:292:CYS:SG	1:O:365:LEU:HB2	2.59	0.43
1:E:587:GLN:NE2	1:Q:490:ARG:O	2.51	0.43
1:F:401:PHE:HE1	1:Q:695:LYS:HB3	1.83	0.43
1:Q:436:LEU:HD21	1:Q:738:LEU:HD22	2.00	0.43
1:R:628:ASP:OD2	1:U:425:SER:OG	2.30	0.43
1:S:247:THR:HG23	1:S:680:GLN:HE22	1.83	0.43
1:T:554:ASN:HB3	1:V:464:LEU:HD23	95.79	0.43
1:U:270:THR:HG23	1:U:272:ASP:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:292:CYS:SG	1:U:365:LEU:HB2	2.59	0.43
1:U:436:LEU:HD21	1:U:738:LEU:HD22	2.00	0.43
1:V:247:THR:HG23	1:V:680:GLN:HE22	1.83	0.43
1:Y:270:THR:HG23	1:Y:272:ASP:H	1.84	0.43
1:Y:292:CYS:SG	1:Y:365:LEU:HB2	2.59	0.43
1:Y:436:LEU:HD21	1:Y:738:LEU:HD22	2.00	0.43
1:2:251:PRO:HG3	1:2:374:MET:CE	2.47	0.43
1:2:436:LEU:HD21	1:2:738:LEU:HD22	2.01	0.43
1:3:406:LEU:HD21	1:3:412:PHE:HB2	2.00	0.43
1:Z:464:LEU:HD23	1:4:554:ASN:HB3	2.00	0.43
1:5:718:ASN:ND2	1:5:722:THR:HB	2.31	0.43
1:6:254:ASN:C	1:6:256:HIS:N	2.72	0.43
1:A:487:ARG:HD2	1:I:583:ALA:O	2.18	0.43
1:A:554:ASN:HB3	1:K:464:LEU:HD23	146.78	0.43
1:B:254:ASN:C	1:B:256:HIS:N	2.72	0.43
1:C:263:ASN:HB2	1:C:275:TYR:CE2	2.53	0.43
1:C:490:ARG:O	1:P:587:GLN:NE2	77.36	0.43
1:D:504:ALA:O	1:D:508:ALA:HB2	2.19	0.43
1:D:718:ASN:ND2	1:D:722:THR:HB	2.31	0.43
1:D:436:LEU:HD21	1:D:738:LEU:HD22	2.00	0.43
1:G:247:THR:HG23	1:G:680:GLN:HE22	1.83	0.43
1:H:263:ASN:HB2	1:H:275:TYR:CE2	2.53	0.43
1:H:718:ASN:ND2	1:H:722:THR:HB	2.31	0.43
1:K:650:LEU:HD13	1:K:650:LEU:HA	1.86	0.43
1:M:292:CYS:SG	1:M:365:LEU:HB2	2.59	0.43
1:P:247:THR:HG23	1:P:680:GLN:HE22	1.83	0.43
1:Q:254:ASN:C	1:Q:256:HIS:N	2.72	0.43
1:Q:292:CYS:SG	1:Q:365:LEU:HB2	2.59	0.43
1:S:406:LEU:HD21	1:S:412:PHE:HB2	2.00	0.43
1:S:436:LEU:HD21	1:S:738:LEU:HD22	2.00	0.43
1:T:650:LEU:HA	1:T:650:LEU:HD13	1.87	0.43
1:D:401:PHE:HE1	1:T:695:LYS:HB3	103.43	0.43
1:V:292:CYS:SG	1:V:365:LEU:HB2	2.59	0.43
1:V:436:LEU:HD21	1:V:738:LEU:HD22	2.01	0.43
1:Y:247:THR:HG23	1:Y:680:GLN:HE22	1.83	0.43
1:H:401:PHE:HE1	1:Y:695:LYS:HB3	1.83	0.43
1:2:270:THR:HG23	1:2:272:ASP:H	1.84	0.43
1:2:504:ALA:O	1:2:508:ALA:HB2	2.19	0.43
1:2:529:HIS:CE1	1:2:534:GLU:HA	2.53	0.43
1:2:622:ALA:HB3	1:2:635:PRO:HG3	2.01	0.43
1:7:312:LYS:O	1:7:418:PHE:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:490:ARG:O	1:7:587:GLN:NE2	2.51	0.43
1:8:616:LEU:HD22	1:8:729:ILE:HD12	1.99	0.43
1:A:504:ALA:O	1:A:508:ALA:HB2	2.19	0.43
1:B:247:THR:HG23	1:B:680:GLN:HE22	1.83	0.43
1:B:406:LEU:HD21	1:B:412:PHE:HB2	2.00	0.43
1:C:270:THR:HG23	1:C:272:ASP:H	1.84	0.43
1:D:270:THR:HG23	1:D:272:ASP:H	1.84	0.43
1:F:718:ASN:ND2	1:F:722:THR:HB	2.31	0.43
1:G:292:CYS:SG	1:G:365:LEU:HB2	2.59	0.43
1:G:435:ARG:HA	1:G:435:ARG:HD3	1.85	0.43
1:G:434:ASP:HB2	1:G:478:LYS:HE2	2.01	0.43
1:H:434:ASP:HB2	1:H:478:LYS:HE2	2.01	0.43
1:K:436:LEU:HD21	1:K:738:LEU:HD22	2.00	0.43
1:L:270:THR:HG23	1:L:272:ASP:H	1.84	0.43
1:L:504:ALA:O	1:L:508:ALA:HB2	2.19	0.43
1:N:461:GLN:H	1:N:461:GLN:CD	2.22	0.43
1:N:434:ASP:HB2	1:N:478:LYS:HE2	2.01	0.43
1:P:434:ASP:HB2	1:P:478:LYS:HE2	2.01	0.43
1:R:270:THR:HG23	1:R:272:ASP:H	1.84	0.43
1:R:434:ASP:HB2	1:R:478:LYS:HE2	2.01	0.43
1:S:270:THR:HG23	1:S:272:ASP:H	1.84	0.43
1:S:292:CYS:SG	1:S:365:LEU:HB2	2.59	0.43
1:S:434:ASP:HB2	1:S:478:LYS:HE2	2.01	0.43
1:T:270:THR:HG23	1:T:272:ASP:H	1.84	0.43
1:T:628:ASP:OD2	1:V:425:SER:OG	106.21	0.43
1:V:406:LEU:HD21	1:V:412:PHE:HB2	2.00	0.43
1:V:434:ASP:HB2	1:V:478:LYS:HE2	2.01	0.43
1:W:254:ASN:C	1:W:256:HIS:N	2.72	0.43
1:X:436:LEU:HD21	1:X:738:LEU:HD22	2.00	0.43
1:Z:292:CYS:SG	1:Z:365:LEU:HB2	2.59	0.43
1:Z:353:LEU:HG	1:Z:401:PHE:HE2	1.84	0.43
1:1:353:LEU:HG	1:1:401:PHE:HE2	1.84	0.43
1:2:406:LEU:HD21	1:2:412:PHE:HB2	2.00	0.43
1:2:461:GLN:CD	1:2:461:GLN:H	2.22	0.43
1:4:461:GLN:CD	1:4:461:GLN:H	2.22	0.43
1:4:434:ASP:HB2	1:4:478:LYS:HE2	2.01	0.43
1:5:401:PHE:HE1	1:7:695:LYS:HB3	1.83	0.43
1:A:254:ASN:C	1:A:256:HIS:N	2.72	0.43
1:A:353:LEU:HG	1:A:401:PHE:HE2	1.84	0.43
1:A:628:ASP:OD2	1:I:425:SER:OG	2.31	0.43
1:C:353:LEU:HG	1:C:401:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:ALA:O	1:C:508:ALA:HB2	2.19	0.43
1:D:434:ASP:HB2	1:D:478:LYS:HE2	2.01	0.43
1:D:622:ALA:HB3	1:D:635:PRO:HG3	2.01	0.43
1:E:292:CYS:SG	1:E:365:LEU:HB2	2.58	0.43
1:G:254:ASN:C	1:G:256:HIS:N	2.72	0.43
1:H:254:ASN:C	1:H:256:HIS:N	2.72	0.43
1:H:622:ALA:HB3	1:H:635:PRO:HG3	2.01	0.43
1:H:436:LEU:HD21	1:H:738:LEU:HD22	2.00	0.43
1:J:610:GLN:HE21	1:K:627:THR:CG2	61.64	0.43
1:J:622:ALA:HB3	1:J:635:PRO:HG3	2.01	0.43
1:K:254:ASN:C	1:K:256:HIS:N	2.72	0.43
1:K:263:ASN:HB2	1:K:275:TYR:CE2	2.53	0.43
1:K:270:THR:HG23	1:K:272:ASP:H	1.84	0.43
1:L:353:LEU:HG	1:L:401:PHE:HE2	1.84	0.43
1:D:464:LEU:HD23	1:L:554:ASN:HB3	153.07	0.43
1:M:270:THR:HG23	1:M:272:ASP:H	1.84	0.43
1:M:353:LEU:HG	1:M:401:PHE:HE2	1.84	0.43
1:M:504:ALA:O	1:M:508:ALA:HB2	2.19	0.43
1:N:270:THR:HG23	1:N:272:ASP:H	1.84	0.43
1:O:353:LEU:HG	1:O:401:PHE:HE2	1.84	0.43
1:P:353:LEU:HG	1:P:401:PHE:HE2	1.84	0.43
1:N:429:HIS:NE2	1:P:627:THR:HG22	2.32	0.43
1:Q:718:ASN:ND2	1:Q:722:THR:HB	2.31	0.43
1:R:436:LEU:HD21	1:R:738:LEU:HD22	2.00	0.43
1:T:401:PHE:HE1	1:V:695:LYS:HB3	69.79	0.43
1:T:434:ASP:HB2	1:T:478:LYS:HE2	2.01	0.43
1:U:434:ASP:HB2	1:U:478:LYS:HE2	2.01	0.43
1:U:512:HIS:CE1	1:U:515:GLY:HA2	2.54	0.43
1:V:353:LEU:HG	1:V:401:PHE:HE2	1.84	0.43
1:V:529:HIS:CE1	1:V:534:GLU:HA	2.53	0.43
1:W:292:CYS:SG	1:W:365:LEU:HB2	2.59	0.43
1:X:650:LEU:HA	1:X:650:LEU:HD13	1.87	0.43
1:Y:353:LEU:HG	1:Y:401:PHE:HE2	1.84	0.43
1:H:490:ARG:O	1:Y:587:GLN:NE2	2.51	0.43
1:Z:254:ASN:C	1:Z:256:HIS:N	2.72	0.43
1:Z:270:THR:HG23	1:Z:272:ASP:H	1.84	0.43
1:Z:490:ARG:O	1:2:587:GLN:NE2	108.74	0.43
1:3:622:ALA:HB3	1:3:635:PRO:HG3	2.01	0.43
1:3:436:LEU:HD21	1:3:738:LEU:HD22	2.00	0.43
1:4:616:LEU:HD22	1:4:729:ILE:HD12	2.00	0.43
1:5:512:HIS:CE1	1:5:515:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:436:LEU:HD21	1:8:738:LEU:HD22	2.00	0.43
1:A:434:ASP:HB2	1:A:478:LYS:HE2	2.01	0.43
1:A:512:HIS:CE1	1:A:515:GLY:HA2	2.54	0.43
1:A:627:THR:HG22	1:I:429:HIS:NE2	2.33	0.43
1:B:504:ALA:O	1:B:508:ALA:HB2	2.19	0.43
1:C:251:PRO:HG3	1:C:374:MET:CE	2.47	0.43
1:C:461:GLN:CD	1:C:461:GLN:H	2.22	0.43
1:E:695:LYS:HB3	1:Q:401:PHE:HE1	1.82	0.43
1:F:353:LEU:HG	1:F:401:PHE:HE2	1.84	0.43
1:F:434:ASP:HB2	1:F:478:LYS:HE2	2.01	0.43
1:F:622:ALA:HB3	1:F:635:PRO:HG3	2.01	0.43
1:G:512:HIS:CE1	1:G:515:GLY:HA2	2.54	0.43
1:H:270:THR:HG23	1:H:272:ASP:H	1.84	0.43
1:H:292:CYS:SG	1:H:365:LEU:HB2	2.59	0.43
1:H:406:LEU:HD21	1:H:412:PHE:HB2	2.00	0.43
1:G:695:LYS:HB3	1:I:401:PHE:HE1	1.83	0.43
1:I:461:GLN:CD	1:I:461:GLN:H	2.22	0.43
1:I:512:HIS:CE1	1:I:515:GLY:HA2	2.54	0.43
1:A:627:THR:CG2	1:I:610:GLN:HE21	2.26	0.43
1:J:270:THR:HG23	1:J:272:ASP:H	1.84	0.43
1:J:434:ASP:HB2	1:J:478:LYS:HE2	2.01	0.43
1:K:434:ASP:HB2	1:K:478:LYS:HE2	2.01	0.43
1:M:512:HIS:CE1	1:M:515:GLY:HA2	2.54	0.43
1:N:254:ASN:C	1:N:256:HIS:N	2.72	0.43
1:O:263:ASN:HB2	1:O:275:TYR:CE2	2.53	0.43
1:O:504:ALA:O	1:O:508:ALA:HB2	2.19	0.43
1:O:622:ALA:HB3	1:O:635:PRO:HG3	2.01	0.43
1:P:436:LEU:HD21	1:P:738:LEU:HD22	2.00	0.43
1:Q:353:LEU:HG	1:Q:401:PHE:HE2	1.84	0.43
1:Q:512:HIS:CE1	1:Q:515:GLY:HA2	2.54	0.43
1:R:512:HIS:CE1	1:R:515:GLY:HA2	2.54	0.43
1:T:353:LEU:HG	1:T:401:PHE:HE2	1.84	0.43
1:U:435:ARG:HD3	1:U:435:ARG:HA	1.85	0.43
1:R:401:PHE:HE1	1:U:695:LYS:HB3	1.82	0.43
1:V:512:HIS:CE1	1:V:515:GLY:HA2	2.54	0.43
1:W:247:THR:HG23	1:W:680:GLN:HE22	1.83	0.43
1:W:353:LEU:HG	1:W:401:PHE:HE2	1.84	0.43
1:X:353:LEU:HG	1:X:401:PHE:HE2	1.84	0.43
1:X:622:ALA:HB3	1:X:635:PRO:HG3	2.01	0.43
1:Z:504:ALA:O	1:Z:508:ALA:HB2	2.19	0.43
1:Z:512:HIS:CE1	1:Z:515:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:504:ALA:O	1:1:508:ALA:HB2	2.19	0.43
1:1:583:ALA:O	1:2:487:ARG:HD2	2.18	0.43
1:3:263:ASN:HB2	1:3:275:TYR:CE2	2.53	0.43
1:3:270:THR:HG23	1:3:272:ASP:H	1.84	0.43
1:3:297:ARG:O	1:3:300:GLN:N	2.48	0.43
1:3:353:LEU:HG	1:3:401:PHE:HE2	1.84	0.43
1:3:461:GLN:H	1:3:461:GLN:CD	2.22	0.43
1:4:270:THR:HG23	1:4:272:ASP:H	1.84	0.43
1:5:504:ALA:O	1:5:508:ALA:HB2	2.19	0.43
1:6:353:LEU:HG	1:6:401:PHE:HE2	1.84	0.43
1:6:718:ASN:ND2	1:6:722:THR:HB	2.31	0.43
1:7:406:LEU:HD21	1:7:412:PHE:HB2	2.00	0.43
1:8:353:LEU:HG	1:8:401:PHE:HE2	1.84	0.43
1:C:622:ALA:HB3	1:C:635:PRO:HG3	2.01	0.43
1:D:247:THR:HG23	1:D:680:GLN:HE22	1.83	0.43
1:D:461:GLN:CD	1:D:461:GLN:H	2.22	0.43
1:D:512:HIS:CE1	1:D:515:GLY:HA2	2.54	0.43
1:E:270:THR:HG23	1:E:272:ASP:H	1.84	0.43
1:I:353:LEU:HG	1:I:401:PHE:HE2	1.84	0.43
1:I:622:ALA:HB3	1:I:635:PRO:HG3	2.01	0.43
1:J:353:LEU:HG	1:J:401:PHE:HE2	1.84	0.43
1:K:512:HIS:CE1	1:K:515:GLY:HA2	2.54	0.43
1:L:286:ASP:O	1:L:364:CYS:HA	2.19	0.43
1:L:461:GLN:CD	1:L:461:GLN:H	2.22	0.43
1:L:512:HIS:CE1	1:L:515:GLY:HA2	2.54	0.43
1:O:254:ASN:C	1:O:256:HIS:N	2.72	0.43
1:O:297:ARG:O	1:O:300:GLN:N	2.48	0.43
1:O:436:LEU:HD21	1:O:738:LEU:HD22	2.00	0.43
1:O:434:ASP:HB2	1:O:478:LYS:HE2	2.01	0.43
1:O:512:HIS:CE1	1:O:515:GLY:HA2	2.54	0.43
1:Q:504:ALA:O	1:Q:508:ALA:HB2	2.19	0.43
1:S:622:ALA:HB3	1:S:635:PRO:HG3	2.01	0.43
1:U:461:GLN:H	1:U:461:GLN:CD	2.22	0.43
1:W:718:ASN:ND2	1:W:722:THR:HB	2.31	0.43
1:Y:254:ASN:C	1:Y:256:HIS:N	2.72	0.43
1:Y:512:HIS:CE1	1:Y:515:GLY:HA2	2.54	0.43
1:Z:286:ASP:O	1:Z:364:CYS:HA	2.19	0.43
1:Z:461:GLN:H	1:Z:461:GLN:CD	2.22	0.43
1:1:251:PRO:HG3	1:1:374:MET:CE	2.47	0.43
1:1:270:THR:HG23	1:1:272:ASP:H	1.84	0.43
1:1:610:GLN:HE21	1:2:627:THR:CG2	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:504:ALA:O	1:3:508:ALA:HB2	2.19	0.43
1:4:292:CYS:SG	1:4:365:LEU:HB2	2.59	0.43
1:4:552:ARG:NH1	1:4:553:ASP:OD2	2.52	0.43
1:6:270:THR:HG23	1:6:272:ASP:H	1.84	0.43
1:6:461:GLN:H	1:6:461:GLN:CD	2.22	0.43
1:6:552:ARG:NH1	1:6:553:ASP:OD2	2.52	0.43
1:7:434:ASP:HB2	1:7:478:LYS:HE2	2.01	0.43
1:A:286:ASP:O	1:A:364:CYS:HA	2.19	0.43
1:B:610:GLN:HE21	1:M:627:THR:CG2	97.92	0.43
1:B:416:TYR:OH	1:B:644:HIS:O	2.33	0.43
1:B:616:LEU:HD22	1:B:729:ILE:HD12	2.00	0.43
1:C:286:ASP:O	1:C:364:CYS:HA	2.19	0.43
1:D:650:LEU:HA	1:D:650:LEU:HD13	1.86	0.43
1:F:270:THR:HG23	1:F:272:ASP:H	1.84	0.43
1:F:461:GLN:H	1:F:461:GLN:CD	2.22	0.43
1:F:552:ARG:NH1	1:F:553:ASP:OD2	2.52	0.43
1:F:610:GLN:HE21	1:H:627:THR:CG2	119.92	0.43
1:G:270:THR:HG23	1:G:272:ASP:H	1.84	0.43
1:H:504:ALA:O	1:H:508:ALA:HB2	2.19	0.43
1:H:552:ARG:NH1	1:H:553:ASP:OD2	2.52	0.43
1:J:461:GLN:CD	1:J:461:GLN:H	2.22	0.43
1:J:512:HIS:CE1	1:J:515:GLY:HA2	2.54	0.43
1:K:435:ARG:HA	1:K:435:ARG:HD3	1.85	0.43
1:K:504:ALA:O	1:K:508:ALA:HB2	2.19	0.43
1:L:254:ASN:C	1:L:256:HIS:N	2.72	0.43
1:L:650:LEU:HA	1:L:650:LEU:HD13	1.86	0.43
1:M:461:GLN:H	1:M:461:GLN:CD	2.22	0.43
1:N:512:HIS:CE1	1:N:515:GLY:HA2	2.54	0.43
1:N:552:ARG:NH1	1:N:553:ASP:OD2	2.52	0.43
1:M:425:SER:OG	1:N:628:ASP:OD2	39.58	0.43
1:O:286:ASP:O	1:O:364:CYS:HA	2.19	0.43
1:O:461:GLN:H	1:O:461:GLN:CD	2.22	0.43
1:O:718:ASN:ND2	1:O:722:THR:HB	2.31	0.43
1:Q:247:THR:HG23	1:Q:680:GLN:HE22	1.83	0.43
1:R:622:ALA:HB3	1:R:635:PRO:HG3	2.01	0.43
1:S:504:ALA:O	1:S:508:ALA:HB2	2.19	0.43
1:T:504:ALA:O	1:T:508:ALA:HB2	2.19	0.43
1:U:247:THR:HG23	1:U:680:GLN:HE22	1.83	0.43
1:V:461:GLN:CD	1:V:461:GLN:H	2.22	0.43
1:V:552:ARG:NH1	1:V:553:ASP:OD2	2.52	0.43
1:V:616:LEU:HD22	1:V:729:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:292:CYS:SG	1:X:365:LEU:HB2	2.59	0.43
1:X:504:ALA:O	1:X:508:ALA:HB2	2.19	0.43
1:Y:622:ALA:HB3	1:Y:635:PRO:HG3	2.01	0.43
1:Z:622:ALA:HB3	1:Z:635:PRO:HG3	2.01	0.43
1:1:512:HIS:CE1	1:1:515:GLY:HA2	2.54	0.42
1:5:353:LEU:HG	1:5:401:PHE:HE2	1.84	0.42
1:5:552:ARG:NH1	1:5:553:ASP:OD2	2.52	0.42
1:5:436:LEU:HD21	1:5:738:LEU:HD22	2.00	0.42
1:6:610:GLN:HE21	1:7:627:THR:CG2	2.25	0.42
1:6:436:LEU:HD21	1:6:738:LEU:HD22	2.01	0.42
1:7:270:THR:HG23	1:7:272:ASP:H	1.84	0.42
1:7:552:ARG:NH1	1:7:553:ASP:OD2	2.52	0.42
1:A:436:LEU:HD21	1:A:738:LEU:HD22	2.00	0.42
1:B:512:HIS:CE1	1:B:515:GLY:HA2	2.54	0.42
1:B:436:LEU:HD21	1:B:738:LEU:HD22	2.00	0.42
1:C:292:CYS:SG	1:C:365:LEU:HB2	2.59	0.42
1:C:512:HIS:CE1	1:C:515:GLY:HA2	2.54	0.42
1:D:254:ASN:C	1:D:256:HIS:N	2.72	0.42
1:D:353:LEU:HG	1:D:401:PHE:HE2	1.84	0.42
1:E:434:ASP:HB2	1:E:478:LYS:HE2	2.01	0.42
1:E:552:ARG:NH1	1:E:553:ASP:OD2	2.52	0.42
1:F:512:HIS:CE1	1:F:515:GLY:HA2	2.54	0.42
1:G:353:LEU:HG	1:G:401:PHE:HE2	1.84	0.42
1:G:504:ALA:O	1:G:508:ALA:HB2	2.19	0.42
1:G:622:ALA:HB3	1:G:635:PRO:HG3	2.01	0.42
1:H:461:GLN:CD	1:H:461:GLN:H	2.22	0.42
1:H:512:HIS:CE1	1:H:515:GLY:HA2	2.54	0.42
1:I:270:THR:HG23	1:I:272:ASP:H	1.84	0.42
1:J:254:ASN:C	1:J:256:HIS:N	2.72	0.42
1:K:353:LEU:HG	1:K:401:PHE:HE2	1.84	0.42
1:L:292:CYS:SG	1:L:365:LEU:HB2	2.59	0.42
1:L:622:ALA:HB3	1:L:635:PRO:HG3	2.01	0.42
1:M:622:ALA:HB3	1:M:635:PRO:HG3	2.01	0.42
1:N:353:LEU:HG	1:N:401:PHE:HE2	1.84	0.42
1:P:622:ALA:HB3	1:P:635:PRO:HG3	2.01	0.42
1:N:481:LEU:HD11	1:P:636:LEU:HD11	2.01	0.42
1:Q:286:ASP:O	1:Q:364:CYS:HA	2.19	0.42
1:Q:552:ARG:NH1	1:Q:553:ASP:OD2	2.52	0.42
1:Q:622:ALA:HB3	1:Q:635:PRO:HG3	2.01	0.42
1:R:552:ARG:NH1	1:R:553:ASP:OD2	2.52	0.42
1:S:353:LEU:HG	1:S:401:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:512:HIS:CE1	1:S:515:GLY:HA2	2.54	0.42
1:S:552:ARG:NH1	1:S:553:ASP:OD2	2.52	0.42
1:T:512:HIS:CE1	1:T:515:GLY:HA2	2.54	0.42
1:U:254:ASN:ND2	1:U:377:GLN:HE22	2.18	0.42
1:U:353:LEU:HG	1:U:401:PHE:HE2	1.84	0.42
1:U:504:ALA:O	1:U:508:ALA:HB2	2.19	0.42
1:U:552:ARG:NH1	1:U:553:ASP:OD2	2.52	0.42
1:T:608:VAL:HG12	1:U:630:ASN:HB3	57.81	0.42
1:V:286:ASP:O	1:V:364:CYS:HA	2.19	0.42
1:V:254:ASN:ND2	1:V:377:GLN:HE22	2.18	0.42
1:V:435:ARG:HA	1:V:435:ARG:HD3	1.85	0.42
1:W:434:ASP:HB2	1:W:478:LYS:HE2	2.01	0.42
1:W:552:ARG:NH1	1:W:553:ASP:OD2	2.52	0.42
1:X:270:THR:HG23	1:X:272:ASP:H	1.84	0.42
1:Y:286:ASP:O	1:Y:364:CYS:HA	2.19	0.42
1:Y:435:ARG:HD3	1:Y:435:ARG:HA	1.85	0.42
1:2:512:HIS:CE1	1:2:515:GLY:HA2	2.54	0.42
1:1:429:HIS:NE2	1:2:627:THR:HG22	2.33	0.42
1:3:254:ASN:ND2	1:3:377:GLN:HE22	2.18	0.42
1:4:254:ASN:ND2	1:4:377:GLN:HE22	2.18	0.42
1:5:247:THR:HG23	1:5:680:GLN:HE22	1.83	0.42
1:6:416:TYR:OH	1:6:644:HIS:O	2.33	0.42
1:7:436:LEU:HD21	1:7:738:LEU:HD22	2.00	0.42
1:8:270:THR:HG23	1:8:272:ASP:H	1.84	0.42
1:8:254:ASN:ND2	1:8:377:GLN:HE22	2.18	0.42
1:8:406:LEU:HD21	1:8:412:PHE:HB2	2.00	0.42
1:C:247:THR:HG23	1:C:680:GLN:HE22	1.83	0.42
1:C:312:LYS:HD2	1:C:312:LYS:HA	1.89	0.42
1:C:552:ARG:NH1	1:C:553:ASP:OD2	2.52	0.42
1:D:503:PHE:HA	1:D:506:THR:OG1	2.20	0.42
1:E:718:ASN:ND2	1:E:722:THR:HB	2.31	0.42
1:G:254:ASN:ND2	1:G:377:GLN:HE22	2.17	0.42
1:G:286:ASP:O	1:G:364:CYS:HA	2.19	0.42
1:I:406:LEU:HD21	1:I:412:PHE:HB2	2.00	0.42
1:I:464:LEU:HD23	1:J:554:ASN:HB3	100.68	0.42
1:I:247:THR:HG23	1:I:680:GLN:HE22	1.83	0.42
1:J:503:PHE:HA	1:J:506:THR:OG1	2.20	0.42
1:J:504:ALA:O	1:J:508:ALA:HB2	2.19	0.42
1:J:552:ARG:NH1	1:J:553:ASP:OD2	2.52	0.42
1:K:286:ASP:O	1:K:364:CYS:HA	2.19	0.42
1:K:254:ASN:ND2	1:K:377:GLN:HE22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:461:GLN:H	1:K:461:GLN:CD	2.22	0.42
1:I:630:ASN:HB3	1:K:608:VAL:HG12	103.11	0.42
1:L:552:ARG:NH1	1:L:553:ASP:OD2	2.52	0.42
1:O:254:ASN:ND2	1:O:377:GLN:HE22	2.18	0.42
1:P:254:ASN:ND2	1:P:377:GLN:HE22	2.18	0.42
1:P:270:THR:HG23	1:P:272:ASP:H	1.84	0.42
1:P:286:ASP:O	1:P:364:CYS:HA	2.19	0.42
1:P:435:ARG:HA	1:P:435:ARG:HD3	1.85	0.42
1:P:504:ALA:O	1:P:508:ALA:HB2	2.19	0.42
1:Q:254:ASN:ND2	1:Q:377:GLN:HE22	2.18	0.42
1:R:353:LEU:HG	1:R:401:PHE:HE2	1.84	0.42
1:T:297:ARG:O	1:T:300:GLN:N	2.48	0.42
1:D:627:THR:CG2	1:T:610:GLN:HE21	116.27	0.42
1:W:286:ASP:O	1:W:364:CYS:HA	2.19	0.42
1:W:464:LEU:HD23	1:X:554:ASN:HB3	59.83	0.42
1:W:512:HIS:CE1	1:W:515:GLY:HA2	2.54	0.42
1:X:512:HIS:CE1	1:X:515:GLY:HA2	2.54	0.42
1:Y:552:ARG:NH1	1:Y:553:ASP:OD2	2.52	0.42
1:Z:254:ASN:ND2	1:Z:377:GLN:HE22	2.18	0.42
1:2:353:LEU:HG	1:2:401:PHE:HE2	1.84	0.42
1:3:286:ASP:O	1:3:364:CYS:HA	2.19	0.42
1:3:552:ARG:NH1	1:3:553:ASP:OD2	2.52	0.42
1:3:616:LEU:HD22	1:3:729:ILE:HD12	1.99	0.42
1:7:292:CYS:SG	1:7:365:LEU:HB2	2.59	0.42
1:A:622:ALA:HB3	1:A:635:PRO:HG3	2.01	0.42
1:A:718:ASN:ND2	1:A:722:THR:HB	2.31	0.42
1:B:434:ASP:HB2	1:B:478:LYS:HE2	2.01	0.42
1:D:434:ASP:N	1:D:434:ASP:OD1	2.53	0.42
1:E:254:ASN:ND2	1:E:377:GLN:HE22	2.18	0.42
1:E:434:ASP:OD1	1:E:434:ASP:N	2.53	0.42
1:E:461:GLN:CD	1:E:461:GLN:H	2.22	0.42
1:G:718:ASN:ND2	1:G:722:THR:HB	2.31	0.42
1:H:286:ASP:O	1:H:364:CYS:HA	2.20	0.42
1:I:292:CYS:SG	1:I:365:LEU:HB2	2.59	0.42
1:I:434:ASP:HB2	1:I:478:LYS:HE2	2.01	0.42
1:G:481:LEU:HD11	1:I:636:LEU:HD11	2.01	0.42
1:J:254:ASN:ND2	1:J:377:GLN:HE22	2.17	0.42
1:K:503:PHE:HA	1:K:506:THR:OG1	2.20	0.42
1:K:552:ARG:NH1	1:K:553:ASP:OD2	2.52	0.42
1:K:622:ALA:HB3	1:K:635:PRO:HG3	2.01	0.42
1:L:254:ASN:ND2	1:L:377:GLN:HE22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:254:ASN:ND2	1:M:377:GLN:HE22	2.18	0.42
1:M:552:ARG:NH1	1:M:553:ASP:OD2	2.52	0.42
1:M:436:LEU:HD21	1:M:738:LEU:HD22	2.01	0.42
1:N:254:ASN:ND2	1:N:377:GLN:HE22	2.18	0.42
1:N:504:ALA:O	1:N:508:ALA:HB2	2.19	0.42
1:O:552:ARG:NH1	1:O:553:ASP:OD2	2.52	0.42
1:Q:434:ASP:HB2	1:Q:478:LYS:HE2	2.01	0.42
1:R:504:ALA:O	1:R:508:ALA:HB2	2.19	0.42
1:Q:608:VAL:HG12	1:R:630:ASN:HB3	63.75	0.42
1:S:254:ASN:C	1:S:256:HIS:N	2.72	0.42
1:T:254:ASN:C	1:T:256:HIS:N	2.72	0.42
1:U:434:ASP:N	1:U:434:ASP:OD1	2.53	0.42
1:T:425:SER:OG	1:U:628:ASP:OD2	39.58	0.42
1:U:622:ALA:HB3	1:U:635:PRO:HG3	2.01	0.42
1:V:504:ALA:O	1:V:508:ALA:HB2	2.19	0.42
1:W:254:ASN:ND2	1:W:377:GLN:HE22	2.18	0.42
1:W:622:ALA:HB3	1:W:635:PRO:HG3	2.01	0.42
1:Y:434:ASP:HB2	1:Y:478:LYS:HE2	2.01	0.42
1:1:254:ASN:C	1:1:256:HIS:N	2.72	0.42
1:1:286:ASP:O	1:1:364:CYS:HA	2.19	0.42
1:1:297:ARG:O	1:1:300:GLN:N	2.48	0.42
1:2:434:ASP:N	1:2:434:ASP:OD1	2.53	0.42
1:2:434:ASP:HB2	1:2:478:LYS:HE2	2.01	0.42
1:2:552:ARG:NH1	1:2:553:ASP:OD2	2.52	0.42
1:4:251:PRO:HG3	1:4:374:MET:CE	2.47	0.42
1:4:504:ALA:O	1:4:508:ALA:HB2	2.19	0.42
1:4:622:ALA:HB3	1:4:635:PRO:HG3	2.01	0.42
1:4:650:LEU:HA	1:4:650:LEU:HD13	1.86	0.42
1:5:254:ASN:ND2	1:5:377:GLN:HE22	2.17	0.42
1:5:434:ASP:HB2	1:5:478:LYS:HE2	2.01	0.42
1:6:286:ASP:O	1:6:364:CYS:HA	2.19	0.42
1:7:254:ASN:ND2	1:7:377:GLN:HE22	2.18	0.42
1:7:353:LEU:HG	1:7:401:PHE:HE2	1.84	0.42
1:7:504:ALA:O	1:7:508:ALA:HB2	2.19	0.42
1:8:504:ALA:O	1:8:508:ALA:HB2	2.19	0.42
1:8:512:HIS:CE1	1:8:515:GLY:HA2	2.54	0.42
1:A:297:ARG:O	1:A:300:GLN:N	2.48	0.42
1:A:503:PHE:HA	1:A:506:THR:OG1	2.20	0.42
1:A:552:ARG:NH1	1:A:553:ASP:OD2	2.52	0.42
1:B:329:ASN:O	1:B:332:THR:OG1	2.21	0.42
1:B:435:ARG:HA	1:B:435:ARG:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:PHE:HA	1:B:506:THR:OG1	2.20	0.42
1:B:552:ARG:NH1	1:B:553:ASP:OD2	2.52	0.42
1:B:610:GLN:HE21	1:J:627:THR:CG2	2.25	0.42
1:D:254:ASN:ND2	1:D:377:GLN:HE22	2.18	0.42
1:D:286:ASP:O	1:D:364:CYS:HA	2.19	0.42
1:E:503:PHE:HA	1:E:506:THR:OG1	2.20	0.42
1:E:504:ALA:O	1:E:508:ALA:HB2	2.19	0.42
1:E:512:HIS:CE1	1:E:515:GLY:HA2	2.54	0.42
1:F:286:ASP:O	1:F:364:CYS:HA	2.19	0.42
1:F:503:PHE:HA	1:F:506:THR:OG1	2.20	0.42
1:G:552:ARG:NH1	1:G:553:ASP:OD2	2.52	0.42
1:I:286:ASP:O	1:I:364:CYS:HA	2.19	0.42
1:I:552:ARG:NH1	1:I:553:ASP:OD2	2.52	0.42
1:B:608:VAL:HG12	1:J:630:ASN:HB3	2.02	0.42
1:L:503:PHE:HA	1:L:506:THR:OG1	2.20	0.42
1:B:608:VAL:HG12	1:M:630:ASN:HB3	91.69	0.42
1:M:718:ASN:ND2	1:M:722:THR:HB	2.31	0.42
1:N:622:ALA:HB3	1:N:635:PRO:HG3	2.01	0.42
1:P:718:ASN:ND2	1:P:722:THR:HB	2.31	0.42
1:R:254:ASN:C	1:R:256:HIS:N	2.72	0.42
1:R:608:VAL:HG12	1:S:630:ASN:HB3	2.01	0.42
1:V:503:PHE:HA	1:V:506:THR:OG1	2.20	0.42
1:W:461:GLN:CD	1:W:461:GLN:H	2.22	0.42
1:W:608:VAL:HG12	1:Y:630:ASN:HB3	2.02	0.42
1:X:718:ASN:ND2	1:X:722:THR:HB	2.31	0.42
1:Y:503:PHE:HA	1:Y:506:THR:OG1	2.20	0.42
1:Z:552:ARG:NH1	1:Z:553:ASP:OD2	2.52	0.42
1:Z:608:VAL:HG12	1:1:630:ASN:HB3	80.17	0.42
1:Z:608:VAL:HG12	1:4:630:ASN:HB3	2.01	0.42
1:Z:718:ASN:ND2	1:Z:722:THR:HB	2.31	0.42
1:3:503:PHE:HA	1:3:506:THR:OG1	2.20	0.42
1:4:353:LEU:HG	1:4:401:PHE:HE2	1.84	0.42
1:5:406:LEU:HD21	1:5:412:PHE:HB2	2.00	0.42
1:6:504:ALA:O	1:6:508:ALA:HB2	2.19	0.42
1:7:254:ASN:C	1:7:256:HIS:N	2.72	0.42
1:7:512:HIS:CE1	1:7:515:GLY:HA2	2.54	0.42
1:D:608:VAL:HG12	1:L:630:ASN:HB3	120.14	0.42
1:E:254:ASN:C	1:E:256:HIS:N	2.72	0.42
1:E:286:ASP:O	1:E:364:CYS:HA	2.19	0.42
1:E:627:THR:CG2	1:F:610:GLN:HE21	2.25	0.42
1:G:284:TYR:HB3	1:G:650:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:435:ARG:HD3	1:H:435:ARG:HA	1.85	0.42
1:G:630:ASN:HB3	1:H:608:VAL:HG12	63.75	0.42
1:I:284:TYR:HB3	1:I:650:LEU:HD13	2.02	0.42
1:K:659:ASP:OD2	1:W:333:LYS:NZ	199.79	0.42
1:M:503:PHE:HA	1:M:506:THR:OG1	2.20	0.42
1:N:503:PHE:HA	1:N:506:THR:OG1	2.20	0.42
1:P:254:ASN:C	1:P:256:HIS:N	2.72	0.42
1:P:503:PHE:HA	1:P:506:THR:OG1	2.20	0.42
1:Q:434:ASP:OD1	1:Q:434:ASP:N	2.53	0.42
1:R:286:ASP:O	1:R:364:CYS:HA	2.19	0.42
1:S:254:ASN:ND2	1:S:377:GLN:HE22	2.18	0.42
1:T:286:ASP:O	1:T:364:CYS:HA	2.19	0.42
1:T:292:CYS:SG	1:T:365:LEU:HB2	2.59	0.42
1:V:622:ALA:HB3	1:V:635:PRO:HG3	2.01	0.42
1:X:254:ASN:ND2	1:X:377:GLN:HE22	2.18	0.42
1:Y:504:ALA:O	1:Y:508:ALA:HB2	2.19	0.42
1:Z:434:ASP:HB2	1:Z:478:LYS:HE2	2.01	0.42
1:Z:503:PHE:HA	1:Z:506:THR:OG1	2.20	0.42
1:1:328:GLN:NE2	1:1:333:LYS:HG3	2.23	0.42
1:2:247:THR:HG23	1:2:680:GLN:HE22	1.83	0.42
1:3:292:CYS:SG	1:3:365:LEU:HB2	2.59	0.42
1:5:286:ASP:O	1:5:364:CYS:HA	2.20	0.42
1:5:434:ASP:OD1	1:5:434:ASP:N	2.53	0.42
1:6:254:ASN:ND2	1:6:377:GLN:HE22	2.18	0.42
1:6:587:GLN:NE2	1:7:490:ARG:O	2.51	0.42
1:8:238:ASP:OD1	1:8:239:ARG:N	2.49	0.42
1:K:630:ASN:HB3	1:8:608:VAL:HG12	2.02	0.42
1:A:254:ASN:ND2	1:A:377:GLN:HE22	2.18	0.42
1:B:254:ASN:ND2	1:B:377:GLN:HE22	2.18	0.42
1:D:552:ARG:NH1	1:D:553:ASP:OD2	2.52	0.42
1:D:554:ASN:HB3	1:T:464:LEU:HD23	148.48	0.42
1:E:338:ASN:ND2	1:E:341:SER:OG	2.53	0.42
1:E:353:LEU:HG	1:E:401:PHE:HE2	1.84	0.42
1:F:312:LYS:O	1:F:418:PHE:N	2.44	0.42
1:F:254:ASN:ND2	1:F:377:GLN:HE22	2.17	0.42
1:F:504:ALA:O	1:F:508:ALA:HB2	2.19	0.42
1:G:503:PHE:HA	1:G:506:THR:OG1	2.20	0.42
1:H:608:VAL:HG12	1:W:630:ASN:HB3	2.02	0.42
1:I:254:ASN:ND2	1:I:377:GLN:HE22	2.18	0.42
1:I:503:PHE:HA	1:I:506:THR:OG1	2.20	0.42
1:K:434:ASP:OD1	1:K:434:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:434:ASP:HB2	1:L:478:LYS:HE2	2.01	0.42
1:M:284:TYR:HB3	1:M:650:LEU:HD13	2.02	0.42
1:M:286:ASP:O	1:M:364:CYS:HA	2.19	0.42
1:M:434:ASP:HB2	1:M:478:LYS:HE2	2.01	0.42
1:O:338:ASN:ND2	1:O:341:SER:OG	2.53	0.42
1:O:481:LEU:HD11	1:P:636:LEU:HD11	73.83	0.42
1:O:503:PHE:HA	1:O:506:THR:OG1	2.20	0.42
1:M:627:THR:CG2	1:O:610:GLN:HE21	101.45	0.42
1:P:338:ASN:ND2	1:P:341:SER:OG	2.53	0.42
1:P:512:HIS:CE1	1:P:515:GLY:HA2	2.54	0.42
1:D:630:ASN:HB3	1:P:608:VAL:HG12	2.02	0.42
1:R:254:ASN:ND2	1:R:377:GLN:HE22	2.17	0.42
1:R:503:PHE:HA	1:R:506:THR:OG1	2.20	0.42
1:S:284:TYR:HB3	1:S:650:LEU:HD13	2.02	0.42
1:R:425:SER:OG	1:S:628:ASP:OD2	2.30	0.42
1:X:552:ARG:NH1	1:X:553:ASP:OD2	2.52	0.42
1:Y:434:ASP:OD1	1:Y:434:ASP:N	2.53	0.42
1:Z:630:ASN:HB3	1:2:608:VAL:HG12	73.93	0.42
1:Z:284:TYR:HB3	1:Z:650:LEU:HD13	2.02	0.42
1:1:292:CYS:SG	1:1:365:LEU:HB2	2.59	0.42
1:1:503:PHE:HA	1:1:506:THR:OG1	2.20	0.42
1:2:286:ASP:O	1:2:364:CYS:HA	2.19	0.42
1:2:290:PHE:HB2	1:2:616:LEU:O	2.20	0.42
1:3:338:ASN:ND2	1:3:341:SER:OG	2.53	0.42
1:3:512:HIS:CE1	1:3:515:GLY:HA2	2.54	0.42
1:4:512:HIS:CE1	1:4:515:GLY:HA2	2.54	0.42
1:5:461:GLN:H	1:5:461:GLN:CD	2.22	0.42
1:5:503:PHE:HA	1:5:506:THR:OG1	2.20	0.42
1:7:286:ASP:O	1:7:364:CYS:HA	2.19	0.42
1:7:338:ASN:ND2	1:7:341:SER:OG	2.53	0.42
1:7:503:PHE:HA	1:7:506:THR:OG1	2.20	0.42
1:8:503:PHE:HA	1:8:506:THR:OG1	2.20	0.42
1:A:338:ASN:ND2	1:A:341:SER:OG	2.53	0.42
1:A:481:LEU:HD11	1:8:636:LEU:HD11	144.85	0.42
1:C:254:ASN:ND2	1:C:377:GLN:HE22	2.17	0.42
1:D:312:LYS:O	1:D:418:PHE:N	2.44	0.42
1:F:338:ASN:ND2	1:F:341:SER:OG	2.53	0.42
1:G:338:ASN:ND2	1:G:341:SER:OG	2.53	0.42
1:H:284:TYR:HB3	1:H:650:LEU:HD13	2.02	0.42
1:H:353:LEU:HG	1:H:401:PHE:HE2	1.84	0.42
1:H:630:ASN:HB3	1:Y:608:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:ASP:O	1:J:364:CYS:HA	2.19	0.42
1:J:481:LEU:HD11	1:K:636:LEU:HD11	65.47	0.42
1:J:284:TYR:HB3	1:J:650:LEU:HD13	2.02	0.42
1:L:608:VAL:HG12	1:T:630:ASN:HB3	190.77	0.42
1:M:481:LEU:HD11	1:N:636:LEU:HD11	73.84	0.42
1:N:286:ASP:O	1:N:364:CYS:HA	2.20	0.42
1:P:552:ARG:NH1	1:P:553:ASP:OD2	2.52	0.42
1:Q:284:TYR:HB3	1:Q:650:LEU:HD13	2.02	0.42
1:Q:461:GLN:CD	1:Q:461:GLN:H	2.22	0.42
1:E:481:LEU:HD11	1:Q:636:LEU:HD11	2.02	0.42
1:R:312:LYS:O	1:R:418:PHE:N	2.44	0.42
1:R:434:ASP:OD1	1:R:434:ASP:N	2.53	0.42
1:Q:630:ASN:HB3	1:S:608:VAL:HG12	82.44	0.42
1:T:254:ASN:ND2	1:T:377:GLN:HE22	2.18	0.42
1:T:503:PHE:HA	1:T:506:THR:OG1	2.20	0.42
1:U:286:ASP:O	1:U:364:CYS:HA	2.19	0.42
1:G:224:SER:C	1:W:407:ARG:HD2	2.40	0.42
1:X:328:GLN:NE2	1:X:333:LYS:HG3	2.23	0.42
1:X:503:PHE:HA	1:X:506:THR:OG1	2.20	0.42
1:Y:254:ASN:ND2	1:Y:377:GLN:HE22	2.17	0.42
1:Z:636:LEU:HD11	1:2:481:LEU:HD11	88.04	0.42
1:Z:650:LEU:HD13	1:Z:650:LEU:HA	1.86	0.42
1:Z:627:THR:CG2	1:3:610:GLN:HE21	2.25	0.42
1:4:338:ASN:ND2	1:4:341:SER:OG	2.53	0.42
1:4:503:PHE:HA	1:4:506:THR:OG1	2.20	0.42
1:5:284:TYR:HB3	1:5:650:LEU:HD13	2.02	0.42
1:5:312:LYS:O	1:5:418:PHE:N	2.44	0.42
1:6:338:ASN:ND2	1:6:341:SER:OG	2.53	0.42
1:O:333:LYS:NZ	1:7:659:ASP:OD2	188.46	0.42
1:8:338:ASN:ND2	1:8:341:SER:OG	2.53	0.42
1:C:284:TYR:HB3	1:C:650:LEU:HD13	2.02	0.42
1:C:290:PHE:HB2	1:C:616:LEU:O	2.20	0.42
1:D:290:PHE:HB2	1:D:616:LEU:O	2.20	0.42
1:E:490:ARG:O	1:F:587:GLN:NE2	2.51	0.42
1:H:338:ASN:ND2	1:H:341:SER:OG	2.53	0.42
1:H:434:ASP:OD1	1:H:434:ASP:N	2.53	0.42
1:I:338:ASN:ND2	1:I:341:SER:OG	2.53	0.42
1:I:504:ALA:O	1:I:508:ALA:HB2	2.19	0.42
1:J:338:ASN:ND2	1:J:341:SER:OG	2.53	0.42
1:K:290:PHE:HB2	1:K:616:LEU:O	2.20	0.42
1:L:338:ASN:ND2	1:L:341:SER:OG	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:338:ASN:ND2	1:N:341:SER:OG	2.53	0.42
1:P:650:LEU:HD13	1:P:650:LEU:HA	1.86	0.42
1:Q:503:PHE:HA	1:Q:506:THR:OG1	2.20	0.42
1:Q:628:ASP:OD2	1:S:425:SER:OG	87.28	0.42
1:R:338:ASN:ND2	1:R:341:SER:OG	2.53	0.42
1:U:338:ASN:ND2	1:U:341:SER:OG	2.53	0.42
1:V:290:PHE:HB2	1:V:616:LEU:O	2.20	0.42
1:V:434:ASP:OD1	1:V:434:ASP:N	2.53	0.42
1:W:503:PHE:HA	1:W:506:THR:OG1	2.20	0.42
1:X:254:ASN:C	1:X:256:HIS:N	2.72	0.42
1:X:481:LEU:HD11	1:Y:636:LEU:HD11	73.83	0.42
1:Y:284:TYR:HB3	1:Y:650:LEU:HD13	2.02	0.42
1:Y:338:ASN:ND2	1:Y:341:SER:OG	2.53	0.42
1:Y:461:GLN:H	1:Y:461:GLN:CD	2.22	0.42
1:Z:338:ASN:ND2	1:Z:341:SER:OG	2.53	0.42
1:2:254:ASN:C	1:2:256:HIS:N	2.72	0.42
1:3:434:ASP:HB2	1:3:478:LYS:HE2	2.01	0.42
1:5:636:LEU:HD11	1:7:481:LEU:HD11	2.02	0.42
1:6:512:HIS:CE1	1:6:515:GLY:HA2	2.54	0.42
1:8:552:ARG:NH1	1:8:553:ASP:OD2	2.52	0.42
1:C:338:ASN:ND2	1:C:341:SER:OG	2.53	0.42
1:E:622:ALA:HB3	1:E:635:PRO:HG3	2.01	0.42
1:F:284:TYR:HB3	1:F:650:LEU:HD13	2.02	0.42
1:F:627:THR:CG2	1:G:610:GLN:HE21	86.13	0.42
1:A:429:HIS:NE2	1:G:627:THR:HG22	2.35	0.42
1:M:338:ASN:ND2	1:M:341:SER:OG	2.53	0.42
1:M:608:VAL:HG12	1:N:630:ASN:HB3	57.80	0.42
1:M:290:PHE:HB2	1:M:616:LEU:O	2.20	0.42
1:C:608:VAL:HG12	1:O:630:ASN:HB3	131.98	0.42
1:Q:312:LYS:O	1:Q:418:PHE:N	2.44	0.42
1:R:461:GLN:H	1:R:461:GLN:CD	2.22	0.42
1:S:338:ASN:ND2	1:S:341:SER:OG	2.53	0.42
1:S:434:ASP:OD1	1:S:434:ASP:N	2.53	0.42
1:S:435:ARG:HD3	1:S:435:ARG:HA	1.85	0.42
1:D:630:ASN:HB3	1:T:608:VAL:HG12	114.85	0.42
1:V:338:ASN:ND2	1:V:341:SER:OG	2.53	0.42
1:W:338:ASN:ND2	1:W:341:SER:OG	2.53	0.42
1:W:504:ALA:O	1:W:508:ALA:HB2	2.19	0.42
1:H:425:SER:OG	1:W:628:ASP:OD2	2.30	0.42
1:Y:290:PHE:HB2	1:Y:616:LEU:O	2.20	0.42
1:1:338:ASN:ND2	1:1:341:SER:OG	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:416:TYR:OH	1:1:644:HIS:O	2.33	0.42
1:2:224:SER:C	1:3:407:ARG:HD2	2.41	0.42
1:2:503:PHE:HA	1:2:506:THR:OG1	2.20	0.42
1:3:284:TYR:HB3	1:3:650:LEU:HD13	2.02	0.42
1:5:610:GLN:HE21	1:6:627:THR:CG2	2.25	0.42
1:8:435:ARG:HA	1:8:435:ARG:HD3	1.85	0.42
1:8:434:ASP:HB2	1:8:478:LYS:HE2	2.01	0.42
1:B:353:LEU:HG	1:B:401:PHE:HE2	1.84	0.42
1:B:622:ALA:HB3	1:B:635:PRO:HG3	2.01	0.42
1:D:636:LEU:HD11	1:P:481:LEU:HD11	2.02	0.42
1:H:290:PHE:HB2	1:H:616:LEU:O	2.20	0.42
1:F:608:VAL:HG12	1:H:630:ASN:HB3	120.14	0.42
1:I:610:GLN:HE21	1:J:627:THR:CG2	45.56	0.42
1:J:434:ASP:OD1	1:J:434:ASP:N	2.53	0.42
1:J:718:ASN:ND2	1:J:722:THR:HB	2.31	0.42
1:K:338:ASN:ND2	1:K:341:SER:OG	2.53	0.42
1:L:290:PHE:HB2	1:L:616:LEU:O	2.20	0.42
1:L:284:TYR:HB3	1:L:650:LEU:HD13	2.02	0.42
1:O:290:PHE:HB2	1:O:616:LEU:O	2.20	0.42
1:O:284:TYR:HB3	1:O:650:LEU:HD13	2.02	0.42
1:R:284:TYR:HB3	1:R:650:LEU:HD13	2.02	0.42
1:T:338:ASN:ND2	1:T:341:SER:OG	2.53	0.42
1:T:290:PHE:HB2	1:T:616:LEU:O	2.20	0.42
1:U:254:ASN:C	1:U:256:HIS:N	2.72	0.42
1:U:503:PHE:HA	1:U:506:THR:OG1	2.20	0.42
1:W:434:ASP:OD1	1:W:434:ASP:N	2.53	0.42
1:X:434:ASP:HB2	1:X:478:LYS:HE2	2.01	0.42
1:X:290:PHE:HB2	1:X:616:LEU:O	2.20	0.42
1:Z:290:PHE:HB2	1:Z:616:LEU:O	2.20	0.42
1:1:290:PHE:HB2	1:1:616:LEU:O	2.20	0.41
1:3:290:PHE:HB2	1:3:616:LEU:O	2.20	0.41
1:Z:630:ASN:HB3	1:3:608:VAL:HG12	2.02	0.41
1:4:254:ASN:C	1:4:256:HIS:N	2.72	0.41
1:4:286:ASP:O	1:4:364:CYS:HA	2.19	0.41
1:5:270:THR:HG23	1:5:272:ASP:H	1.83	0.41
1:6:608:VAL:HG12	1:7:630:ASN:HB3	2.02	0.41
1:8:254:ASN:C	1:8:256:HIS:N	2.72	0.41
1:D:407:ARG:HD2	1:S:224:SER:C	94.50	0.41
1:E:481:LEU:HD11	1:X:636:LEU:HD11	137.26	0.41
1:H:254:ASN:ND2	1:H:377:GLN:HE22	2.17	0.41
1:J:608:VAL:HG12	1:K:630:ASN:HB3	63.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:636:LEU:HD11	1:8:481:LEU:HD11	2.02	0.41
1:M:434:ASP:OD1	1:M:434:ASP:N	2.53	0.41
1:C:636:LEU:HD11	1:M:481:LEU:HD11	2.02	0.41
1:M:630:ASN:HB3	1:O:608:VAL:HG12	103.11	0.41
1:B:481:LEU:HD11	1:M:636:LEU:HD11	103.61	0.41
1:D:481:LEU:HD11	1:N:636:LEU:HD11	2.02	0.41
1:P:290:PHE:HB2	1:P:616:LEU:O	2.20	0.41
1:Q:290:PHE:HB2	1:Q:616:LEU:O	2.20	0.41
1:F:627:THR:CG2	1:Q:610:GLN:HE21	2.25	0.41
1:T:284:TYR:HB3	1:T:650:LEU:HD13	2.02	0.41
1:U:290:PHE:HB2	1:U:616:LEU:O	2.20	0.41
1:U:284:TYR:HB3	1:U:650:LEU:HD13	2.02	0.41
1:V:284:TYR:HB3	1:V:650:LEU:HD13	2.02	0.41
1:T:630:ASN:HB3	1:V:608:VAL:HG12	103.11	0.41
1:V:636:LEU:HD11	1:X:481:LEU:HD11	2.02	0.41
1:H:636:LEU:HD11	1:Y:481:LEU:HD11	2.02	0.41
1:1:552:ARG:NH1	1:1:553:ASP:OD2	2.52	0.41
1:1:622:ALA:HB3	1:1:635:PRO:HG3	2.01	0.41
1:5:297:ARG:O	1:5:300:GLN:N	2.48	0.41
1:5:338:ASN:ND2	1:5:341:SER:OG	2.53	0.41
1:6:290:PHE:HB2	1:6:616:LEU:O	2.20	0.41
1:A:284:TYR:HB3	1:A:650:LEU:HD13	2.02	0.41
1:A:435:ARG:HA	1:A:435:ARG:HD3	1.85	0.41
1:B:286:ASP:O	1:B:364:CYS:HA	2.19	0.41
1:B:284:TYR:HB3	1:B:650:LEU:HD13	2.02	0.41
1:D:481:LEU:HD11	1:L:636:LEU:HD11	129.47	0.41
1:E:610:GLN:HE21	1:Q:627:THR:CG2	2.25	0.41
1:F:290:PHE:HB2	1:F:616:LEU:O	2.20	0.41
1:H:503:PHE:HA	1:H:506:THR:OG1	2.20	0.41
1:J:481:LEU:HD11	1:L:636:LEU:HD11	2.02	0.41
1:J:290:PHE:HB2	1:J:616:LEU:O	2.20	0.41
1:I:608:VAL:HG12	1:J:630:ASN:HB3	57.80	0.41
1:M:636:LEU:HD11	1:O:481:LEU:HD11	106.79	0.41
1:P:434:ASP:OD1	1:P:434:ASP:N	2.53	0.41
1:Q:338:ASN:ND2	1:Q:341:SER:OG	2.53	0.41
1:F:636:LEU:HD11	1:Q:481:LEU:HD11	2.02	0.41
1:S:503:PHE:HA	1:S:506:THR:OG1	2.20	0.41
1:S:290:PHE:HB2	1:S:616:LEU:O	2.20	0.41
1:T:622:ALA:HB3	1:T:635:PRO:HG3	2.01	0.41
1:U:608:VAL:HG12	1:V:630:ASN:HB3	63.75	0.41
1:W:290:PHE:HB2	1:W:616:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:434:ASP:OD1	1:X:434:ASP:N	2.53	0.41
1:W:481:LEU:HD11	1:Y:636:LEU:HD11	2.02	0.41
1:Z:312:LYS:O	1:Z:418:PHE:N	2.44	0.41
1:1:608:VAL:HG12	1:2:630:ASN:HB3	2.02	0.41
1:6:503:PHE:HA	1:6:506:THR:OG1	2.20	0.41
1:7:284:TYR:HB3	1:7:650:LEU:HD13	2.02	0.41
1:8:434:ASP:N	1:8:434:ASP:OD1	2.53	0.41
1:A:290:PHE:HB2	1:A:616:LEU:O	2.20	0.41
1:C:636:LEU:HD11	1:P:481:LEU:HD11	66.89	0.41
1:D:490:ARG:HB2	1:D:576:THR:HB	2.03	0.41
1:E:284:TYR:HB3	1:E:650:LEU:HD13	2.02	0.41
1:G:608:VAL:HG12	1:I:630:ASN:HB3	2.02	0.41
1:G:290:PHE:HB2	1:G:616:LEU:O	2.20	0.41
1:G:636:LEU:HD11	1:H:481:LEU:HD11	65.47	0.41
1:B:481:LEU:HD11	1:J:636:LEU:HD11	2.02	0.41
1:L:297:ARG:O	1:L:300:GLN:N	2.48	0.41
1:M:254:ASN:C	1:M:256:HIS:N	2.72	0.41
1:O:435:ARG:HA	1:O:435:ARG:HD3	1.85	0.41
1:P:284:TYR:HB3	1:P:650:LEU:HD13	2.02	0.41
1:R:630:ASN:HB3	1:U:608:VAL:HG12	2.02	0.41
1:S:650:LEU:HA	1:S:650:LEU:HD13	1.86	0.41
1:T:552:ARG:NH1	1:T:553:ASP:OD2	2.52	0.41
1:E:407:ARG:HD2	1:U:224:SER:C	145.23	0.41
1:S:481:LEU:HD11	1:U:636:LEU:HD11	2.01	0.41
1:X:338:ASN:ND2	1:X:341:SER:OG	2.53	0.41
1:Z:636:LEU:HD11	1:3:481:LEU:HD11	2.02	0.41
1:1:254:ASN:ND2	1:1:377:GLN:HE22	2.18	0.41
1:2:338:ASN:ND2	1:2:341:SER:OG	2.53	0.41
1:2:490:ARG:HB2	1:2:576:THR:HB	2.03	0.41
1:3:490:ARG:HB2	1:3:576:THR:HB	2.03	0.41
1:6:434:ASP:HB2	1:6:478:LYS:HE2	2.01	0.41
1:7:461:GLN:CD	1:7:461:GLN:H	2.22	0.41
1:7:290:PHE:HB2	1:7:616:LEU:O	2.20	0.41
1:7:622:ALA:HB3	1:7:635:PRO:HG3	2.01	0.41
1:8:286:ASP:O	1:8:364:CYS:HA	2.19	0.41
1:A:407:ARG:HD2	1:B:224:SER:C	2.41	0.41
1:C:503:PHE:HA	1:C:506:THR:OG1	2.20	0.41
1:B:630:ASN:HB3	1:C:608:VAL:HG12	57.80	0.41
1:D:338:ASN:ND2	1:D:341:SER:OG	2.53	0.41
1:E:290:PHE:HB2	1:E:616:LEU:O	2.20	0.41
1:E:630:ASN:HB3	1:V:608:VAL:HG12	120.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:630:ASN:HB3	1:F:608:VAL:HG12	2.02	0.41
1:I:290:PHE:HB2	1:I:616:LEU:O	2.20	0.41
1:I:432:SER:HA	1:I:570:THR:HB	2.03	0.41
1:K:432:SER:HA	1:K:570:THR:HB	2.03	0.41
1:K:628:ASP:OD2	1:8:425:SER:OG	2.30	0.41
1:L:260:GLN:NE2	1:L:276:PHE:CE1	2.88	0.41
1:B:630:ASN:HB3	1:L:608:VAL:HG12	2.01	0.41
1:M:446:TYR:CE1	1:M:467:GLN:HG3	2.56	0.41
1:M:432:SER:HA	1:M:570:THR:HB	2.03	0.41
1:N:284:TYR:HB3	1:N:650:LEU:HD13	2.02	0.41
1:N:290:PHE:HB2	1:N:616:LEU:O	2.20	0.41
1:O:490:ARG:HB2	1:O:576:THR:HB	2.03	0.41
1:R:290:PHE:HB2	1:R:616:LEU:O	2.20	0.41
1:Q:481:LEU:HD11	1:R:636:LEU:HD11	65.48	0.41
1:S:286:ASP:O	1:S:364:CYS:HA	2.19	0.41
1:M:224:SER:C	1:S:407:ARG:HD2	100.54	0.41
1:S:490:ARG:HB2	1:S:576:THR:HB	2.03	0.41
1:U:490:ARG:HB2	1:U:576:THR:HB	2.03	0.41
1:V:432:SER:HA	1:V:570:THR:HB	2.03	0.41
1:V:490:ARG:HB2	1:V:576:THR:HB	2.03	0.41
1:V:630:ASN:HB3	1:X:608:VAL:HG12	2.02	0.41
1:W:446:TYR:CE1	1:W:467:GLN:HG3	2.56	0.41
1:X:432:SER:HA	1:X:570:THR:HB	2.03	0.41
1:Y:490:ARG:HB2	1:Y:576:THR:HB	2.03	0.41
1:W:630:ASN:HB3	1:Y:608:VAL:HG12	18.45	0.41
1:Z:260:GLN:NE2	1:Z:276:PHE:CE1	2.88	0.41
1:Z:432:SER:HA	1:Z:570:THR:HB	2.03	0.41
1:2:432:SER:HA	1:2:570:THR:HB	2.03	0.41
1:5:622:ALA:HB3	1:5:635:PRO:HG3	2.01	0.41
1:6:312:LYS:HA	1:6:312:LYS:HD2	1.88	0.41
1:8:432:SER:HA	1:8:570:THR:HB	2.03	0.41
1:B:338:ASN:ND2	1:B:341:SER:OG	2.53	0.41
1:B:636:LEU:HD11	1:L:481:LEU:HD11	2.02	0.41
1:B:659:ASP:OD1	1:B:659:ASP:N	2.54	0.41
1:C:434:ASP:HB2	1:C:478:LYS:HE2	2.01	0.41
1:C:490:ARG:HB2	1:C:576:THR:HB	2.03	0.41
1:F:630:ASN:HB3	1:G:608:VAL:HG12	82.44	0.41
1:G:434:ASP:OD1	1:G:434:ASP:N	2.53	0.41
1:H:446:TYR:CE1	1:H:467:GLN:HG3	2.56	0.41
1:H:432:SER:HA	1:H:570:THR:HB	2.03	0.41
1:J:224:SER:C	1:X:407:ARG:HD2	111.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:446:TYR:CE1	1:J:467:GLN:HG3	2.56	0.41
1:L:718:ASN:ND2	1:L:722:THR:HB	2.31	0.41
1:N:435:ARG:HA	1:N:435:ARG:HD3	1.85	0.41
1:C:481:LEU:HD11	1:O:636:LEU:HD11	136.13	0.41
1:Q:446:TYR:CE1	1:Q:467:GLN:HG3	2.56	0.41
1:Q:490:ARG:HB2	1:Q:576:THR:HB	2.03	0.41
1:R:636:LEU:HD11	1:U:481:LEU:HD11	2.01	0.41
1:R:650:LEU:HD13	1:R:650:LEU:HA	1.86	0.41
1:T:718:ASN:ND2	1:T:722:THR:HB	2.31	0.41
1:U:446:TYR:CE1	1:U:467:GLN:HG3	2.56	0.41
1:U:432:SER:HA	1:U:570:THR:HB	2.03	0.41
1:V:254:ASN:C	1:V:256:HIS:N	2.72	0.41
1:V:446:TYR:CE1	1:V:467:GLN:HG3	2.56	0.41
1:X:286:ASP:O	1:X:364:CYS:HA	2.19	0.41
1:X:490:ARG:HB2	1:X:576:THR:HB	2.03	0.41
1:Z:446:TYR:CE1	1:Z:467:GLN:HG3	2.56	0.41
1:Z:481:LEU:HD11	1:4:636:LEU:HD11	2.03	0.41
1:1:434:ASP:HB2	1:1:478:LYS:HE2	2.01	0.41
1:1:284:TYR:HB3	1:1:650:LEU:HD13	2.02	0.41
1:3:446:TYR:CE1	1:3:467:GLN:HG3	2.56	0.41
1:4:446:TYR:CE1	1:4:467:GLN:HG3	2.56	0.41
1:5:432:SER:HA	1:5:570:THR:HB	2.03	0.41
1:5:490:ARG:HB2	1:5:576:THR:HB	2.03	0.41
1:8:622:ALA:HB3	1:8:635:PRO:HG3	2.01	0.41
1:8:650:LEU:HD13	1:8:650:LEU:HA	1.87	0.41
1:A:446:TYR:CE1	1:A:467:GLN:HG3	2.56	0.41
1:A:490:ARG:HB2	1:A:576:THR:HB	2.03	0.41
1:B:636:LEU:HD11	1:C:481:LEU:HD11	73.84	0.41
1:D:432:SER:HA	1:D:570:THR:HB	2.03	0.41
1:D:659:ASP:N	1:D:659:ASP:OD1	2.54	0.41
1:E:446:TYR:CE1	1:E:467:GLN:HG3	2.56	0.41
1:G:432:SER:HA	1:G:570:THR:HB	2.03	0.41
1:H:407:ARG:HD2	1:Z:224:SER:C	2.41	0.41
1:J:407:ARG:HD2	1:L:224:SER:C	90.17	0.41
1:A:630:ASN:HB3	1:K:608:VAL:HG12	106.22	0.41
1:L:446:TYR:CE1	1:L:467:GLN:HG3	2.56	0.41
1:L:481:LEU:HD11	1:T:636:LEU:HD11	204.06	0.41
1:L:490:ARG:HB2	1:L:576:THR:HB	2.03	0.41
1:M:224:SER:C	1:N:407:ARG:HD2	2.41	0.41
1:M:650:LEU:HA	1:M:650:LEU:HD13	1.86	0.41
1:O:608:VAL:HG12	1:P:630:ASN:HB3	57.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:446:TYR:CE1	1:P:467:GLN:HG3	2.56	0.41
1:P:432:SER:HA	1:P:570:THR:HB	2.03	0.41
1:Q:432:SER:HA	1:Q:570:THR:HB	2.03	0.41
1:R:432:SER:HA	1:R:570:THR:HB	2.03	0.41
1:Q:224:SER:C	1:S:407:ARG:HD2	2.41	0.41
1:S:461:GLN:CD	1:S:461:GLN:H	2.22	0.41
1:S:446:TYR:CE1	1:S:467:GLN:HG3	2.56	0.41
1:V:260:GLN:NE2	1:V:276:PHE:CE1	2.88	0.41
1:H:627:THR:CG2	1:Y:610:GLN:HE21	2.25	0.41
1:1:490:ARG:HB2	1:1:576:THR:HB	2.03	0.41
1:3:434:ASP:N	1:3:434:ASP:OD1	2.53	0.41
1:3:630:ASN:HB3	1:4:608:VAL:HG12	2.02	0.41
1:4:290:PHE:HB2	1:4:616:LEU:O	2.20	0.41
1:6:260:GLN:NE2	1:6:276:PHE:CE1	2.88	0.41
1:6:481:LEU:HD11	1:7:636:LEU:HD11	2.02	0.41
1:8:446:TYR:CE1	1:8:467:GLN:HG3	2.56	0.41
1:A:636:LEU:HD11	1:K:481:LEU:HD11	123.69	0.41
1:B:432:SER:HA	1:B:570:THR:HB	2.03	0.41
1:C:446:TYR:CE1	1:C:467:GLN:HG3	2.56	0.41
1:F:636:LEU:HD11	1:G:481:LEU:HD11	83.03	0.41
1:G:490:ARG:HB2	1:G:576:THR:HB	2.03	0.41
1:F:481:LEU:HD11	1:H:636:LEU:HD11	129.47	0.41
1:H:650:LEU:HA	1:H:650:LEU:HD13	1.86	0.41
1:I:434:ASP:OD1	1:I:434:ASP:N	2.53	0.41
1:I:446:TYR:CE1	1:I:467:GLN:HG3	2.56	0.41
1:I:490:ARG:HB2	1:I:576:THR:HB	2.03	0.41
1:I:636:LEU:HD11	1:K:481:LEU:HD11	106.79	0.41
1:K:659:ASP:OD1	1:K:659:ASP:N	2.54	0.41
1:M:407:ARG:HD2	1:N:224:SER:C	21.98	0.41
1:D:608:VAL:HG12	1:N:630:ASN:HB3	2.02	0.41
1:O:434:ASP:N	1:O:434:ASP:OD1	2.53	0.41
1:O:446:TYR:CE1	1:O:467:GLN:HG3	2.56	0.41
1:R:233:SER:OG	1:R:298:ASP:OD2	2.34	0.41
1:R:446:TYR:CE1	1:R:467:GLN:HG3	2.56	0.41
1:T:461:GLN:H	1:T:461:GLN:CD	2.22	0.41
1:T:446:TYR:CE1	1:T:467:GLN:HG3	2.56	0.41
1:T:636:LEU:HD11	1:V:481:LEU:HD11	106.80	0.41
1:T:481:LEU:HD11	1:U:636:LEU:HD11	73.84	0.41
1:W:608:VAL:HG12	1:X:630:ASN:HB3	63.75	0.41
1:W:284:TYR:HB3	1:W:650:LEU:HD13	2.02	0.41
1:Y:260:GLN:NE2	1:Y:276:PHE:CE1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:636:LEU:HD11	1:Y:481:LEU:HD11	23.70	0.41
1:Y:432:SER:HA	1:Y:570:THR:HB	2.03	0.41
1:1:718:ASN:ND2	1:1:722:THR:HB	2.31	0.41
1:3:432:SER:HA	1:3:570:THR:HB	2.03	0.41
1:6:622:ALA:HB3	1:6:635:PRO:HG3	2.01	0.41
1:B:224:SER:C	1:O:407:ARG:HD2	111.55	0.41
1:E:636:LEU:HD11	1:F:481:LEU:HD11	2.02	0.41
1:N:446:TYR:CE1	1:N:467:GLN:HG3	2.56	0.41
1:O:432:SER:HA	1:O:570:THR:HB	2.03	0.41
1:N:608:VAL:HG12	1:O:630:ASN:HB3	63.75	0.41
1:P:224:SER:C	1:Q:407:ARG:HD2	2.41	0.41
1:C:630:ASN:HB3	1:P:608:VAL:HG12	63.73	0.41
1:R:260:GLN:NE2	1:R:276:PHE:CE1	2.88	0.41
1:R:490:ARG:HB2	1:R:576:THR:HB	2.03	0.41
1:R:659:ASP:OD1	1:R:659:ASP:N	2.54	0.41
1:S:432:SER:HA	1:S:570:THR:HB	2.03	0.41
1:T:407:ARG:HD2	1:Y:224:SER:C	112.59	0.41
1:T:490:ARG:HB2	1:T:576:THR:HB	2.03	0.41
1:S:608:VAL:HG12	1:U:630:ASN:HB3	2.02	0.41
1:E:636:LEU:HD11	1:V:481:LEU:HD11	141.61	0.41
1:F:224:SER:C	1:X:407:ARG:HD2	101.21	0.41
1:X:608:VAL:HG12	1:Y:630:ASN:HB3	57.80	0.41
1:1:446:TYR:CE1	1:1:467:GLN:HG3	2.56	0.41
1:1:561:MET:SD	1:1:727:ARG:HA	2.61	0.41
1:1:481:LEU:HD11	1:2:636:LEU:HD11	2.02	0.41
1:3:224:SER:C	1:8:407:ARG:HD2	2.41	0.41
1:4:284:TYR:HB3	1:4:650:LEU:HD13	2.02	0.41
1:5:254:ASN:C	1:5:256:HIS:N	2.72	0.41
1:5:290:PHE:HB2	1:5:616:LEU:O	2.20	0.41
1:6:561:MET:SD	1:6:727:ARG:HA	2.61	0.41
1:7:434:ASP:N	1:7:434:ASP:OD1	2.53	0.41
1:7:659:ASP:N	1:7:659:ASP:OD1	2.54	0.41
1:B:290:PHE:HB2	1:B:616:LEU:O	2.20	0.41
1:K:284:TYR:HB3	1:K:650:LEU:HD13	2.02	0.41
1:K:224:SER:C	1:L:407:ARG:HD2	2.41	0.41
1:L:434:ASP:N	1:L:434:ASP:OD1	2.53	0.41
1:P:461:GLN:CD	1:P:461:GLN:H	2.22	0.41
1:P:512:HIS:ND1	1:P:517:ASP:OD1	2.38	0.41
1:T:224:SER:C	1:6:407:ARG:HD2	160.44	0.41
1:T:561:MET:SD	1:T:727:ARG:HA	2.61	0.41
1:T:659:ASP:N	1:T:659:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:224:SER:C	1:U:407:ARG:HD2	2.42	0.41
1:X:446:TYR:CE1	1:X:467:GLN:HG3	2.56	0.41
1:3:254:ASN:C	1:3:256:HIS:N	2.72	0.41
1:4:561:MET:SD	1:4:727:ARG:HA	2.61	0.41
1:5:481:LEU:HD11	1:6:636:LEU:HD11	2.03	0.41
1:8:461:GLN:CD	1:8:461:GLN:H	2.22	0.41
1:A:425:SER:OG	1:8:628:ASP:OD2	128.20	0.41
1:A:224:SER:C	1:E:407:ARG:HD2	2.41	0.41
1:A:260:GLN:NE2	1:A:276:PHE:CE1	2.88	0.41
1:B:260:GLN:NE2	1:B:276:PHE:CE1	2.88	0.41
1:B:461:GLN:H	1:B:461:GLN:CD	2.22	0.41
1:C:432:SER:HA	1:C:570:THR:HB	2.03	0.41
1:C:718:ASN:ND2	1:C:722:THR:HB	2.31	0.41
1:D:446:TYR:CE1	1:D:467:GLN:HG3	2.56	0.41
1:E:608:VAL:HG12	1:X:630:ASN:HB3	131.11	0.41
1:E:659:ASP:N	1:E:659:ASP:OD1	2.54	0.41
1:F:659:ASP:N	1:F:659:ASP:OD1	2.54	0.41
1:G:224:SER:C	1:1:407:ARG:HD2	151.47	0.41
1:E:224:SER:C	1:H:407:ARG:HD2	111.59	0.41
1:J:608:VAL:HG12	1:L:630:ASN:HB3	2.02	0.41
1:K:446:TYR:CE1	1:K:467:GLN:HG3	2.56	0.41
1:L:368:PHE:HA	1:L:369:PRO:HD3	1.98	0.41
1:C:630:ASN:HB3	1:M:608:VAL:HG12	2.02	0.41
1:L:407:ARG:HD2	1:N:224:SER:C	111.59	0.41
1:D:224:SER:C	1:O:407:ARG:HD2	101.70	0.41
1:O:659:ASP:N	1:O:659:ASP:OD1	2.54	0.41
1:R:407:ARG:HD2	1:V:224:SER:C	2.41	0.41
1:S:233:SER:OG	1:S:298:ASP:OD2	2.34	0.41
1:S:561:MET:SD	1:S:727:ARG:HA	2.61	0.41
1:U:561:MET:SD	1:U:727:ARG:HA	2.61	0.41
1:V:368:PHE:HA	1:V:369:PRO:HD3	1.98	0.41
1:V:407:ARG:HD2	1:1:224:SER:C	152.36	0.41
1:W:659:ASP:N	1:W:659:ASP:OD1	2.54	0.41
1:R:661:PRO:O	1:X:374:MET:HE3	78.88	0.41
1:X:561:MET:SD	1:X:727:ARG:HA	2.61	0.41
1:Z:434:ASP:N	1:Z:434:ASP:OD1	2.53	0.41
1:Z:490:ARG:HB2	1:Z:576:THR:HB	2.03	0.41
1:5:608:VAL:HG12	1:6:630:ASN:HB3	2.01	0.41
1:5:630:ASN:HB3	1:7:608:VAL:HG12	2.02	0.41
1:7:561:MET:SD	1:7:727:ARG:HA	2.61	0.41
1:B:490:ARG:HB2	1:B:576:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ARG:HD2	1:D:224:SER:C	2.42	0.41
1:D:284:TYR:HB3	1:D:650:LEU:HD13	2.02	0.41
1:E:561:MET:SD	1:E:727:ARG:HA	2.61	0.41
1:F:561:MET:SD	1:F:727:ARG:HA	2.61	0.41
1:G:446:TYR:CE1	1:G:467:GLN:HG3	2.56	0.41
1:G:659:ASP:OD1	1:G:659:ASP:N	2.54	0.41
1:I:718:ASN:ND2	1:I:722:THR:HB	2.31	0.41
1:A:407:ARG:HD2	1:J:224:SER:C	84.39	0.41
1:J:650:LEU:HD13	1:J:650:LEU:HA	1.86	0.41
1:J:659:ASP:N	1:J:659:ASP:OD1	2.54	0.41
1:N:260:GLN:NE2	1:N:276:PHE:CE1	2.88	0.41
1:N:718:ASN:ND2	1:N:722:THR:HB	2.31	0.41
1:N:481:LEU:HD11	1:O:636:LEU:HD11	65.47	0.41
1:O:224:SER:C	1:P:407:ARG:HD2	2.41	0.41
1:P:561:MET:SD	1:P:727:ARG:HA	2.61	0.41
1:P:659:ASP:OD1	1:P:659:ASP:N	2.54	0.41
1:R:481:LEU:HD11	1:S:636:LEU:HD11	2.02	0.41
1:T:434:ASP:OD1	1:T:434:ASP:N	2.53	0.41
1:V:487:ARG:HH22	1:V:578:GLN:HB3	1.86	0.41
1:Y:446:TYR:CE1	1:Y:467:GLN:HG3	2.56	0.41
1:1:659:ASP:OD1	1:1:659:ASP:N	2.54	0.40
1:4:432:SER:HA	1:4:570:THR:HB	2.03	0.40
1:6:446:TYR:CE1	1:6:467:GLN:HG3	2.56	0.40
1:A:224:SER:C	1:Z:407:ARG:HD2	103.46	0.40
1:A:636:LEU:HD11	1:I:481:LEU:HD11	2.03	0.40
1:A:561:MET:SD	1:A:727:ARG:HA	2.61	0.40
1:C:561:MET:SD	1:C:727:ARG:HA	2.61	0.40
1:C:659:ASP:OD1	1:C:659:ASP:N	2.54	0.40
1:E:490:ARG:HB2	1:E:576:THR:HB	2.03	0.40
1:F:407:ARG:HD2	1:R:224:SER:C	2.41	0.40
1:F:490:ARG:HB2	1:F:576:THR:HB	2.03	0.40
1:G:487:ARG:HH22	1:G:578:GLN:HB3	1.87	0.40
1:G:512:HIS:ND1	1:G:517:ASP:OD1	2.38	0.40
1:H:487:ARG:HH22	1:H:578:GLN:HB3	1.87	0.40
1:H:561:MET:SD	1:H:727:ARG:HA	2.61	0.40
1:I:260:GLN:NE2	1:I:276:PHE:CE1	2.88	0.40
1:I:304:ASN:O	1:I:734:LEU:HD11	2.22	0.40
1:I:487:ARG:HH22	1:I:578:GLN:HB3	1.87	0.40
1:A:630:ASN:HB3	1:I:608:VAL:HG12	2.03	0.40
1:I:659:ASP:OD1	1:I:659:ASP:N	2.54	0.40
1:I:561:MET:SD	1:I:727:ARG:HA	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:481:LEU:HD11	1:J:636:LEU:HD11	73.83	0.40
1:K:561:MET:SD	1:K:727:ARG:HA	2.61	0.40
1:L:487:ARG:HH22	1:L:578:GLN:HB3	1.87	0.40
1:L:561:MET:SD	1:L:727:ARG:HA	2.61	0.40
1:L:432:SER:HA	1:L:570:THR:HB	2.03	0.40
1:M:435:ARG:HA	1:M:435:ARG:HD3	1.85	0.40
1:M:490:ARG:HB2	1:M:576:THR:HB	2.03	0.40
1:M:659:ASP:OD1	1:M:659:ASP:N	2.54	0.40
1:N:432:SER:HA	1:N:570:THR:HB	2.03	0.40
1:N:490:ARG:HB2	1:N:576:THR:HB	2.03	0.40
1:N:561:MET:SD	1:N:727:ARG:HA	2.61	0.40
1:O:652:LYS:NZ	1:O:655:PRO:HD3	2.37	0.40
1:F:630:ASN:HB3	1:Q:608:VAL:HG12	2.01	0.40
1:Q:636:LEU:HD11	1:S:481:LEU:HD11	83.03	0.40
1:Q:652:LYS:NZ	1:Q:655:PRO:HD3	2.37	0.40
1:Q:659:ASP:OD1	1:Q:659:ASP:N	2.54	0.40
1:X:487:ARG:HH22	1:X:578:GLN:HB3	1.87	0.40
1:W:481:LEU:HD11	1:X:636:LEU:HD11	65.47	0.40
1:Y:487:ARG:HH22	1:Y:578:GLN:HB3	1.87	0.40
1:Z:561:MET:SD	1:Z:727:ARG:HA	2.61	0.40
1:2:254:ASN:ND2	1:2:377:GLN:HE22	2.18	0.40
1:3:652:LYS:NZ	1:3:655:PRO:HD3	2.37	0.40
1:Z:407:ARG:HD2	1:4:224:SER:C	90.17	0.40
1:Z:736:ARG:NH2	1:4:626:HIS:CD2	2.89	0.40
1:5:652:LYS:NZ	1:5:655:PRO:HD3	2.37	0.40
1:6:284:TYR:HB3	1:6:650:LEU:HD13	2.02	0.40
1:6:490:ARG:HB2	1:6:576:THR:HB	2.03	0.40
1:A:434:ASP:N	1:A:434:ASP:OD1	2.53	0.40
1:A:652:LYS:NZ	1:A:655:PRO:HD3	2.37	0.40
1:B:304:ASN:O	1:B:734:LEU:HD11	2.22	0.40
1:C:304:ASN:O	1:C:734:LEU:HD11	2.22	0.40
1:C:487:ARG:HH22	1:C:578:GLN:HB3	1.87	0.40
1:F:312:LYS:HD2	1:F:312:LYS:HA	1.88	0.40
1:F:446:TYR:CE1	1:F:467:GLN:HG3	2.56	0.40
1:G:561:MET:SD	1:G:727:ARG:HA	2.61	0.40
1:H:304:ASN:O	1:H:734:LEU:HD11	2.22	0.40
1:H:652:LYS:NZ	1:H:655:PRO:HD3	2.37	0.40
1:K:304:ASN:O	1:K:734:LEU:HD11	2.22	0.40
1:K:487:ARG:HH22	1:K:578:GLN:HB3	1.87	0.40
1:L:304:ASN:O	1:L:734:LEU:HD11	2.22	0.40
1:N:434:ASP:N	1:N:434:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:561:MET:SD	1:O:727:ARG:HA	2.61	0.40
1:P:652:LYS:NZ	1:P:655:PRO:HD3	2.37	0.40
1:S:304:ASN:O	1:S:734:LEU:HD11	2.22	0.40
1:S:652:LYS:NZ	1:S:655:PRO:HD3	2.37	0.40
1:U:304:ASN:O	1:U:734:LEU:HD11	2.22	0.40
1:V:224:SER:C	1:W:407:ARG:HD2	21.98	0.40
1:V:304:ASN:O	1:V:734:LEU:HD11	2.22	0.40
1:V:561:MET:SD	1:V:727:ARG:HA	2.61	0.40
1:X:284:TYR:HB3	1:X:650:LEU:HD13	2.02	0.40
1:X:224:SER:C	1:Y:407:ARG:HD2	2.41	0.40
1:Z:487:ARG:HH22	1:Z:578:GLN:HB3	1.87	0.40
1:1:434:ASP:OD1	1:1:434:ASP:N	2.53	0.40
1:2:328:GLN:NE2	1:2:333:LYS:HG3	2.23	0.40
1:2:652:LYS:NZ	1:2:655:PRO:HD3	2.37	0.40
1:2:304:ASN:O	1:2:734:LEU:HD11	2.22	0.40
1:3:636:LEU:HD11	1:4:481:LEU:HD11	2.02	0.40
1:4:434:ASP:OD1	1:4:434:ASP:N	2.53	0.40
1:U:407:ARG:HD2	1:5:224:SER:C	162.74	0.40
1:6:652:LYS:NZ	1:6:655:PRO:HD3	2.37	0.40
1:7:432:SER:HA	1:7:570:THR:HB	2.03	0.40
1:7:490:ARG:HB2	1:7:576:THR:HB	2.03	0.40
1:8:284:TYR:HB3	1:8:650:LEU:HD13	2.02	0.40
1:8:652:LYS:NZ	1:8:655:PRO:HD3	2.37	0.40
1:8:659:ASP:N	1:8:659:ASP:OD1	2.54	0.40
1:8:561:MET:SD	1:8:727:ARG:HA	2.61	0.40
1:A:461:GLN:H	1:A:461:GLN:CD	2.22	0.40
1:B:407:ARG:HD2	1:C:224:SER:C	2.41	0.40
1:B:487:ARG:HH22	1:B:578:GLN:HB3	1.87	0.40
1:C:407:ARG:HD2	1:S:224:SER:C	102.46	0.40
1:C:434:ASP:OD1	1:C:434:ASP:N	2.53	0.40
1:D:652:LYS:NZ	1:D:655:PRO:HD3	2.37	0.40
1:D:304:ASN:O	1:D:734:LEU:HD11	2.22	0.40
1:E:432:SER:HA	1:E:570:THR:HB	2.03	0.40
1:F:652:LYS:NZ	1:F:655:PRO:HD3	2.37	0.40
1:A:608:VAL:HG12	1:G:630:ASN:HB3	2.03	0.40
1:H:490:ARG:HB2	1:H:576:THR:HB	2.03	0.40
1:H:659:ASP:OD1	1:H:659:ASP:N	2.54	0.40
1:I:224:SER:C	1:T:407:ARG:HD2	163.55	0.40
1:J:304:ASN:O	1:J:734:LEU:HD11	2.22	0.40
1:M:304:ASN:O	1:M:734:LEU:HD11	2.22	0.40
1:N:652:LYS:NZ	1:N:655:PRO:HD3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:608:VAL:HG12	1:Q:630:ASN:HB3	2.02	0.40
1:R:487:ARG:HH22	1:R:578:GLN:HB3	1.87	0.40
1:S:487:ARG:HH22	1:S:578:GLN:HB3	1.87	0.40
1:T:260:GLN:NE2	1:T:276:PHE:CE1	2.88	0.40
1:U:652:LYS:NZ	1:U:655:PRO:HD3	2.37	0.40
1:W:561:MET:SD	1:W:727:ARG:HA	2.61	0.40
1:W:652:LYS:NZ	1:W:655:PRO:HD3	2.37	0.40
1:Y:561:MET:SD	1:Y:727:ARG:HA	2.61	0.40
1:4:490:ARG:HB2	1:4:576:THR:HB	2.03	0.40
1:5:446:TYR:CE1	1:5:467:GLN:HG3	2.56	0.40
1:6:452:GLN:HE21	1:6:459:GLY:HA2	1.87	0.40
1:5:407:ARG:HD2	1:8:224:SER:C	2.42	0.40
1:B:561:MET:SD	1:B:727:ARG:HA	2.61	0.40
1:D:636:LEU:HD11	1:T:481:LEU:HD11	128.44	0.40
1:E:652:LYS:NZ	1:E:655:PRO:HD3	2.37	0.40
1:F:407:ARG:HD2	1:Z:224:SER:C	101.63	0.40
1:F:452:GLN:HE21	1:F:459:GLY:HA2	1.87	0.40
1:G:461:GLN:CD	1:G:461:GLN:H	2.22	0.40
1:G:652:LYS:NZ	1:G:655:PRO:HD3	2.37	0.40
1:F:736:ARG:NH2	1:H:626:HIS:CD2	110.87	0.40
1:J:561:MET:SD	1:J:727:ARG:HA	2.61	0.40
1:K:407:ARG:HD2	1:W:224:SER:C	158.71	0.40
1:M:260:GLN:NE2	1:M:276:PHE:CE1	2.88	0.40
1:M:561:MET:SD	1:M:727:ARG:HA	2.61	0.40
1:D:425:SER:OG	1:N:628:ASP:OD2	2.30	0.40
1:Q:561:MET:SD	1:Q:727:ARG:HA	2.61	0.40
1:U:481:LEU:HD11	1:V:636:LEU:HD11	65.47	0.40
1:Y:659:ASP:N	1:Y:659:ASP:OD1	2.54	0.40
1:2:284:TYR:HB3	1:2:650:LEU:HD13	2.02	0.40
1:2:561:MET:SD	1:2:727:ARG:HA	2.61	0.40
1:4:435:ARG:HA	1:4:435:ARG:HD3	1.85	0.40
1:7:446:TYR:CE1	1:7:467:GLN:HG3	2.56	0.40
1:K:627:THR:CG2	1:8:610:GLN:HE21	2.25	0.40
1:8:290:PHE:HB2	1:8:616:LEU:O	2.20	0.40
1:A:608:VAL:HG12	1:8:630:ASN:HB3	130.66	0.40
1:A:432:SER:HA	1:A:570:THR:HB	2.03	0.40
1:B:407:ARG:HD2	1:L:224:SER:C	76.30	0.40
1:B:446:TYR:CE1	1:B:467:GLN:HG3	2.56	0.40
1:D:452:GLN:HE21	1:D:459:GLY:HA2	1.87	0.40
1:D:487:ARG:HH22	1:D:578:GLN:HB3	1.86	0.40
1:E:312:LYS:HD2	1:E:312:LYS:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:ASN:O	1:E:734:LEU:HD11	2.22	0.40
1:F:304:ASN:O	1:F:734:LEU:HD11	2.22	0.40
1:H:224:SER:C	1:I:407:ARG:HD2	2.42	0.40
1:J:435:ARG:HA	1:J:435:ARG:HD3	1.85	0.40
1:K:490:ARG:HB2	1:K:576:THR:HB	2.03	0.40
1:M:652:LYS:NZ	1:M:655:PRO:HD3	2.37	0.40
1:R:304:ASN:O	1:R:734:LEU:HD11	2.22	0.40
1:S:659:ASP:OD1	1:S:659:ASP:N	2.54	0.40
1:T:304:ASN:O	1:T:734:LEU:HD11	2.22	0.40
1:V:659:ASP:N	1:V:659:ASP:OD1	2.54	0.40
1:W:432:SER:HA	1:W:570:THR:HB	2.03	0.40
1:W:490:ARG:HB2	1:W:576:THR:HB	2.03	0.40
1:W:304:ASN:O	1:W:734:LEU:HD11	2.22	0.40
1:X:659:ASP:N	1:X:659:ASP:OD1	2.54	0.40
1:Q:224:SER:C	1:Y:407:ARG:HD2	144.83	0.40
1:Y:452:GLN:HE21	1:Y:459:GLY:HA2	1.87	0.40
1:Y:652:LYS:NZ	1:Y:655:PRO:HD3	2.37	0.40
1:Z:481:LEU:HD11	1:1:636:LEU:HD11	85.95	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	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	2	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	3	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	4	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	5	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	6	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	8	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	A	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	B	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	C	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	D	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	E	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	F	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	G	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	H	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	I	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	J	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	K	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	L	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	M	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	N	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	O	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	P	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	Q	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	R	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	S	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	T	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	U	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	V	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	W	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	X	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	Y	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	Z	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	a	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	b	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	c	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	e	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	f	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	g	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	h	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	i	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	j	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	k	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	l	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	m	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	n	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	o	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	p	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	q	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	r	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	s	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	t	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	u	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	v	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	w	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	x	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	y	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	z	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
All	All	31200/31260 (100%)	30240 (97%)	840 (3%)	120 (0%)	40	75

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	408	THR
1	B	255	ASN
1	B	408	THR
1	C	255	ASN
1	C	408	THR

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Mol	Chain	Res	Type
1	D	255	ASN
1	D	408	THR
1	E	255	ASN
1	E	408	THR
1	F	255	ASN
1	F	408	THR
1	G	255	ASN
1	G	408	THR
1	H	255	ASN
1	H	408	THR
1	I	255	ASN
1	I	408	THR
1	J	255	ASN
1	J	408	THR
1	K	255	ASN
1	K	408	THR
1	L	255	ASN
1	L	408	THR
1	M	255	ASN
1	M	408	THR
1	N	255	ASN
1	N	408	THR
1	O	255	ASN
1	O	408	THR
1	P	255	ASN
1	P	408	THR
1	Q	255	ASN
1	Q	408	THR
1	R	255	ASN
1	R	408	THR
1	S	255	ASN
1	S	408	THR
1	T	255	ASN
1	T	408	THR
1	U	255	ASN
1	U	408	THR
1	V	255	ASN
1	V	408	THR
1	W	255	ASN
1	W	408	THR
1	X	255	ASN
1	X	408	THR

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Mol	Chain	Res	Type
1	Y	255	ASN
1	Y	408	THR
1	Z	255	ASN
1	Z	408	THR
1	a	255	ASN
1	a	408	THR
1	b	255	ASN
1	b	408	THR
1	c	255	ASN
1	c	408	THR
1	d	255	ASN
1	d	408	THR
1	e	255	ASN
1	e	408	THR
1	f	255	ASN
1	f	408	THR
1	g	255	ASN
1	g	408	THR
1	h	255	ASN
1	h	408	THR
1	i	255	ASN
1	i	408	THR
1	j	255	ASN
1	j	408	THR
1	k	255	ASN
1	k	408	THR
1	l	255	ASN
1	l	408	THR
1	m	255	ASN
1	m	408	THR
1	n	255	ASN
1	n	408	THR
1	o	255	ASN
1	o	408	THR
1	p	255	ASN
1	p	408	THR
1	q	255	ASN
1	q	408	THR
1	r	255	ASN
1	r	408	THR
1	s	255	ASN
1	s	408	THR

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Mol	Chain	Res	Type
1	t	255	ASN
1	t	408	THR
1	u	255	ASN
1	u	408	THR
1	v	255	ASN
1	v	408	THR
1	w	255	ASN
1	w	408	THR
1	x	255	ASN
1	x	408	THR
1	y	255	ASN
1	y	408	THR
1	z	255	ASN
1	z	408	THR
1	1	255	ASN
1	1	408	THR
1	2	255	ASN
1	2	408	THR
1	3	255	ASN
1	3	408	THR
1	4	255	ASN
1	4	408	THR
1	5	255	ASN
1	5	408	THR
1	6	255	ASN
1	6	408	THR
1	7	255	ASN
1	7	408	THR
1	8	255	ASN
1	8	408	THR

### 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	455/454 (100%)	454 (100%)	1 (0%)	94 98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	3	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	4	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	5	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	6	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	7	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	8	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	A	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	B	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	C	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	D	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	E	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	F	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	G	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	H	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	I	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	J	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	K	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	L	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	M	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	N	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	O	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	P	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	Q	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	R	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	S	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	T	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	U	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	V	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	W	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	X	455/454 (100%)	454 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	Z	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	a	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	b	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	c	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	d	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	e	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	f	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	g	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	h	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	i	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	j	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	k	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	l	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	m	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	n	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	o	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	p	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	q	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	r	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	s	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	t	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	u	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	v	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	w	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	x	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	y	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	z	455/454 (100%)	454 (100%)	1 (0%)	94	98
All	All	27300/27240 (100%)	27240 (100%)	60 (0%)	94	98

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	448	LEU
1	B	448	LEU
1	C	448	LEU
1	D	448	LEU
1	E	448	LEU
1	F	448	LEU
1	G	448	LEU
1	H	448	LEU
1	I	448	LEU
1	J	448	LEU
1	K	448	LEU
1	L	448	LEU
1	M	448	LEU
1	N	448	LEU
1	O	448	LEU
1	P	448	LEU
1	Q	448	LEU
1	R	448	LEU
1	S	448	LEU
1	T	448	LEU
1	U	448	LEU
1	V	448	LEU
1	W	448	LEU
1	X	448	LEU
1	Y	448	LEU
1	Z	448	LEU
1	a	448	LEU
1	b	448	LEU
1	c	448	LEU
1	d	448	LEU
1	e	448	LEU
1	f	448	LEU
1	g	448	LEU
1	h	448	LEU
1	i	448	LEU
1	j	448	LEU
1	k	448	LEU
1	l	448	LEU
1	m	448	LEU
1	n	448	LEU
1	o	448	LEU
1	p	448	LEU
1	q	448	LEU

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Mol	Chain	Res	Type
1	r	448	LEU
1	s	448	LEU
1	t	448	LEU
1	u	448	LEU
1	v	448	LEU
1	w	448	LEU
1	x	448	LEU
1	y	448	LEU
1	z	448	LEU
1	1	448	LEU
1	2	448	LEU
1	3	448	LEU
1	4	448	LEU
1	5	448	LEU
1	6	448	LEU
1	7	448	LEU
1	8	448	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (660) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	ASN
1	A	328	GLN
1	A	377	GLN
1	A	431	GLN
1	A	587	GLN
1	A	597	ASN
1	A	610	GLN
1	A	626	HIS
1	A	653	ASN
1	A	675	GLN
1	A	737	ASN
1	B	305	ASN
1	B	328	GLN
1	B	377	GLN
1	B	431	GLN
1	B	587	GLN
1	B	597	ASN
1	B	610	GLN
1	B	626	HIS
1	B	653	ASN
1	B	675	GLN

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Mol	Chain	Res	Type
1	B	737	ASN
1	C	305	ASN
1	C	328	GLN
1	C	377	GLN
1	C	431	GLN
1	C	587	GLN
1	C	597	ASN
1	C	610	GLN
1	C	626	HIS
1	C	653	ASN
1	C	675	GLN
1	C	737	ASN
1	D	305	ASN
1	D	328	GLN
1	D	377	GLN
1	D	431	GLN
1	D	587	GLN
1	D	597	ASN
1	D	610	GLN
1	D	626	HIS
1	D	653	ASN
1	D	675	GLN
1	D	737	ASN
1	E	305	ASN
1	E	328	GLN
1	E	377	GLN
1	E	431	GLN
1	E	587	GLN
1	E	597	ASN
1	E	610	GLN
1	E	626	HIS
1	E	653	ASN
1	E	675	GLN
1	E	737	ASN
1	F	305	ASN
1	F	328	GLN
1	F	377	GLN
1	F	431	GLN
1	F	587	GLN
1	F	597	ASN
1	F	610	GLN
1	F	626	HIS

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Mol	Chain	Res	Type
1	F	653	ASN
1	F	675	GLN
1	F	737	ASN
1	G	305	ASN
1	G	328	GLN
1	G	377	GLN
1	G	431	GLN
1	G	587	GLN
1	G	597	ASN
1	G	610	GLN
1	G	626	HIS
1	G	653	ASN
1	G	675	GLN
1	G	737	ASN
1	H	305	ASN
1	H	328	GLN
1	H	377	GLN
1	H	431	GLN
1	H	587	GLN
1	H	597	ASN
1	H	610	GLN
1	H	626	HIS
1	H	653	ASN
1	H	675	GLN
1	H	737	ASN
1	I	305	ASN
1	I	328	GLN
1	I	377	GLN
1	I	431	GLN
1	I	587	GLN
1	I	597	ASN
1	I	610	GLN
1	I	626	HIS
1	I	653	ASN
1	I	675	GLN
1	I	737	ASN
1	J	305	ASN
1	J	328	GLN
1	J	377	GLN
1	J	431	GLN
1	J	587	GLN
1	J	597	ASN

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Mol	Chain	Res	Type
1	J	610	GLN
1	J	626	HIS
1	J	653	ASN
1	J	675	GLN
1	J	737	ASN
1	K	305	ASN
1	K	328	GLN
1	K	377	GLN
1	K	431	GLN
1	K	587	GLN
1	K	597	ASN
1	K	610	GLN
1	K	626	HIS
1	K	653	ASN
1	K	675	GLN
1	K	737	ASN
1	L	305	ASN
1	L	328	GLN
1	L	377	GLN
1	L	431	GLN
1	L	587	GLN
1	L	597	ASN
1	L	610	GLN
1	L	626	HIS
1	L	653	ASN
1	L	675	GLN
1	L	737	ASN
1	M	305	ASN
1	M	328	GLN
1	M	377	GLN
1	M	431	GLN
1	M	587	GLN
1	M	597	ASN
1	M	610	GLN
1	M	626	HIS
1	M	653	ASN
1	M	675	GLN
1	M	737	ASN
1	N	305	ASN
1	N	328	GLN
1	N	377	GLN
1	N	431	GLN

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Mol	Chain	Res	Type
1	N	587	GLN
1	N	597	ASN
1	N	610	GLN
1	N	626	HIS
1	N	653	ASN
1	N	675	GLN
1	N	737	ASN
1	O	305	ASN
1	O	328	GLN
1	O	377	GLN
1	O	431	GLN
1	O	587	GLN
1	O	597	ASN
1	O	610	GLN
1	O	626	HIS
1	O	653	ASN
1	O	675	GLN
1	O	737	ASN
1	P	305	ASN
1	P	328	GLN
1	P	377	GLN
1	P	431	GLN
1	P	587	GLN
1	P	597	ASN
1	P	610	GLN
1	P	626	HIS
1	P	653	ASN
1	P	675	GLN
1	P	737	ASN
1	Q	305	ASN
1	Q	328	GLN
1	Q	377	GLN
1	Q	431	GLN
1	Q	587	GLN
1	Q	597	ASN
1	Q	610	GLN
1	Q	626	HIS
1	Q	653	ASN
1	Q	675	GLN
1	Q	737	ASN
1	R	305	ASN
1	R	328	GLN

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Mol	Chain	Res	Type
1	R	377	GLN
1	R	431	GLN
1	R	587	GLN
1	R	597	ASN
1	R	610	GLN
1	R	626	HIS
1	R	653	ASN
1	R	675	GLN
1	R	737	ASN
1	S	305	ASN
1	S	328	GLN
1	S	377	GLN
1	S	431	GLN
1	S	587	GLN
1	S	597	ASN
1	S	610	GLN
1	S	626	HIS
1	S	653	ASN
1	S	675	GLN
1	S	737	ASN
1	T	305	ASN
1	T	328	GLN
1	T	377	GLN
1	T	431	GLN
1	T	587	GLN
1	T	597	ASN
1	T	610	GLN
1	T	626	HIS
1	T	653	ASN
1	T	675	GLN
1	T	737	ASN
1	U	305	ASN
1	U	328	GLN
1	U	377	GLN
1	U	431	GLN
1	U	587	GLN
1	U	597	ASN
1	U	610	GLN
1	U	626	HIS
1	U	653	ASN
1	U	675	GLN
1	U	737	ASN

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Mol	Chain	Res	Type
1	V	305	ASN
1	V	328	GLN
1	V	377	GLN
1	V	431	GLN
1	V	587	GLN
1	V	597	ASN
1	V	610	GLN
1	V	626	HIS
1	V	653	ASN
1	V	675	GLN
1	V	737	ASN
1	W	305	ASN
1	W	328	GLN
1	W	377	GLN
1	W	431	GLN
1	W	587	GLN
1	W	597	ASN
1	W	610	GLN
1	W	626	HIS
1	W	653	ASN
1	W	675	GLN
1	W	737	ASN
1	X	305	ASN
1	X	328	GLN
1	X	377	GLN
1	X	431	GLN
1	X	587	GLN
1	X	597	ASN
1	X	610	GLN
1	X	626	HIS
1	X	653	ASN
1	X	675	GLN
1	X	737	ASN
1	Y	305	ASN
1	Y	328	GLN
1	Y	377	GLN
1	Y	431	GLN
1	Y	587	GLN
1	Y	597	ASN
1	Y	610	GLN
1	Y	626	HIS
1	Y	653	ASN

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Mol	Chain	Res	Type
1	Y	675	GLN
1	Y	737	ASN
1	Z	305	ASN
1	Z	328	GLN
1	Z	377	GLN
1	Z	431	GLN
1	Z	587	GLN
1	Z	597	ASN
1	Z	610	GLN
1	Z	626	HIS
1	Z	653	ASN
1	Z	675	GLN
1	Z	737	ASN
1	a	305	ASN
1	a	328	GLN
1	a	377	GLN
1	a	431	GLN
1	a	587	GLN
1	a	597	ASN
1	a	610	GLN
1	a	626	HIS
1	a	653	ASN
1	a	675	GLN
1	a	737	ASN
1	b	305	ASN
1	b	328	GLN
1	b	377	GLN
1	b	431	GLN
1	b	587	GLN
1	b	597	ASN
1	b	610	GLN
1	b	626	HIS
1	b	653	ASN
1	b	675	GLN
1	b	737	ASN
1	c	305	ASN
1	c	328	GLN
1	c	377	GLN
1	c	431	GLN
1	c	587	GLN
1	c	597	ASN
1	c	610	GLN

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Mol	Chain	Res	Type
1	c	626	HIS
1	c	653	ASN
1	c	675	GLN
1	c	737	ASN
1	d	305	ASN
1	d	328	GLN
1	d	377	GLN
1	d	431	GLN
1	d	587	GLN
1	d	597	ASN
1	d	610	GLN
1	d	626	HIS
1	d	653	ASN
1	d	675	GLN
1	d	737	ASN
1	e	305	ASN
1	e	328	GLN
1	e	377	GLN
1	e	431	GLN
1	e	587	GLN
1	e	597	ASN
1	e	610	GLN
1	e	626	HIS
1	e	653	ASN
1	e	675	GLN
1	e	737	ASN
1	f	305	ASN
1	f	328	GLN
1	f	377	GLN
1	f	431	GLN
1	f	587	GLN
1	f	597	ASN
1	f	610	GLN
1	f	626	HIS
1	f	653	ASN
1	f	675	GLN
1	f	737	ASN
1	g	305	ASN
1	g	328	GLN
1	g	377	GLN
1	g	431	GLN
1	g	587	GLN

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Mol	Chain	Res	Type
1	g	597	ASN
1	g	610	GLN
1	g	626	HIS
1	g	653	ASN
1	g	675	GLN
1	g	737	ASN
1	h	305	ASN
1	h	328	GLN
1	h	377	GLN
1	h	431	GLN
1	h	587	GLN
1	h	597	ASN
1	h	610	GLN
1	h	626	HIS
1	h	653	ASN
1	h	675	GLN
1	h	737	ASN
1	i	305	ASN
1	i	328	GLN
1	i	377	GLN
1	i	431	GLN
1	i	587	GLN
1	i	597	ASN
1	i	610	GLN
1	i	626	HIS
1	i	653	ASN
1	i	675	GLN
1	i	737	ASN
1	j	305	ASN
1	j	328	GLN
1	j	377	GLN
1	j	431	GLN
1	j	587	GLN
1	j	597	ASN
1	j	610	GLN
1	j	626	HIS
1	j	653	ASN
1	j	675	GLN
1	j	737	ASN
1	k	305	ASN
1	k	328	GLN
1	k	377	GLN

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Mol	Chain	Res	Type
1	k	431	GLN
1	k	587	GLN
1	k	597	ASN
1	k	610	GLN
1	k	626	HIS
1	k	653	ASN
1	k	675	GLN
1	k	737	ASN
1	l	305	ASN
1	l	328	GLN
1	l	377	GLN
1	l	431	GLN
1	l	587	GLN
1	l	597	ASN
1	l	610	GLN
1	l	626	HIS
1	l	653	ASN
1	l	675	GLN
1	l	737	ASN
1	m	305	ASN
1	m	328	GLN
1	m	377	GLN
1	m	431	GLN
1	m	587	GLN
1	m	597	ASN
1	m	610	GLN
1	m	626	HIS
1	m	653	ASN
1	m	675	GLN
1	m	737	ASN
1	n	305	ASN
1	n	328	GLN
1	n	377	GLN
1	n	431	GLN
1	n	587	GLN
1	n	597	ASN
1	n	610	GLN
1	n	626	HIS
1	n	653	ASN
1	n	675	GLN
1	n	737	ASN
1	o	305	ASN

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Mol	Chain	Res	Type
1	o	328	GLN
1	o	377	GLN
1	o	431	GLN
1	o	587	GLN
1	o	597	ASN
1	o	610	GLN
1	o	626	HIS
1	o	653	ASN
1	o	675	GLN
1	o	737	ASN
1	p	305	ASN
1	p	328	GLN
1	p	377	GLN
1	p	431	GLN
1	p	587	GLN
1	p	597	ASN
1	p	610	GLN
1	p	626	HIS
1	p	653	ASN
1	p	675	GLN
1	p	737	ASN
1	q	305	ASN
1	q	328	GLN
1	q	377	GLN
1	q	431	GLN
1	q	587	GLN
1	q	597	ASN
1	q	610	GLN
1	q	626	HIS
1	q	653	ASN
1	q	675	GLN
1	q	737	ASN
1	r	305	ASN
1	r	328	GLN
1	r	377	GLN
1	r	431	GLN
1	r	587	GLN
1	r	597	ASN
1	r	610	GLN
1	r	626	HIS
1	r	653	ASN
1	r	675	GLN

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Mol	Chain	Res	Type
1	r	737	ASN
1	s	305	ASN
1	s	328	GLN
1	s	377	GLN
1	s	431	GLN
1	s	587	GLN
1	s	597	ASN
1	s	610	GLN
1	s	626	HIS
1	s	653	ASN
1	s	675	GLN
1	s	737	ASN
1	t	305	ASN
1	t	328	GLN
1	t	377	GLN
1	t	431	GLN
1	t	587	GLN
1	t	597	ASN
1	t	610	GLN
1	t	626	HIS
1	t	653	ASN
1	t	675	GLN
1	t	737	ASN
1	u	305	ASN
1	u	328	GLN
1	u	377	GLN
1	u	431	GLN
1	u	587	GLN
1	u	597	ASN
1	u	610	GLN
1	u	626	HIS
1	u	653	ASN
1	u	675	GLN
1	u	737	ASN
1	v	305	ASN
1	v	328	GLN
1	v	377	GLN
1	v	431	GLN
1	v	587	GLN
1	v	597	ASN
1	v	610	GLN
1	v	626	HIS

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Mol	Chain	Res	Type
1	v	653	ASN
1	v	675	GLN
1	v	737	ASN
1	w	305	ASN
1	w	328	GLN
1	w	377	GLN
1	w	431	GLN
1	w	587	GLN
1	w	597	ASN
1	w	610	GLN
1	w	626	HIS
1	w	653	ASN
1	w	675	GLN
1	w	737	ASN
1	x	305	ASN
1	x	328	GLN
1	x	377	GLN
1	x	431	GLN
1	x	587	GLN
1	x	597	ASN
1	x	610	GLN
1	x	626	HIS
1	x	653	ASN
1	x	675	GLN
1	x	737	ASN
1	y	305	ASN
1	y	328	GLN
1	y	377	GLN
1	y	431	GLN
1	y	587	GLN
1	y	597	ASN
1	y	610	GLN
1	y	626	HIS
1	y	653	ASN
1	y	675	GLN
1	y	737	ASN
1	z	305	ASN
1	z	328	GLN
1	z	377	GLN
1	z	431	GLN
1	z	587	GLN
1	z	597	ASN

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Mol	Chain	Res	Type
1	z	610	GLN
1	z	626	HIS
1	z	653	ASN
1	z	675	GLN
1	z	737	ASN
1	1	305	ASN
1	1	328	GLN
1	1	377	GLN
1	1	431	GLN
1	1	587	GLN
1	1	597	ASN
1	1	610	GLN
1	1	626	HIS
1	1	653	ASN
1	1	675	GLN
1	1	737	ASN
1	2	305	ASN
1	2	328	GLN
1	2	377	GLN
1	2	431	GLN
1	2	587	GLN
1	2	597	ASN
1	2	610	GLN
1	2	626	HIS
1	2	653	ASN
1	2	675	GLN
1	2	737	ASN
1	3	305	ASN
1	3	328	GLN
1	3	377	GLN
1	3	431	GLN
1	3	587	GLN
1	3	597	ASN
1	3	610	GLN
1	3	626	HIS
1	3	653	ASN
1	3	675	GLN
1	3	737	ASN
1	4	305	ASN
1	4	328	GLN
1	4	377	GLN
1	4	431	GLN

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Mol	Chain	Res	Type
1	4	587	GLN
1	4	597	ASN
1	4	610	GLN
1	4	626	HIS
1	4	653	ASN
1	4	675	GLN
1	4	737	ASN
1	5	305	ASN
1	5	328	GLN
1	5	377	GLN
1	5	431	GLN
1	5	587	GLN
1	5	597	ASN
1	5	610	GLN
1	5	626	HIS
1	5	653	ASN
1	5	675	GLN
1	5	737	ASN
1	6	305	ASN
1	6	328	GLN
1	6	377	GLN
1	6	431	GLN
1	6	587	GLN
1	6	597	ASN
1	6	610	GLN
1	6	626	HIS
1	6	653	ASN
1	6	675	GLN
1	6	737	ASN
1	7	305	ASN
1	7	328	GLN
1	7	377	GLN
1	7	431	GLN
1	7	587	GLN
1	7	597	ASN
1	7	610	GLN
1	7	626	HIS
1	7	653	ASN
1	7	675	GLN
1	7	737	ASN
1	8	305	ASN
1	8	328	GLN

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Mol	Chain	Res	Type
1	8	377	GLN
1	8	431	GLN
1	8	587	GLN
1	8	597	ASN
1	8	610	GLN
1	8	626	HIS
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 ⓘ

There are no chain breaks in this entry.