



Full wwPDB EM Model Validation Report ⓘ

May 18, 2020 – 12:00 PM EDT

PDB ID : 6U3Q
EMDB ID : EMD-20630
Title : The atomic structure of a human adeno-associated virus capsid isolate (AAVhu69/AAVv66)
Authors : Hsu, H.-L.; Brown, A.; Loveland, A.; Tai, P.; Korostelev, A.; Gao, G.
Deposited on : 2019-08-22
Resolution : 2.46 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

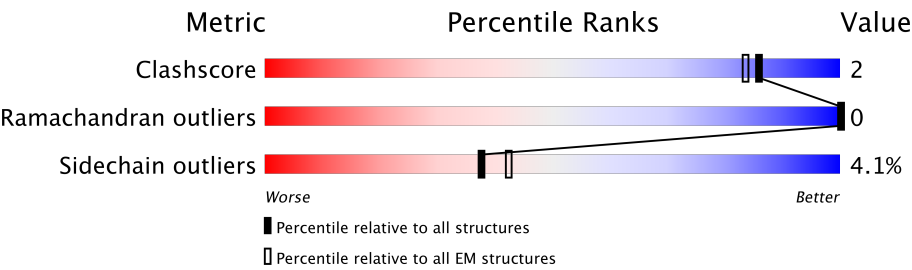
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 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 and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	0	735	<div><div>63%7%•29%</div></div>
1	1	735	<div><div>63%7%•29%</div></div>
1	2	735	<div><div>63%7%•29%</div></div>
1	3	735	<div><div>63%7%•29%</div></div>
1	4	735	<div><div>62%8%•29%</div></div>
1	5	735	<div><div>62%8%•29%</div></div>
1	6	735	<div><div>63%7%•29%</div></div>
1	7	735	<div><div>63%7%•29%</div></div>
1	A	735	<div><div>62%8%•29%</div></div>


























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Mol	Chain	Length	Quality of chain
1	B	735	
1	C	735	
1	D	735	
1	E	735	
1	F	735	
1	G	735	
1	H	735	
1	I	735	
1	J	735	
1	K	735	
1	L	735	
1	M	735	
1	N	735	
1	O	735	
1	P	735	
1	Q	735	
1	R	735	
1	S	735	
1	T	735	
1	U	735	
1	V	735	
1	W	735	
1	X	735	
1	Y	735	
1	Z	735	

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Mol	Chain	Length	Quality of chain
1	a	735	
1	b	735	
1	c	735	
1	d	735	
1	e	735	
1	f	735	
1	g	735	
1	h	735	
1	i	735	
1	j	735	
1	k	735	
1	l	735	
1	m	735	
1	n	735	
1	o	735	
1	p	735	
1	q	735	
1	r	735	
1	s	735	
1	t	735	
1	u	735	
1	v	735	
1	w	735	
1	x	735	
1	y	735	

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Mol	Chain	Length	Quality of chain
1	z	735	<div><div></div><div>68%</div><div></div><div>•</div><div>29%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 248280 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	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	K	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	L	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	M	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	N	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	O	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	P	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	Q	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	R	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	S	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	T	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	B	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	U	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	V	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	W	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	X	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	Y	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	a	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	b	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	c	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	d	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	C	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	e	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	f	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	g	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	h	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	i	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	j	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	k	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	l	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	m	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	n	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	D	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	o	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	p	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	q	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	r	519	Total 4138	C 2605	N 716	O 803	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	s	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	t	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	u	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	v	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	w	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	x	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	E	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	y	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	z	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	0	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	1	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	2	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	3	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	4	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	5	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	6	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	7	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	F	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	G	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	H	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	I	519	Total 4138	C 2605	N 716	O 803	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLN	LYS	conflict	UNP Q670R6
A	164	GLN	ASN	conflict	UNP Q670R6
A	312	ASN	SER	conflict	UNP Q670R6
A	447	LYS	ARG	conflict	UNP Q670R6
A	450	ALA	THR	conflict	UNP Q670R6
A	593	THR	SER	conflict	UNP Q670R6
K	39	GLN	LYS	conflict	UNP Q670R6
K	164	GLN	ASN	conflict	UNP Q670R6
K	312	ASN	SER	conflict	UNP Q670R6
K	447	LYS	ARG	conflict	UNP Q670R6
K	450	ALA	THR	conflict	UNP Q670R6
K	593	THR	SER	conflict	UNP Q670R6
L	39	GLN	LYS	conflict	UNP Q670R6
L	164	GLN	ASN	conflict	UNP Q670R6
L	312	ASN	SER	conflict	UNP Q670R6
L	447	LYS	ARG	conflict	UNP Q670R6
L	450	ALA	THR	conflict	UNP Q670R6
L	593	THR	SER	conflict	UNP Q670R6
M	39	GLN	LYS	conflict	UNP Q670R6
M	164	GLN	ASN	conflict	UNP Q670R6
M	312	ASN	SER	conflict	UNP Q670R6
M	447	LYS	ARG	conflict	UNP Q670R6
M	450	ALA	THR	conflict	UNP Q670R6
M	593	THR	SER	conflict	UNP Q670R6
N	39	GLN	LYS	conflict	UNP Q670R6
N	164	GLN	ASN	conflict	UNP Q670R6
N	312	ASN	SER	conflict	UNP Q670R6
N	447	LYS	ARG	conflict	UNP Q670R6
N	450	ALA	THR	conflict	UNP Q670R6
N	593	THR	SER	conflict	UNP Q670R6
O	39	GLN	LYS	conflict	UNP Q670R6
O	164	GLN	ASN	conflict	UNP Q670R6
O	312	ASN	SER	conflict	UNP Q670R6
O	447	LYS	ARG	conflict	UNP Q670R6
O	450	ALA	THR	conflict	UNP Q670R6
O	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
P	39	GLN	LYS	conflict	UNP Q670R6
P	164	GLN	ASN	conflict	UNP Q670R6
P	312	ASN	SER	conflict	UNP Q670R6
P	447	LYS	ARG	conflict	UNP Q670R6
P	450	ALA	THR	conflict	UNP Q670R6
P	593	THR	SER	conflict	UNP Q670R6
Q	39	GLN	LYS	conflict	UNP Q670R6
Q	164	GLN	ASN	conflict	UNP Q670R6
Q	312	ASN	SER	conflict	UNP Q670R6
Q	447	LYS	ARG	conflict	UNP Q670R6
Q	450	ALA	THR	conflict	UNP Q670R6
Q	593	THR	SER	conflict	UNP Q670R6
R	39	GLN	LYS	conflict	UNP Q670R6
R	164	GLN	ASN	conflict	UNP Q670R6
R	312	ASN	SER	conflict	UNP Q670R6
R	447	LYS	ARG	conflict	UNP Q670R6
R	450	ALA	THR	conflict	UNP Q670R6
R	593	THR	SER	conflict	UNP Q670R6
S	39	GLN	LYS	conflict	UNP Q670R6
S	164	GLN	ASN	conflict	UNP Q670R6
S	312	ASN	SER	conflict	UNP Q670R6
S	447	LYS	ARG	conflict	UNP Q670R6
S	450	ALA	THR	conflict	UNP Q670R6
S	593	THR	SER	conflict	UNP Q670R6
T	39	GLN	LYS	conflict	UNP Q670R6
T	164	GLN	ASN	conflict	UNP Q670R6
T	312	ASN	SER	conflict	UNP Q670R6
T	447	LYS	ARG	conflict	UNP Q670R6
T	450	ALA	THR	conflict	UNP Q670R6
T	593	THR	SER	conflict	UNP Q670R6
B	39	GLN	LYS	conflict	UNP Q670R6
B	164	GLN	ASN	conflict	UNP Q670R6
B	312	ASN	SER	conflict	UNP Q670R6
B	447	LYS	ARG	conflict	UNP Q670R6
B	450	ALA	THR	conflict	UNP Q670R6
B	593	THR	SER	conflict	UNP Q670R6
U	39	GLN	LYS	conflict	UNP Q670R6
U	164	GLN	ASN	conflict	UNP Q670R6
U	312	ASN	SER	conflict	UNP Q670R6
U	447	LYS	ARG	conflict	UNP Q670R6
U	450	ALA	THR	conflict	UNP Q670R6
U	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
V	39	GLN	LYS	conflict	UNP Q670R6
V	164	GLN	ASN	conflict	UNP Q670R6
V	312	ASN	SER	conflict	UNP Q670R6
V	447	LYS	ARG	conflict	UNP Q670R6
V	450	ALA	THR	conflict	UNP Q670R6
V	593	THR	SER	conflict	UNP Q670R6
W	39	GLN	LYS	conflict	UNP Q670R6
W	164	GLN	ASN	conflict	UNP Q670R6
W	312	ASN	SER	conflict	UNP Q670R6
W	447	LYS	ARG	conflict	UNP Q670R6
W	450	ALA	THR	conflict	UNP Q670R6
W	593	THR	SER	conflict	UNP Q670R6
X	39	GLN	LYS	conflict	UNP Q670R6
X	164	GLN	ASN	conflict	UNP Q670R6
X	312	ASN	SER	conflict	UNP Q670R6
X	447	LYS	ARG	conflict	UNP Q670R6
X	450	ALA	THR	conflict	UNP Q670R6
X	593	THR	SER	conflict	UNP Q670R6
Y	39	GLN	LYS	conflict	UNP Q670R6
Y	164	GLN	ASN	conflict	UNP Q670R6
Y	312	ASN	SER	conflict	UNP Q670R6
Y	447	LYS	ARG	conflict	UNP Q670R6
Y	450	ALA	THR	conflict	UNP Q670R6
Y	593	THR	SER	conflict	UNP Q670R6
Z	39	GLN	LYS	conflict	UNP Q670R6
Z	164	GLN	ASN	conflict	UNP Q670R6
Z	312	ASN	SER	conflict	UNP Q670R6
Z	447	LYS	ARG	conflict	UNP Q670R6
Z	450	ALA	THR	conflict	UNP Q670R6
Z	593	THR	SER	conflict	UNP Q670R6
a	39	GLN	LYS	conflict	UNP Q670R6
a	164	GLN	ASN	conflict	UNP Q670R6
a	312	ASN	SER	conflict	UNP Q670R6
a	447	LYS	ARG	conflict	UNP Q670R6
a	450	ALA	THR	conflict	UNP Q670R6
a	593	THR	SER	conflict	UNP Q670R6
b	39	GLN	LYS	conflict	UNP Q670R6
b	164	GLN	ASN	conflict	UNP Q670R6
b	312	ASN	SER	conflict	UNP Q670R6
b	447	LYS	ARG	conflict	UNP Q670R6
b	450	ALA	THR	conflict	UNP Q670R6
b	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
c	39	GLN	LYS	conflict	UNP Q670R6
c	164	GLN	ASN	conflict	UNP Q670R6
c	312	ASN	SER	conflict	UNP Q670R6
c	447	LYS	ARG	conflict	UNP Q670R6
c	450	ALA	THR	conflict	UNP Q670R6
c	593	THR	SER	conflict	UNP Q670R6
d	39	GLN	LYS	conflict	UNP Q670R6
d	164	GLN	ASN	conflict	UNP Q670R6
d	312	ASN	SER	conflict	UNP Q670R6
d	447	LYS	ARG	conflict	UNP Q670R6
d	450	ALA	THR	conflict	UNP Q670R6
d	593	THR	SER	conflict	UNP Q670R6
C	39	GLN	LYS	conflict	UNP Q670R6
C	164	GLN	ASN	conflict	UNP Q670R6
C	312	ASN	SER	conflict	UNP Q670R6
C	447	LYS	ARG	conflict	UNP Q670R6
C	450	ALA	THR	conflict	UNP Q670R6
C	593	THR	SER	conflict	UNP Q670R6
e	39	GLN	LYS	conflict	UNP Q670R6
e	164	GLN	ASN	conflict	UNP Q670R6
e	312	ASN	SER	conflict	UNP Q670R6
e	447	LYS	ARG	conflict	UNP Q670R6
e	450	ALA	THR	conflict	UNP Q670R6
e	593	THR	SER	conflict	UNP Q670R6
f	39	GLN	LYS	conflict	UNP Q670R6
f	164	GLN	ASN	conflict	UNP Q670R6
f	312	ASN	SER	conflict	UNP Q670R6
f	447	LYS	ARG	conflict	UNP Q670R6
f	450	ALA	THR	conflict	UNP Q670R6
f	593	THR	SER	conflict	UNP Q670R6
g	39	GLN	LYS	conflict	UNP Q670R6
g	164	GLN	ASN	conflict	UNP Q670R6
g	312	ASN	SER	conflict	UNP Q670R6
g	447	LYS	ARG	conflict	UNP Q670R6
g	450	ALA	THR	conflict	UNP Q670R6
g	593	THR	SER	conflict	UNP Q670R6
h	39	GLN	LYS	conflict	UNP Q670R6
h	164	GLN	ASN	conflict	UNP Q670R6
h	312	ASN	SER	conflict	UNP Q670R6
h	447	LYS	ARG	conflict	UNP Q670R6
h	450	ALA	THR	conflict	UNP Q670R6
h	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
i	39	GLN	LYS	conflict	UNP Q670R6
i	164	GLN	ASN	conflict	UNP Q670R6
i	312	ASN	SER	conflict	UNP Q670R6
i	447	LYS	ARG	conflict	UNP Q670R6
i	450	ALA	THR	conflict	UNP Q670R6
i	593	THR	SER	conflict	UNP Q670R6
j	39	GLN	LYS	conflict	UNP Q670R6
j	164	GLN	ASN	conflict	UNP Q670R6
j	312	ASN	SER	conflict	UNP Q670R6
j	447	LYS	ARG	conflict	UNP Q670R6
j	450	ALA	THR	conflict	UNP Q670R6
j	593	THR	SER	conflict	UNP Q670R6
k	39	GLN	LYS	conflict	UNP Q670R6
k	164	GLN	ASN	conflict	UNP Q670R6
k	312	ASN	SER	conflict	UNP Q670R6
k	447	LYS	ARG	conflict	UNP Q670R6
k	450	ALA	THR	conflict	UNP Q670R6
k	593	THR	SER	conflict	UNP Q670R6
l	39	GLN	LYS	conflict	UNP Q670R6
l	164	GLN	ASN	conflict	UNP Q670R6
l	312	ASN	SER	conflict	UNP Q670R6
l	447	LYS	ARG	conflict	UNP Q670R6
l	450	ALA	THR	conflict	UNP Q670R6
l	593	THR	SER	conflict	UNP Q670R6
m	39	GLN	LYS	conflict	UNP Q670R6
m	164	GLN	ASN	conflict	UNP Q670R6
m	312	ASN	SER	conflict	UNP Q670R6
m	447	LYS	ARG	conflict	UNP Q670R6
m	450	ALA	THR	conflict	UNP Q670R6
m	593	THR	SER	conflict	UNP Q670R6
n	39	GLN	LYS	conflict	UNP Q670R6
n	164	GLN	ASN	conflict	UNP Q670R6
n	312	ASN	SER	conflict	UNP Q670R6
n	447	LYS	ARG	conflict	UNP Q670R6
n	450	ALA	THR	conflict	UNP Q670R6
n	593	THR	SER	conflict	UNP Q670R6
D	39	GLN	LYS	conflict	UNP Q670R6
D	164	GLN	ASN	conflict	UNP Q670R6
D	312	ASN	SER	conflict	UNP Q670R6
D	447	LYS	ARG	conflict	UNP Q670R6
D	450	ALA	THR	conflict	UNP Q670R6
D	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
o	39	GLN	LYS	conflict	UNP Q670R6
o	164	GLN	ASN	conflict	UNP Q670R6
o	312	ASN	SER	conflict	UNP Q670R6
o	447	LYS	ARG	conflict	UNP Q670R6
o	450	ALA	THR	conflict	UNP Q670R6
o	593	THR	SER	conflict	UNP Q670R6
p	39	GLN	LYS	conflict	UNP Q670R6
p	164	GLN	ASN	conflict	UNP Q670R6
p	312	ASN	SER	conflict	UNP Q670R6
p	447	LYS	ARG	conflict	UNP Q670R6
p	450	ALA	THR	conflict	UNP Q670R6
p	593	THR	SER	conflict	UNP Q670R6
q	39	GLN	LYS	conflict	UNP Q670R6
q	164	GLN	ASN	conflict	UNP Q670R6
q	312	ASN	SER	conflict	UNP Q670R6
q	447	LYS	ARG	conflict	UNP Q670R6
q	450	ALA	THR	conflict	UNP Q670R6
q	593	THR	SER	conflict	UNP Q670R6
r	39	GLN	LYS	conflict	UNP Q670R6
r	164	GLN	ASN	conflict	UNP Q670R6
r	312	ASN	SER	conflict	UNP Q670R6
r	447	LYS	ARG	conflict	UNP Q670R6
r	450	ALA	THR	conflict	UNP Q670R6
r	593	THR	SER	conflict	UNP Q670R6
s	39	GLN	LYS	conflict	UNP Q670R6
s	164	GLN	ASN	conflict	UNP Q670R6
s	312	ASN	SER	conflict	UNP Q670R6
s	447	LYS	ARG	conflict	UNP Q670R6
s	450	ALA	THR	conflict	UNP Q670R6
s	593	THR	SER	conflict	UNP Q670R6
t	39	GLN	LYS	conflict	UNP Q670R6
t	164	GLN	ASN	conflict	UNP Q670R6
t	312	ASN	SER	conflict	UNP Q670R6
t	447	LYS	ARG	conflict	UNP Q670R6
t	450	ALA	THR	conflict	UNP Q670R6
t	593	THR	SER	conflict	UNP Q670R6
u	39	GLN	LYS	conflict	UNP Q670R6
u	164	GLN	ASN	conflict	UNP Q670R6
u	312	ASN	SER	conflict	UNP Q670R6
u	447	LYS	ARG	conflict	UNP Q670R6
u	450	ALA	THR	conflict	UNP Q670R6
u	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
v	39	GLN	LYS	conflict	UNP Q670R6
v	164	GLN	ASN	conflict	UNP Q670R6
v	312	ASN	SER	conflict	UNP Q670R6
v	447	LYS	ARG	conflict	UNP Q670R6
v	450	ALA	THR	conflict	UNP Q670R6
v	593	THR	SER	conflict	UNP Q670R6
w	39	GLN	LYS	conflict	UNP Q670R6
w	164	GLN	ASN	conflict	UNP Q670R6
w	312	ASN	SER	conflict	UNP Q670R6
w	447	LYS	ARG	conflict	UNP Q670R6
w	450	ALA	THR	conflict	UNP Q670R6
w	593	THR	SER	conflict	UNP Q670R6
x	39	GLN	LYS	conflict	UNP Q670R6
x	164	GLN	ASN	conflict	UNP Q670R6
x	312	ASN	SER	conflict	UNP Q670R6
x	447	LYS	ARG	conflict	UNP Q670R6
x	450	ALA	THR	conflict	UNP Q670R6
x	593	THR	SER	conflict	UNP Q670R6
E	39	GLN	LYS	conflict	UNP Q670R6
E	164	GLN	ASN	conflict	UNP Q670R6
E	312	ASN	SER	conflict	UNP Q670R6
E	447	LYS	ARG	conflict	UNP Q670R6
E	450	ALA	THR	conflict	UNP Q670R6
E	593	THR	SER	conflict	UNP Q670R6
y	39	GLN	LYS	conflict	UNP Q670R6
y	164	GLN	ASN	conflict	UNP Q670R6
y	312	ASN	SER	conflict	UNP Q670R6
y	447	LYS	ARG	conflict	UNP Q670R6
y	450	ALA	THR	conflict	UNP Q670R6
y	593	THR	SER	conflict	UNP Q670R6
z	39	GLN	LYS	conflict	UNP Q670R6
z	164	GLN	ASN	conflict	UNP Q670R6
z	312	ASN	SER	conflict	UNP Q670R6
z	447	LYS	ARG	conflict	UNP Q670R6
z	450	ALA	THR	conflict	UNP Q670R6
z	593	THR	SER	conflict	UNP Q670R6
0	39	GLN	LYS	conflict	UNP Q670R6
0	164	GLN	ASN	conflict	UNP Q670R6
0	312	ASN	SER	conflict	UNP Q670R6
0	447	LYS	ARG	conflict	UNP Q670R6
0	450	ALA	THR	conflict	UNP Q670R6
0	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
1	39	GLN	LYS	conflict	UNP Q670R6
1	164	GLN	ASN	conflict	UNP Q670R6
1	312	ASN	SER	conflict	UNP Q670R6
1	447	LYS	ARG	conflict	UNP Q670R6
1	450	ALA	THR	conflict	UNP Q670R6
1	593	THR	SER	conflict	UNP Q670R6
2	39	GLN	LYS	conflict	UNP Q670R6
2	164	GLN	ASN	conflict	UNP Q670R6
2	312	ASN	SER	conflict	UNP Q670R6
2	447	LYS	ARG	conflict	UNP Q670R6
2	450	ALA	THR	conflict	UNP Q670R6
2	593	THR	SER	conflict	UNP Q670R6
3	39	GLN	LYS	conflict	UNP Q670R6
3	164	GLN	ASN	conflict	UNP Q670R6
3	312	ASN	SER	conflict	UNP Q670R6
3	447	LYS	ARG	conflict	UNP Q670R6
3	450	ALA	THR	conflict	UNP Q670R6
3	593	THR	SER	conflict	UNP Q670R6
4	39	GLN	LYS	conflict	UNP Q670R6
4	164	GLN	ASN	conflict	UNP Q670R6
4	312	ASN	SER	conflict	UNP Q670R6
4	447	LYS	ARG	conflict	UNP Q670R6
4	450	ALA	THR	conflict	UNP Q670R6
4	593	THR	SER	conflict	UNP Q670R6
5	39	GLN	LYS	conflict	UNP Q670R6
5	164	GLN	ASN	conflict	UNP Q670R6
5	312	ASN	SER	conflict	UNP Q670R6
5	447	LYS	ARG	conflict	UNP Q670R6
5	450	ALA	THR	conflict	UNP Q670R6
5	593	THR	SER	conflict	UNP Q670R6
6	39	GLN	LYS	conflict	UNP Q670R6
6	164	GLN	ASN	conflict	UNP Q670R6
6	312	ASN	SER	conflict	UNP Q670R6
6	447	LYS	ARG	conflict	UNP Q670R6
6	450	ALA	THR	conflict	UNP Q670R6
6	593	THR	SER	conflict	UNP Q670R6
7	39	GLN	LYS	conflict	UNP Q670R6
7	164	GLN	ASN	conflict	UNP Q670R6
7	312	ASN	SER	conflict	UNP Q670R6
7	447	LYS	ARG	conflict	UNP Q670R6
7	450	ALA	THR	conflict	UNP Q670R6
7	593	THR	SER	conflict	UNP Q670R6

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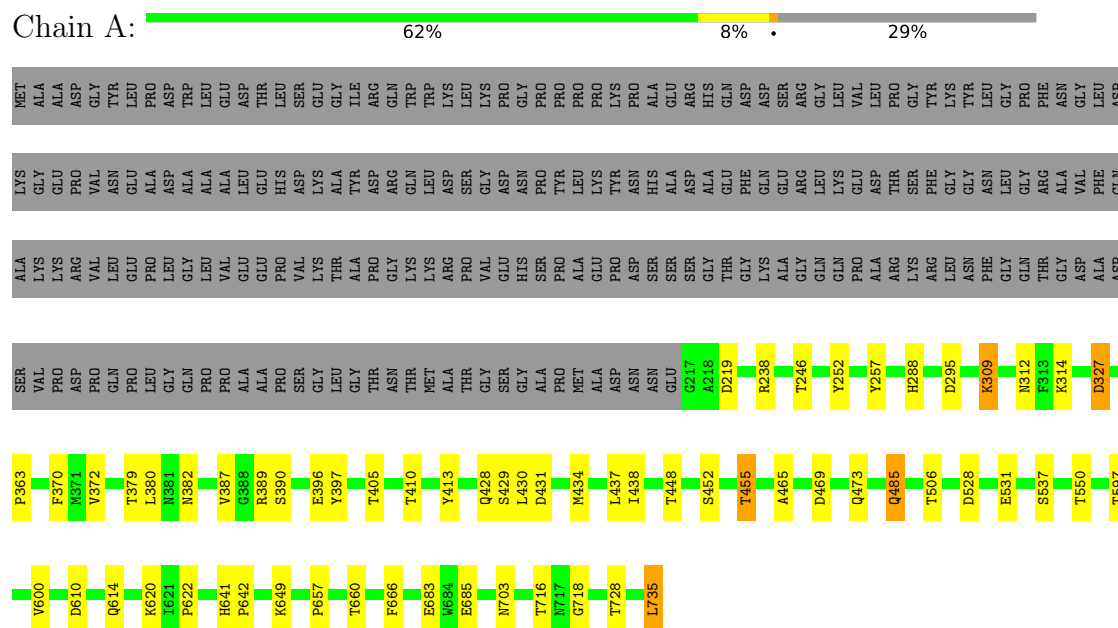
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Chain	Residue	Modelled	Actual	Comment	Reference
F	39	GLN	LYS	conflict	UNP Q670R6
F	164	GLN	ASN	conflict	UNP Q670R6
F	312	ASN	SER	conflict	UNP Q670R6
F	447	LYS	ARG	conflict	UNP Q670R6
F	450	ALA	THR	conflict	UNP Q670R6
F	593	THR	SER	conflict	UNP Q670R6
G	39	GLN	LYS	conflict	UNP Q670R6
G	164	GLN	ASN	conflict	UNP Q670R6
G	312	ASN	SER	conflict	UNP Q670R6
G	447	LYS	ARG	conflict	UNP Q670R6
G	450	ALA	THR	conflict	UNP Q670R6
G	593	THR	SER	conflict	UNP Q670R6
H	39	GLN	LYS	conflict	UNP Q670R6
H	164	GLN	ASN	conflict	UNP Q670R6
H	312	ASN	SER	conflict	UNP Q670R6
H	447	LYS	ARG	conflict	UNP Q670R6
H	450	ALA	THR	conflict	UNP Q670R6
H	593	THR	SER	conflict	UNP Q670R6
I	39	GLN	LYS	conflict	UNP Q670R6
I	164	GLN	ASN	conflict	UNP Q670R6
I	312	ASN	SER	conflict	UNP Q670R6
I	447	LYS	ARG	conflict	UNP Q670R6
I	450	ALA	THR	conflict	UNP Q670R6
I	593	THR	SER	conflict	UNP Q670R6
J	39	GLN	LYS	conflict	UNP Q670R6
J	164	GLN	ASN	conflict	UNP Q670R6
J	312	ASN	SER	conflict	UNP Q670R6
J	447	LYS	ARG	conflict	UNP Q670R6
J	450	ALA	THR	conflict	UNP Q670R6
J	593	THR	SER	conflict	UNP Q670R6

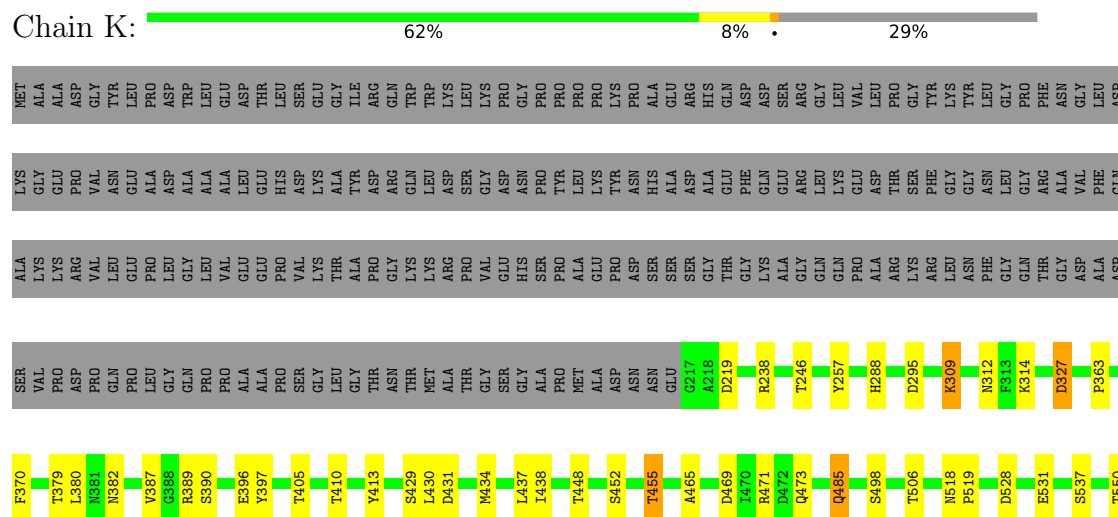
3 Residue-property plots [i](#)

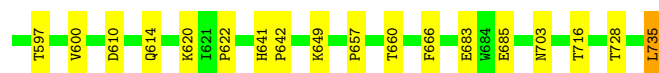
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



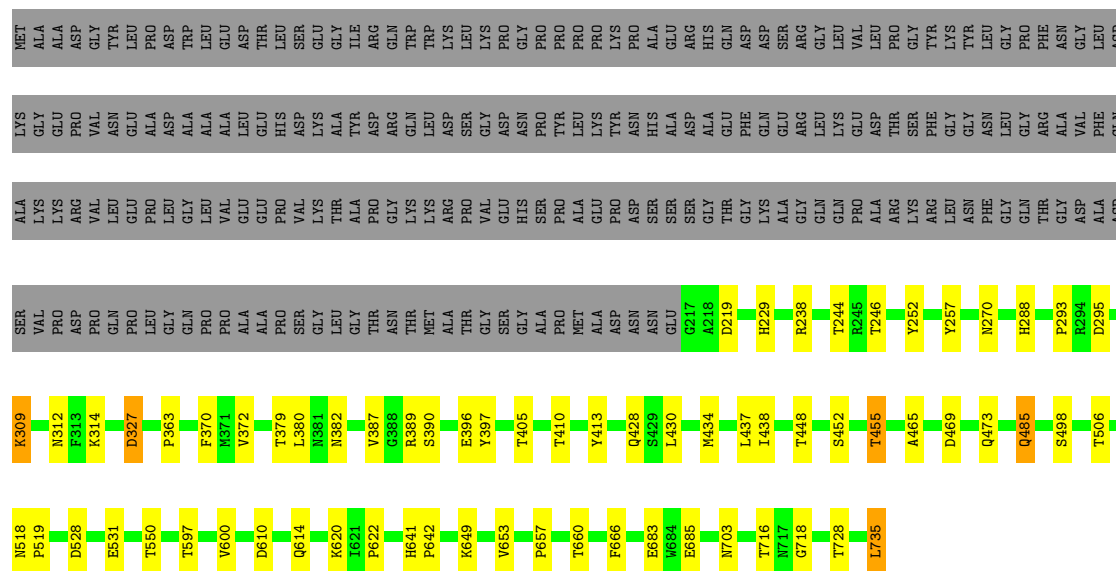
• Molecule 1: Capsid protein VP1





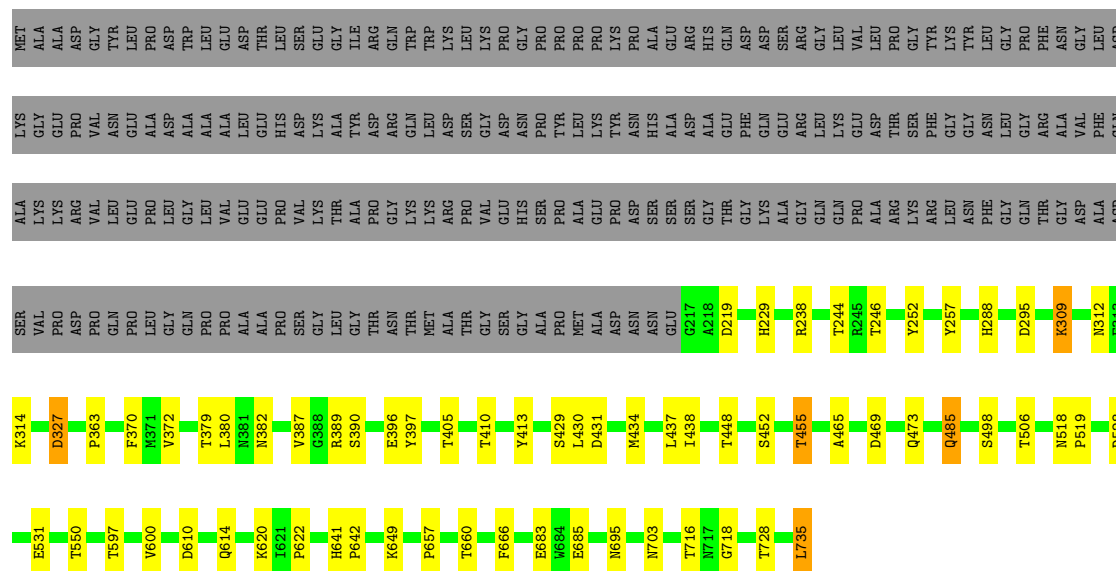
• Molecule 1: Capsid protein VP1

Chain L: 61% 9% 29%



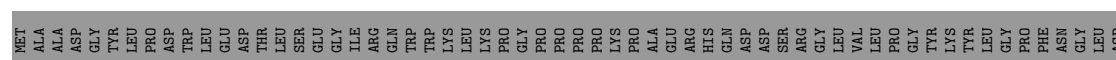
• Molecule 1: Capsid protein VP1

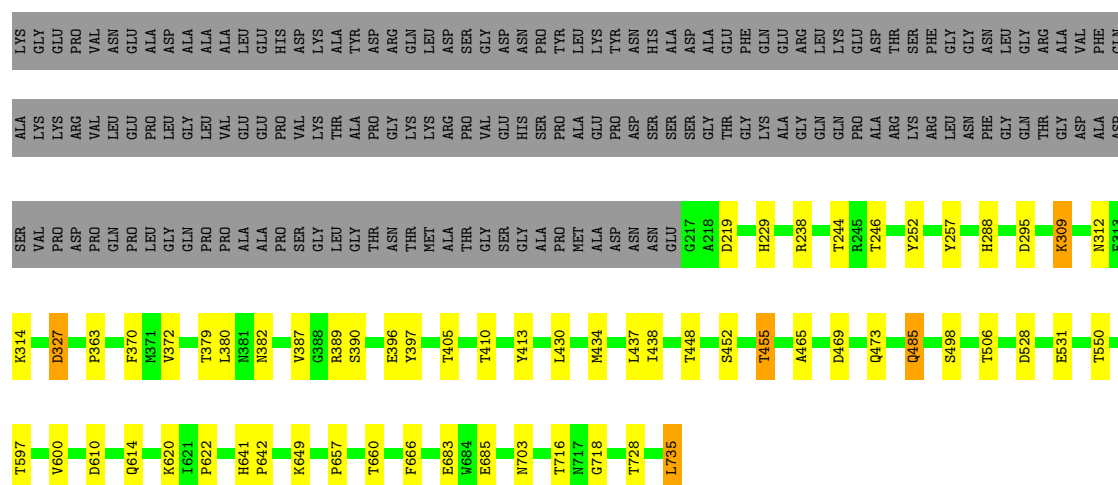
Chain M: 61% 8% 29%



• Molecule 1: Capsid protein VP1

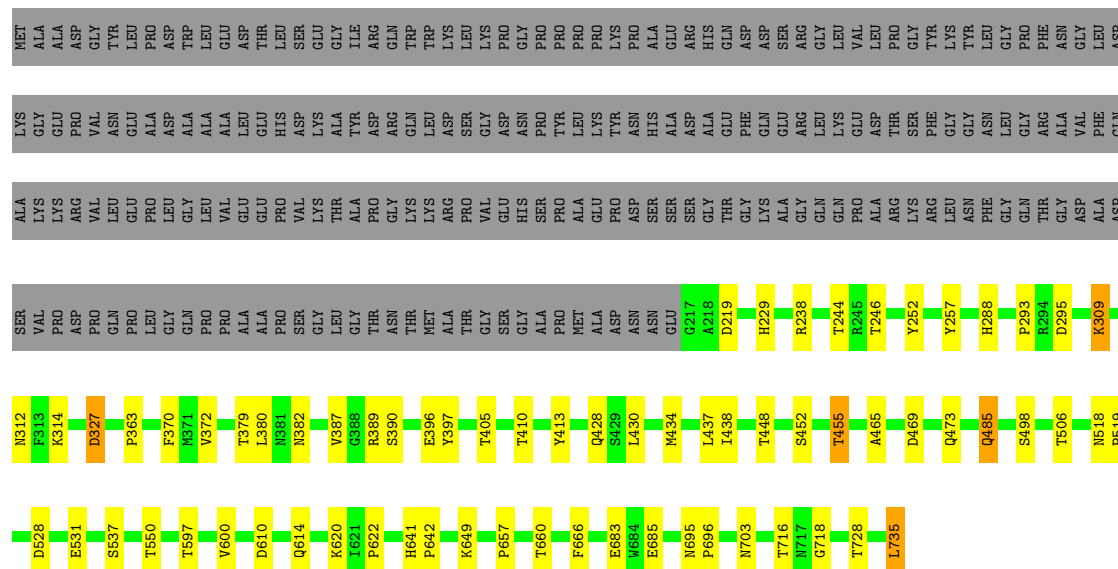
Chain N: 62% 8% 29%





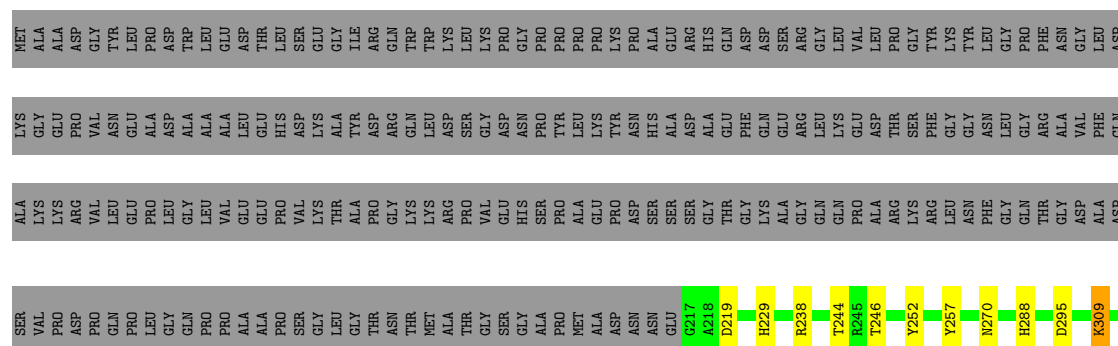
• Molecule 1: Capsid protein VP1

Chain O: 61% 9% 29%



• Molecule 1: Capsid protein VP1

Chain P: 62% 8% 29%





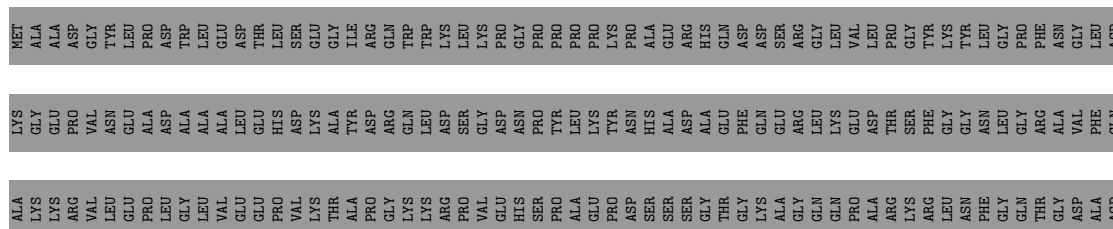
Response	Percentage
Yes, the U.S. is a democracy	62%
No, the U.S. is not a democracy	8%
Don't know	29%

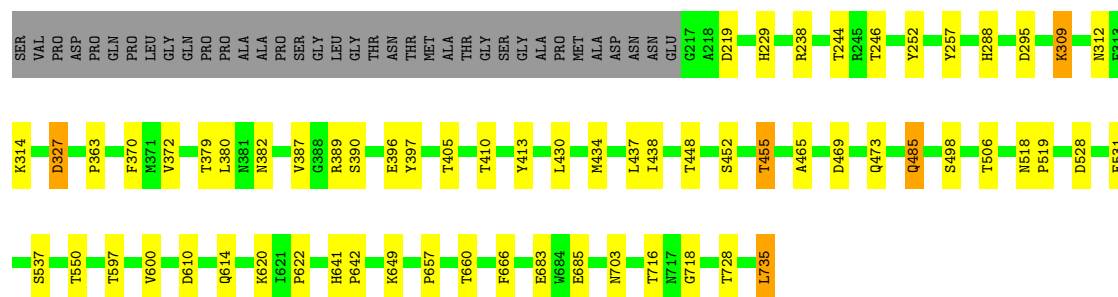


Response	Percentage
Yes	63%
No	7%
Don't know	29%



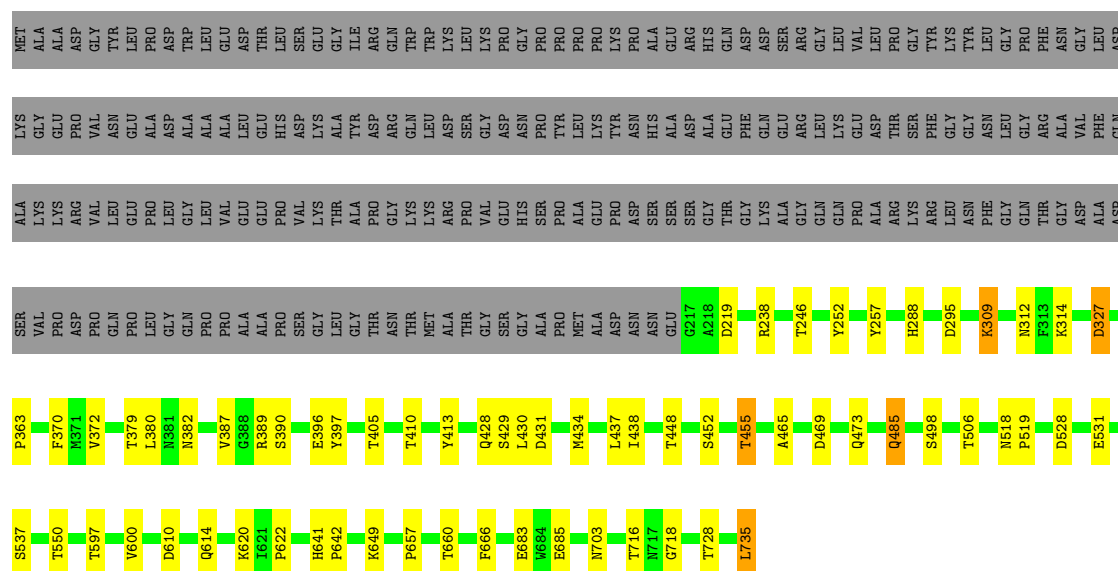
Response	Percentage
Yes	62%
No	8%
Don't know	29%





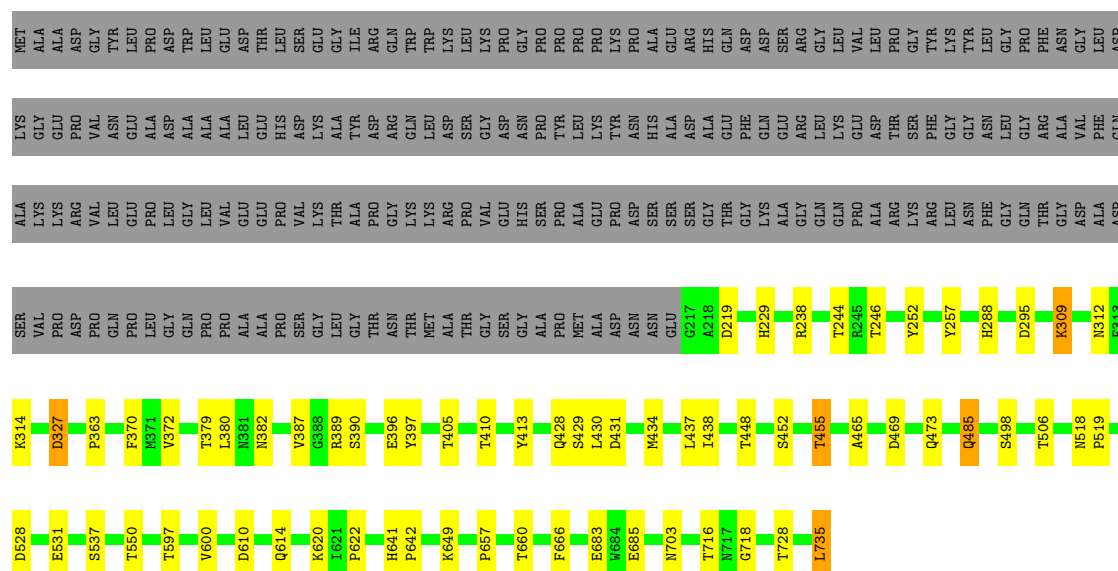
• Molecule 1: Capsid protein VP1

Chain U: 62% 8% 29%

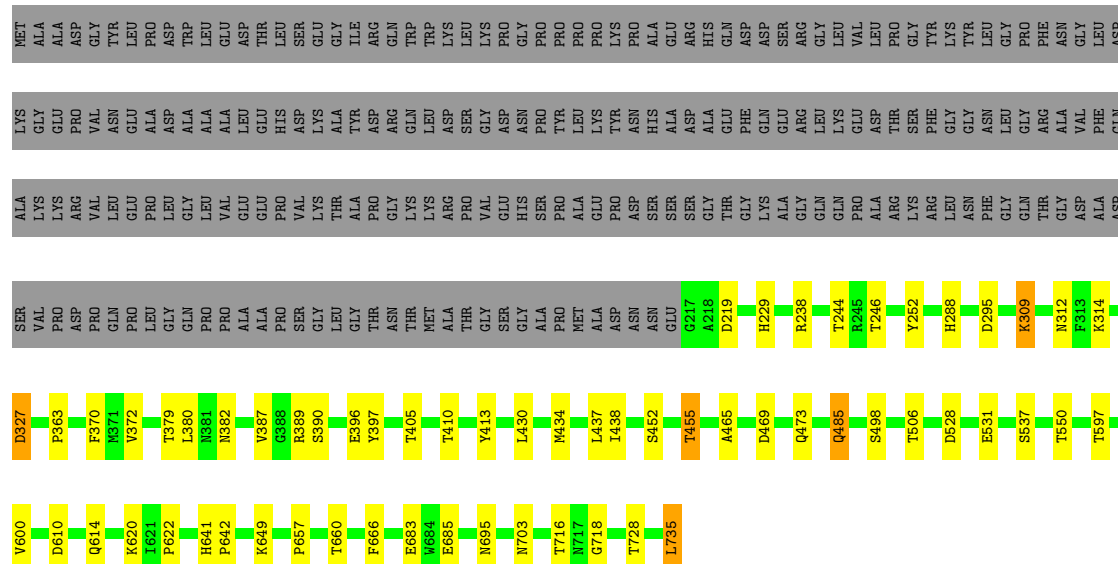


• Molecule 1: Capsid protein VP1

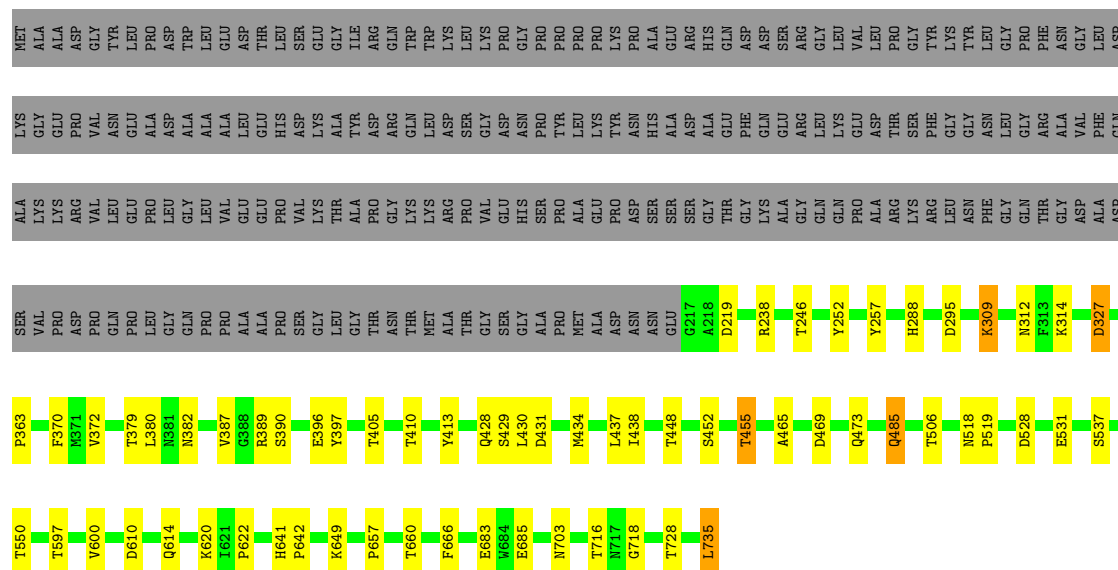
Chain V: 61% 9% 29%



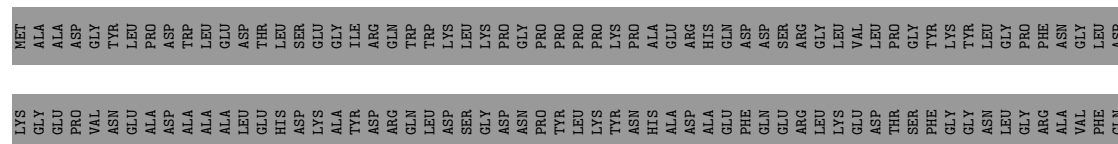
● Molecule 1: Capsid protein VP1

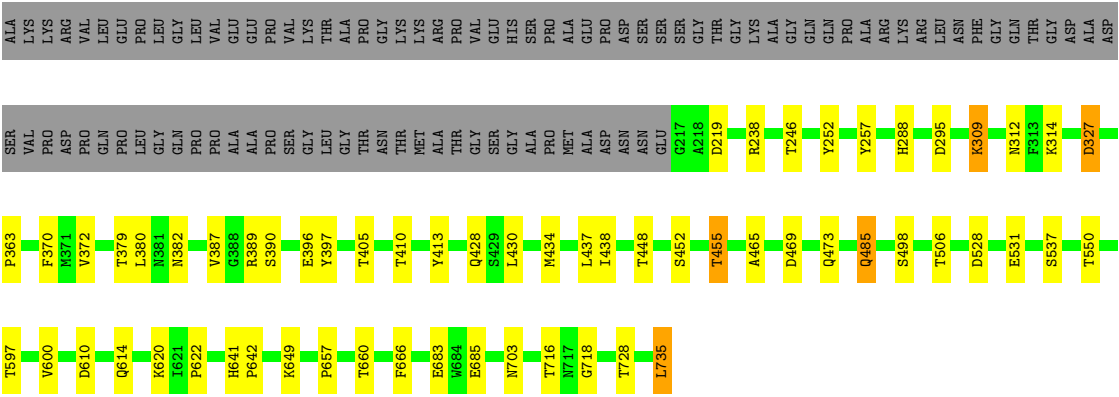
Chain W:  62% 8% 29%

● Molecule 1: Capsid protein VP1

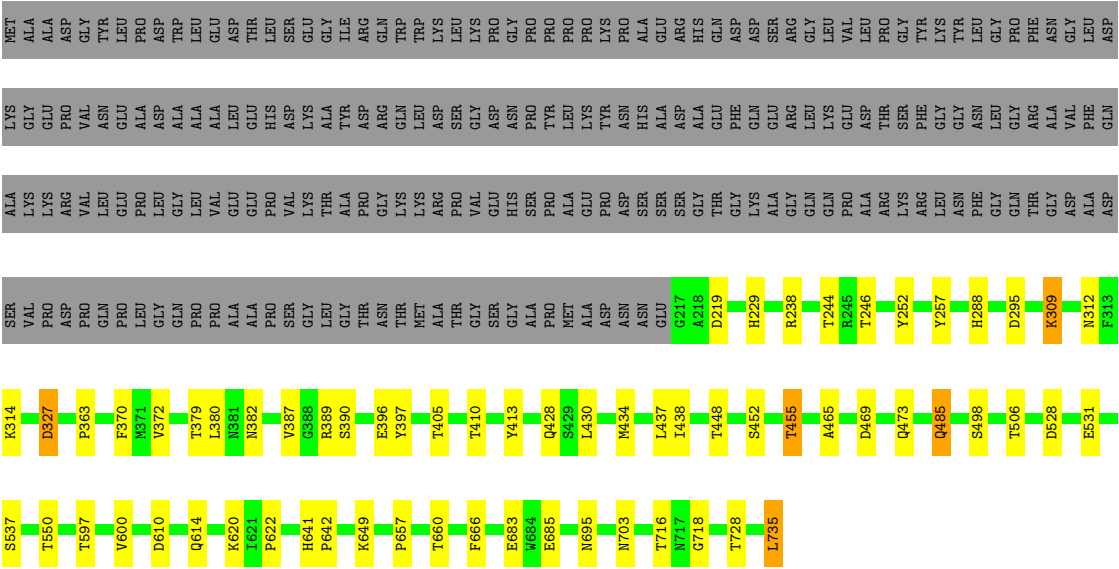
Chain X:  62% 8% 29%

● Molecule 1: Capsid protein VP1

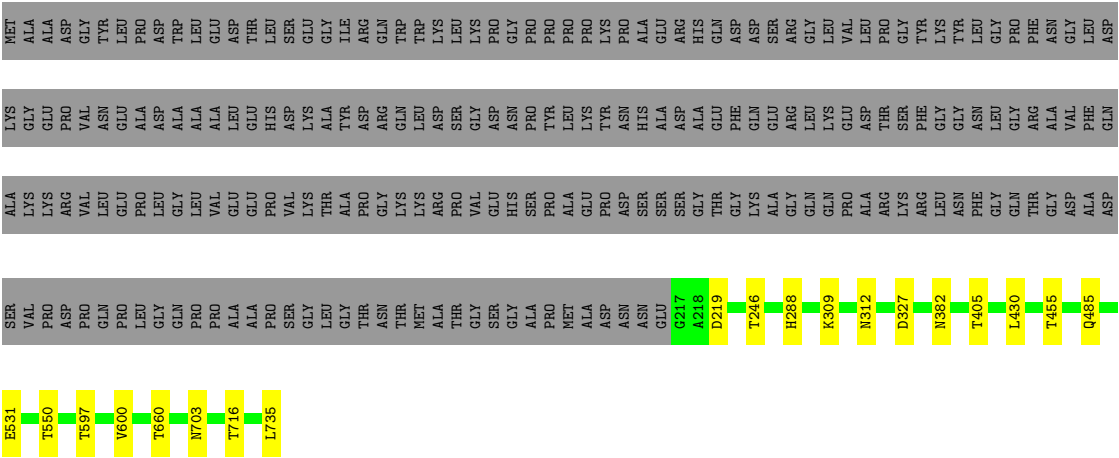
Chain Y:  62% 8% 29%



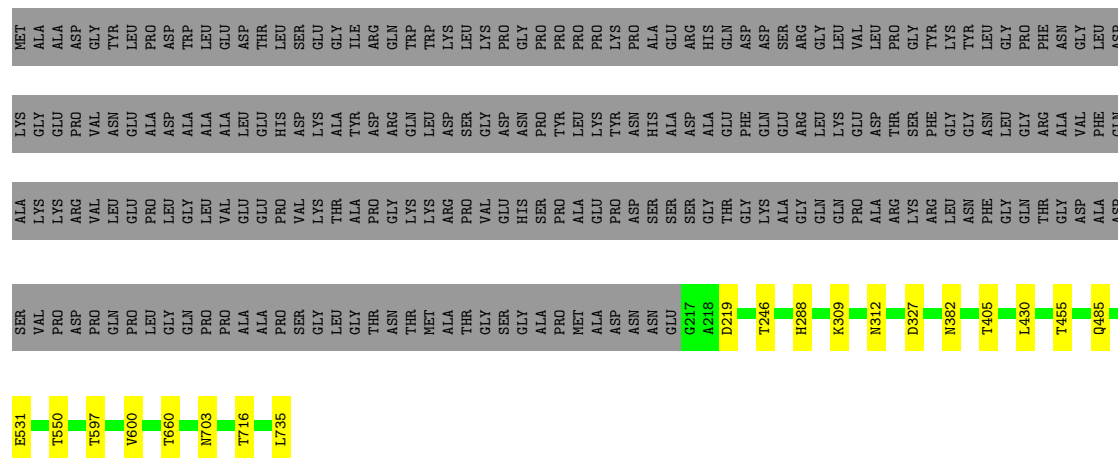
• Molecule 1: Capsid protein VP1



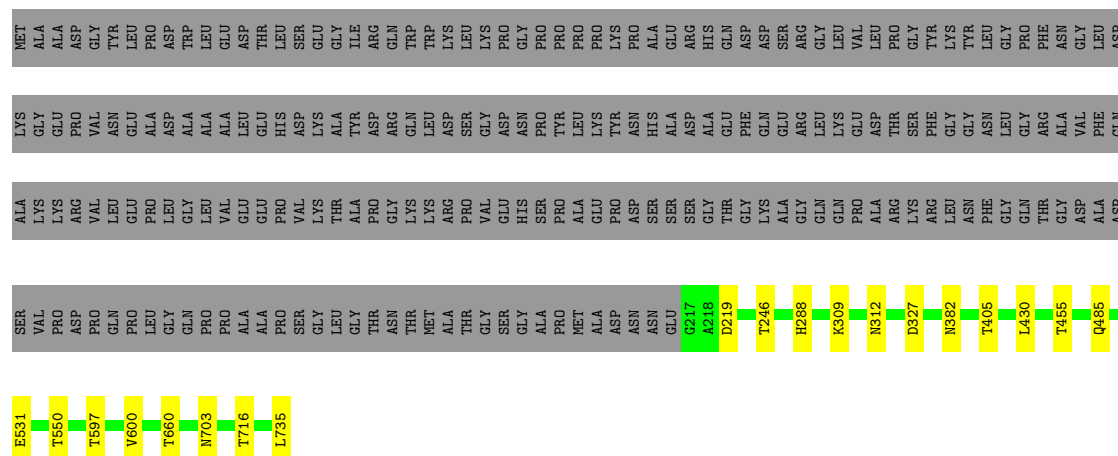
• Molecule 1: Capsid protein VP1



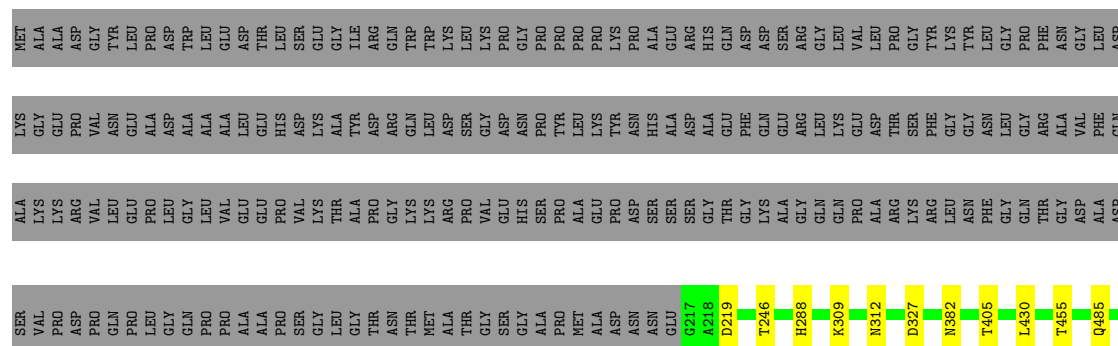
Chain b: 68% 29%

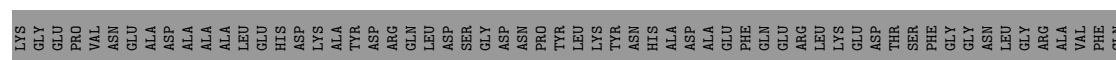


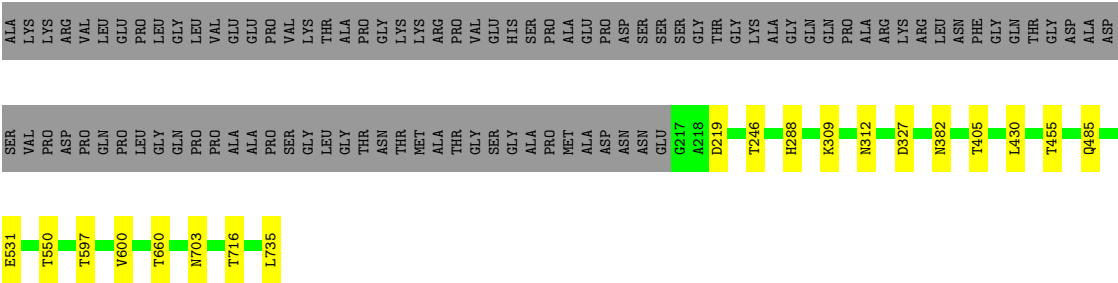
Chain c: 68% . 29%



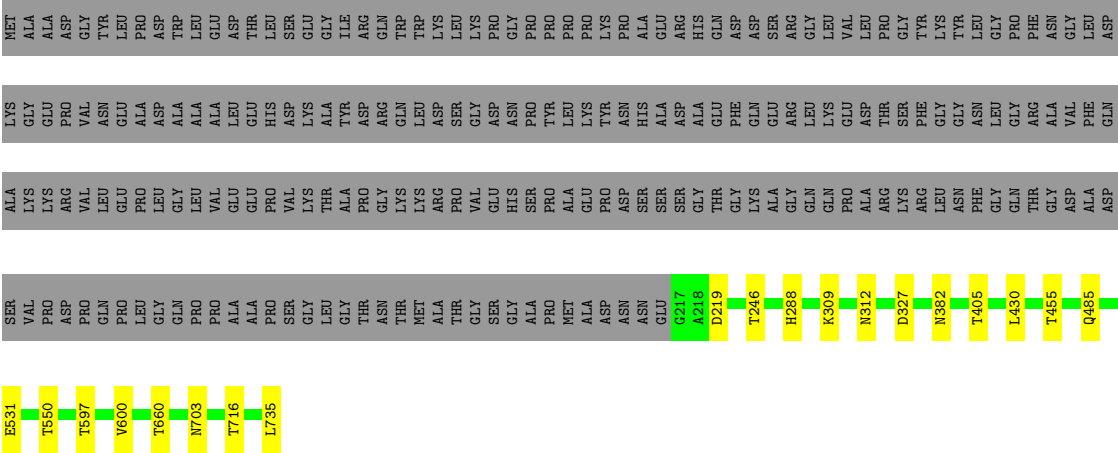
Chain d: 68% 29%



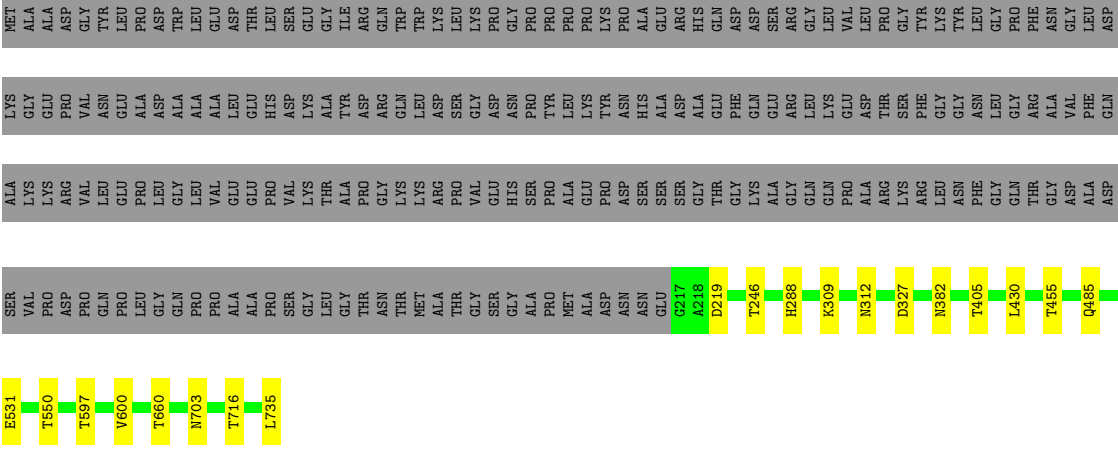




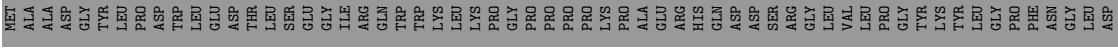
• Molecule 1: Capsid protein VP1

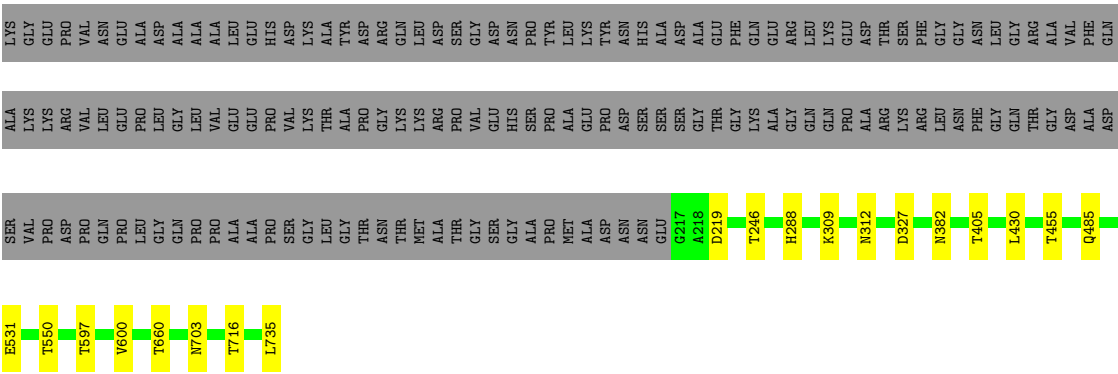


• Molecule 1: Capsid protein VP1

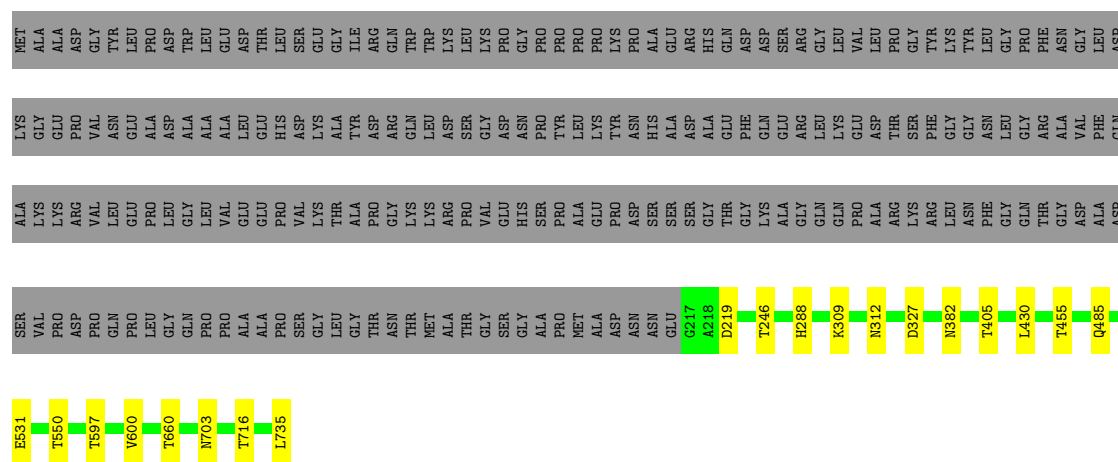


• Molecule 1: Capsid protein VP1

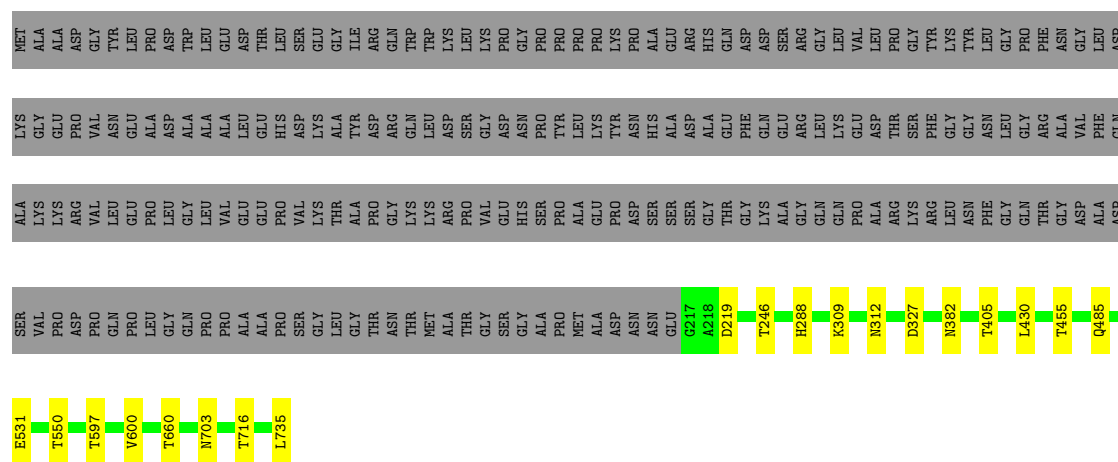




- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

Response	Percentage
Yes	62%
No	8%
Don't know	29%

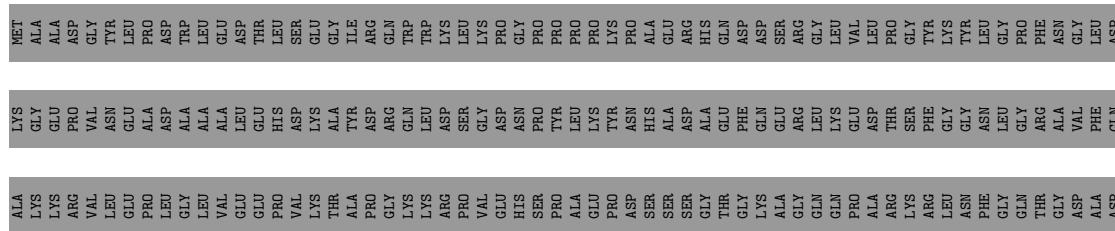


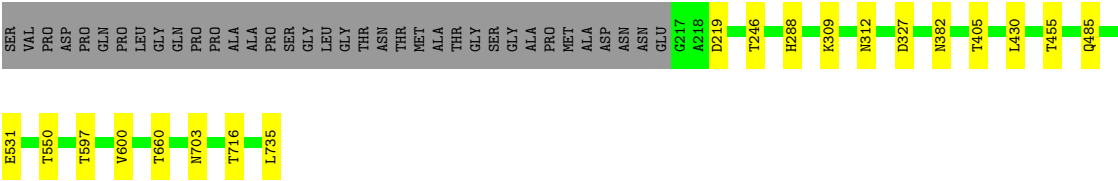
68% . 29%



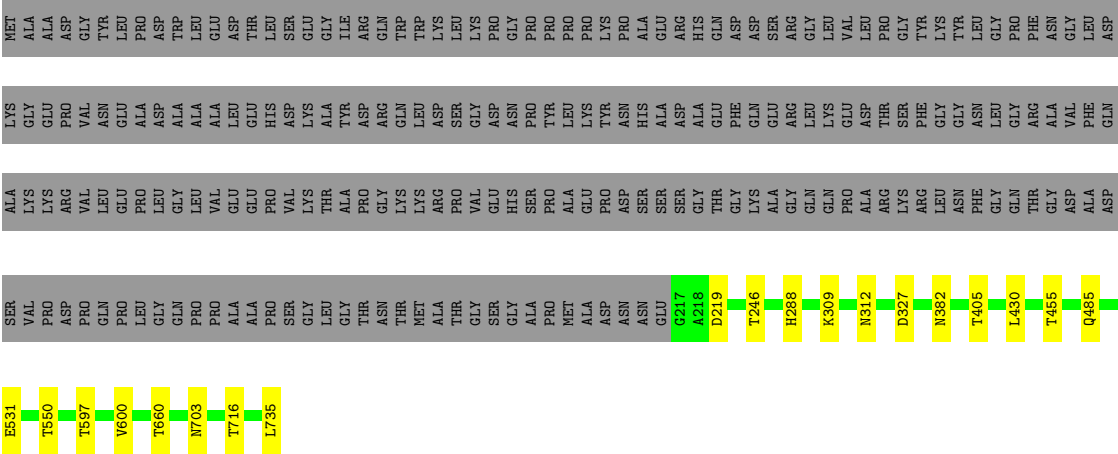
Response	Percentage
Yes, the U.S. is a democracy	68%
No, the U.S. is not a democracy	29%



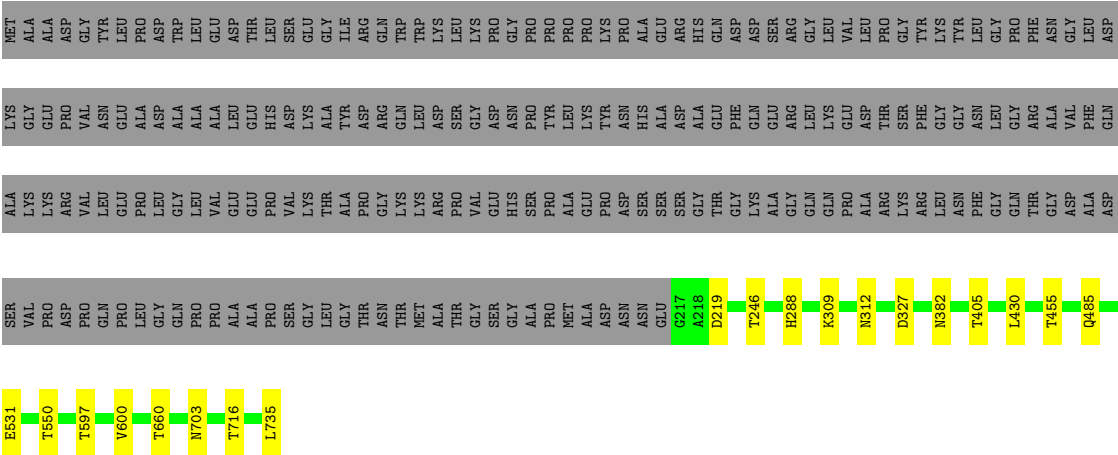




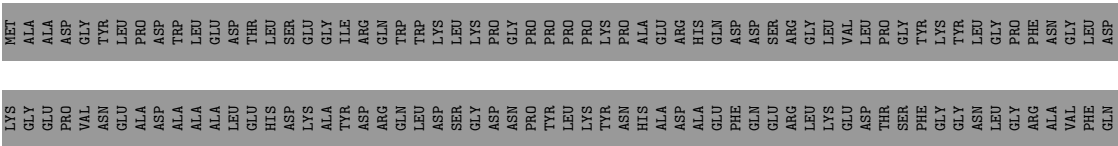
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



29%

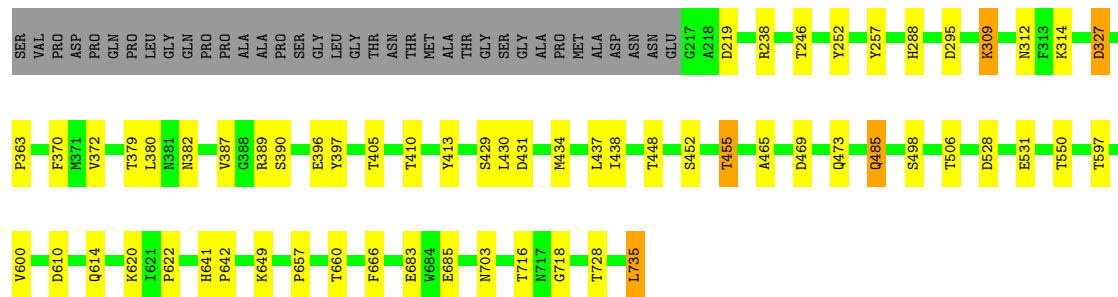
- Molecule 1: Capsid protein VP1

29%

- Molecule 1: Capsid protein VP1

29%

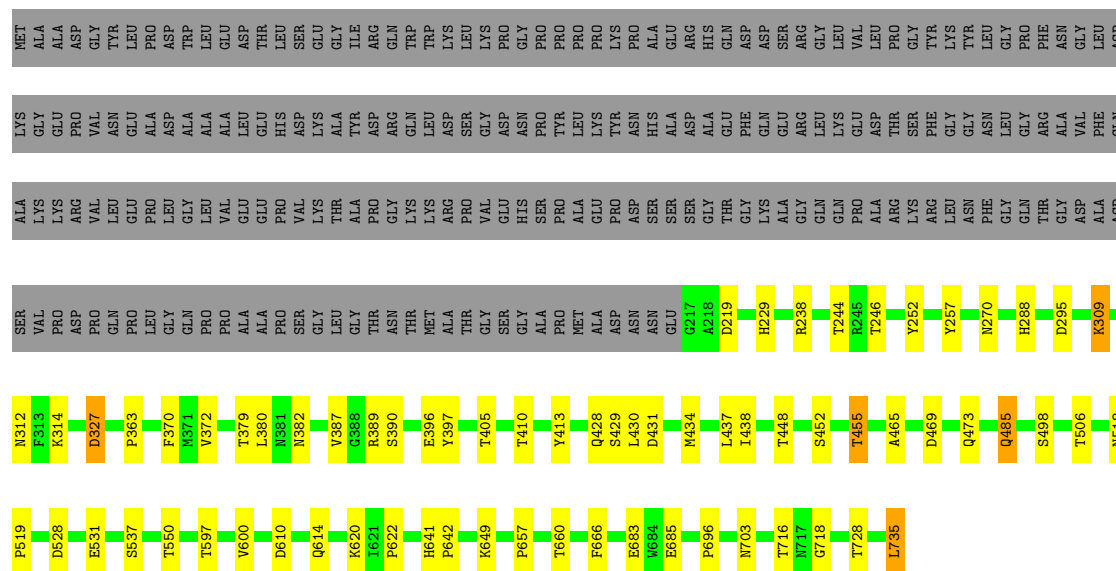






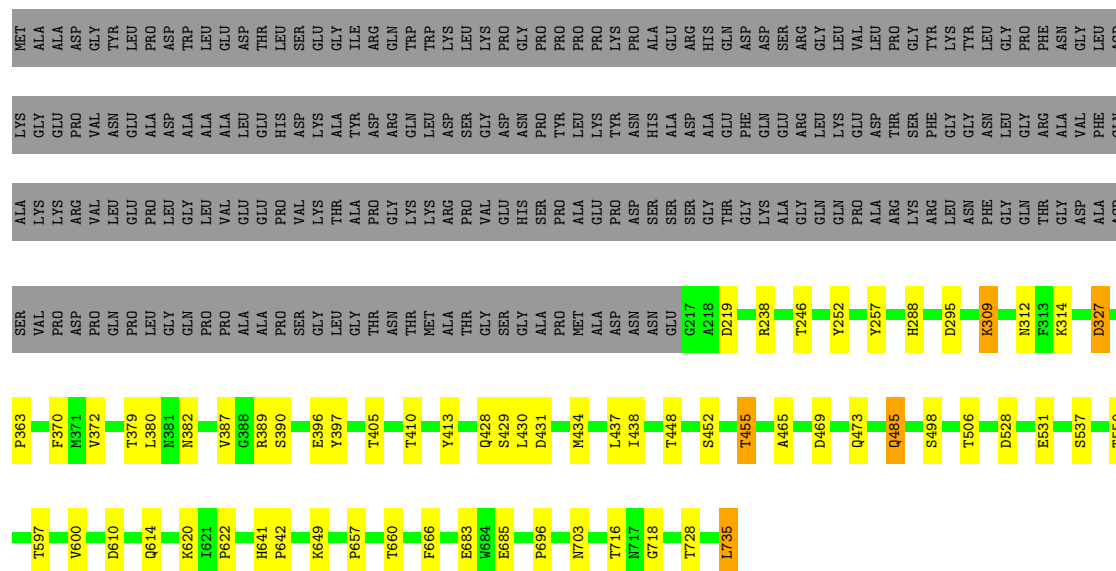
• Molecule 1: Capsid protein VP1

Chain H: 61% 9% 29%



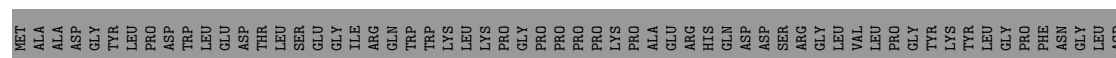
• Molecule 1: Capsid protein VP1

Chain I: 62% 8% 29%



• Molecule 1: Capsid protein VP1

Chain J: 62% 8% 29%



LYS	LYS	ALA	SER	P363	V600
GLY	GLY	LYS	VAL		
PRO	LYS	LYS	ASP	F370	D610
ARG	ARG	ARG	ASP	N371	
VAL	VAL	VAL	PRO	V372	Q614
ASN	ASN	LEU	GLN		
GLU	GLU	GLU	PRO	T379	K620
ALA	ALA	PRO	LEU	L380	F621
ASP	ASP	LEU	GLY	N381	P622
ALA	GLY	GLN	GLN	N382	
ALA	LEU	LEU	PRO		
ALA	ALA	VAL	PRO	V387	H641
LEU	LEU	GLU	ALA	G388	P642
GLU	GLU	GLU	ALA	R389	
HIS	HIS	PRO	PRO	S390	K649
ASP	VAL	VAL	SER		
LYS	LYS	THR	GLY	E396	P657
ALA	ALA	THR	LEU	Y397	
TYR	TYR	ALA	GLY		T660
ASP	ASP	PRO	THR	T405	
ARG	ARG	GLY	ASN		F666
GLN	GLN	LYS	THR	T410	
LEU	LEU	MET	THR		E683
ASP	ASP	ALA	ALA	Y413	F684
SER	SER	PRO	THR		E685
GLY	GLY	VAL	GLY	L430	
ASP	ASP	GLU	SER		N695
ASN	ASN	HIS	GLY	M434	
PRO	PRO	SER	ALA		N703
TYR	TYR	PRO	PRO	L437	
LEU	LEU	ALA	MET	I438	T716
LYS	LYS	GLU	ALA		H717
TYR	TYR	PRO	ASP	T448	G718
HIS	HIS	ASN	ASN	S452	
ALA	ALA	SER	GLU		T728
ASP	ASP	SER	GLU	T455	L735
ALA	ALA	GLY	A217		
GLU	GLU	THR	A218		
PHE	PHE	GLY	D219	A465	
GLN	GLN	LYS	R238	Q473	
ALA	ALA	ALA			
ARG	ARG	GLY	T246	Q485	
LEU	LEU	GLN			S498
LYS	LYS	GLN	Y252		
GLU	GLU	PRO		Y257	T506
ASP	ASP	ALA			
THR	THR	ARG	ARG	H288	N518
SER	SER	LYS	ARG		P519
PHE	PHE	LEU	D295		
GLY	GLY	ASN		D528	
ASN	ASN	PHE	K309	E531	
LEU	LEU	GLN	N312		S537
GLY	GLY	THR	F313		
ARG	ARG	GLY	K314		T550
ALA	ALA	VAL			
PHE	PHE	ALA	D327		
GLN	GLN	ASP		T597	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	52874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.62	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.46	0/4261	0.46	0/5811
1	1	0.46	0/4261	0.46	0/5811
1	2	0.46	0/4261	0.46	0/5811
1	3	0.46	0/4261	0.46	0/5811
1	4	0.46	0/4261	0.46	0/5811
1	5	0.46	0/4261	0.46	0/5811
1	6	0.46	0/4261	0.46	0/5811
1	7	0.46	0/4261	0.46	0/5811
1	A	0.46	0/4261	0.46	0/5811
1	B	0.46	0/4261	0.46	0/5811
1	C	0.46	0/4261	0.46	0/5811
1	D	0.46	0/4261	0.46	0/5811
1	E	0.46	0/4261	0.46	0/5811
1	F	0.46	0/4261	0.46	0/5811
1	G	0.46	0/4261	0.46	0/5811
1	H	0.46	0/4261	0.46	0/5811
1	I	0.46	0/4261	0.46	0/5811
1	J	0.46	0/4261	0.46	0/5811
1	K	0.46	0/4261	0.46	0/5811
1	L	0.46	0/4261	0.46	0/5811
1	M	0.46	0/4261	0.46	0/5811
1	N	0.46	0/4261	0.46	0/5811
1	O	0.46	0/4261	0.46	0/5811
1	P	0.46	0/4261	0.46	0/5811
1	Q	0.46	0/4261	0.46	0/5811
1	R	0.46	0/4261	0.46	0/5811
1	S	0.46	0/4261	0.46	0/5811
1	T	0.46	0/4261	0.46	0/5811
1	U	0.46	0/4261	0.46	0/5811
1	V	0.46	0/4261	0.46	0/5811
1	W	0.46	0/4261	0.46	0/5811
1	X	0.46	0/4261	0.46	0/5811
1	Y	0.46	0/4261	0.46	0/5811
1	Z	0.46	0/4261	0.46	0/5811

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.46	0/4261	0.46	0/5811
1	b	0.46	0/4261	0.46	0/5811
1	c	0.46	0/4261	0.46	0/5811
1	d	0.46	0/4261	0.46	0/5811
1	e	0.46	0/4261	0.46	0/5811
1	f	0.46	0/4261	0.46	0/5811
1	g	0.46	0/4261	0.46	0/5811
1	h	0.46	0/4261	0.46	0/5811
1	i	0.46	0/4261	0.46	0/5811
1	j	0.46	0/4261	0.46	0/5811
1	k	0.46	0/4261	0.46	0/5811
1	l	0.46	0/4261	0.46	0/5811
1	m	0.46	0/4261	0.46	0/5811
1	n	0.46	0/4261	0.46	0/5811
1	o	0.46	0/4261	0.46	0/5811
1	p	0.46	0/4261	0.46	0/5811
1	q	0.46	0/4261	0.46	0/5811
1	r	0.46	0/4261	0.46	0/5811
1	s	0.46	0/4261	0.46	0/5811
1	t	0.46	0/4261	0.46	0/5811
1	u	0.46	0/4261	0.46	0/5811
1	v	0.46	0/4261	0.46	0/5811
1	w	0.46	0/4261	0.46	0/5811
1	x	0.46	0/4261	0.46	0/5811
1	y	0.46	0/4261	0.46	0/5811
1	z	0.46	0/4261	0.46	0/5811
All	All	0.46	0/255660	0.46	0/348660

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	0	4138	0	3887	30	0
1	1	4138	0	3887	30	0
1	2	4138	0	3887	28	0
1	3	4138	0	3887	29	0
1	4	4138	0	3887	34	0
1	5	4138	0	3887	32	0
1	6	4138	0	3887	29	0
1	7	4138	0	3887	26	0
1	A	4138	0	3887	40	0
1	B	4138	0	3887	42	0
1	C	4138	0	3887	38	0
1	D	4138	0	3887	40	0
1	E	4138	0	3887	39	0
1	F	4138	0	3887	36	0
1	G	4138	0	3887	40	0
1	H	4138	0	3887	42	0
1	I	4138	0	3887	42	0
1	J	4138	0	3887	38	0
1	K	4138	0	3887	38	0
1	L	4138	0	3887	44	0
1	M	4138	0	3887	41	0
1	N	4138	0	3887	35	0
1	O	4138	0	3887	41	0
1	P	4138	0	3887	36	0
1	Q	4138	0	3887	39	0
1	R	4138	0	3887	43	0
1	S	4138	0	3887	37	0
1	T	4138	0	3887	37	0
1	U	4138	0	3887	43	0
1	V	4138	0	3887	43	0
1	W	4138	0	3887	39	0
1	X	4138	0	3887	41	0
1	Y	4138	0	3887	37	0
1	Z	4138	0	3887	43	0
1	a	4138	0	3887	0	0
1	b	4138	0	3887	0	0
1	c	4138	0	3887	0	0
1	d	4138	0	3887	0	0
1	e	4138	0	3887	0	0
1	f	4138	0	3887	0	0
1	g	4138	0	3887	0	0
1	h	4138	0	3887	0	0
1	i	4138	0	3887	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4138	0	3887	0	0
1	k	4138	0	3887	0	0
1	l	4138	0	3887	0	0
1	m	4138	0	3887	0	0
1	n	4138	0	3887	0	0
1	o	4138	0	3887	0	0
1	p	4138	0	3887	0	0
1	q	4138	0	3887	0	0
1	r	4138	0	3887	0	0
1	s	4138	0	3887	0	0
1	t	4138	0	3887	0	0
1	u	4138	0	3887	0	0
1	v	4138	0	3887	0	0
1	w	4138	0	3887	0	0
1	x	4138	0	3887	0	0
1	y	4138	0	3887	0	0
1	z	4138	0	3887	0	0
All	All	248280	0	233220	1086	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 2.

All (1086) 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:N:657:PRO:HB3	1:N:666:PHE:HZ	1.59	0.68
1:E:657:PRO:HB3	1:E:666:PHE:HZ	1.59	0.68
1:L:657:PRO:HB3	1:L:666:PHE:HZ	1.59	0.68
1:O:657:PRO:HB3	1:O:666:PHE:HZ	1.59	0.68
1:4:657:PRO:HB3	1:4:666:PHE:HZ	1.59	0.68
1:A:657:PRO:HB3	1:A:666:PHE:HZ	1.59	0.68
1:C:657:PRO:HB3	1:C:666:PHE:HZ	1.59	0.68
1:P:657:PRO:HB3	1:P:666:PHE:HZ	1.59	0.68
1:S:657:PRO:HB3	1:S:666:PHE:HZ	1.59	0.68
1:2:657:PRO:HB3	1:2:666:PHE:HZ	1.59	0.68
1:G:657:PRO:HB3	1:G:666:PHE:HZ	1.59	0.68
1:F:657:PRO:HB3	1:F:666:PHE:HZ	1.59	0.67
1:J:657:PRO:HB3	1:J:666:PHE:HZ	1.59	0.67
1:U:657:PRO:HB3	1:U:666:PHE:HZ	1.59	0.67
1:H:657:PRO:HB3	1:H:666:PHE:HZ	1.59	0.67
1:D:657:PRO:HB3	1:D:666:PHE:HZ	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:657:PRO:HB3	1:K:666:PHE:HZ	1.59	0.67
1:X:657:PRO:HB3	1:X:666:PHE:HZ	1.59	0.67
1:Y:657:PRO:HB3	1:Y:666:PHE:HZ	1.59	0.67
1:Z:657:PRO:HB3	1:Z:666:PHE:HZ	1.59	0.67
1:5:657:PRO:HB3	1:5:666:PHE:HZ	1.59	0.67
1:B:657:PRO:HB3	1:B:666:PHE:HZ	1.59	0.67
1:W:657:PRO:HB3	1:W:666:PHE:HZ	1.59	0.67
1:R:657:PRO:HB3	1:R:666:PHE:HZ	1.59	0.67
1:V:657:PRO:HB3	1:V:666:PHE:HZ	1.59	0.67
1:Q:657:PRO:HB3	1:Q:666:PHE:HZ	1.59	0.67
1:O:657:PRO:HB3	1:O:666:PHE:HZ	1.59	0.67
1:T:657:PRO:HB3	1:T:666:PHE:HZ	1.59	0.66
1:M:657:PRO:HB3	1:M:666:PHE:HZ	1.59	0.66
1:1:657:PRO:HB3	1:1:666:PHE:HZ	1.59	0.66
1:I:657:PRO:HB3	1:I:666:PHE:HZ	1.59	0.66
1:3:657:PRO:HB3	1:3:666:PHE:HZ	1.59	0.65
1:6:657:PRO:HB3	1:6:666:PHE:HZ	1.59	0.65
1:7:657:PRO:HB3	1:7:666:PHE:HZ	1.59	0.65
1:N:238:ARG:NH1	1:N:683:GLU:OE2	2.33	0.62
1:2:238:ARG:NH1	1:2:683:GLU:OE2	2.33	0.62
1:Q:238:ARG:NH1	1:Q:683:GLU:OE2	2.33	0.62
1:3:238:ARG:NH1	1:3:683:GLU:OE2	2.33	0.62
1:B:238:ARG:NH1	1:B:683:GLU:OE2	2.33	0.62
1:E:238:ARG:NH1	1:E:683:GLU:OE2	2.33	0.62
1:H:238:ARG:NH1	1:H:683:GLU:OE2	2.33	0.62
1:I:238:ARG:NH1	1:I:683:GLU:OE2	2.33	0.62
1:J:238:ARG:NH1	1:J:683:GLU:OE2	2.33	0.62
1:M:238:ARG:NH1	1:M:683:GLU:OE2	2.33	0.62
1:R:238:ARG:NH1	1:R:683:GLU:OE2	2.33	0.62
1:S:238:ARG:NH1	1:S:683:GLU:OE2	2.33	0.62
1:T:238:ARG:NH1	1:T:683:GLU:OE2	2.33	0.62
1:W:238:ARG:NH1	1:W:683:GLU:OE2	2.33	0.62
1:5:238:ARG:NH1	1:5:683:GLU:OE2	2.33	0.62
1:G:238:ARG:NH1	1:G:683:GLU:OE2	2.33	0.62
1:L:238:ARG:NH1	1:L:683:GLU:OE2	2.33	0.62
1:P:238:ARG:NH1	1:P:683:GLU:OE2	2.33	0.62
1:U:238:ARG:NH1	1:U:683:GLU:OE2	2.33	0.62
1:A:238:ARG:NH1	1:A:683:GLU:OE2	2.33	0.62
1:O:238:ARG:NH1	1:O:683:GLU:OE2	2.33	0.62
1:X:238:ARG:NH1	1:X:683:GLU:OE2	2.33	0.62
1:Z:238:ARG:NH1	1:Z:683:GLU:OE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:238:ARG:NH1	1:7:683:GLU:OE2	2.33	0.61
1:6:238:ARG:NH1	1:6:683:GLU:OE2	2.33	0.61
1:D:238:ARG:NH1	1:D:683:GLU:OE2	2.33	0.61
1:K:238:ARG:NH1	1:K:683:GLU:OE2	2.33	0.61
1:Y:238:ARG:NH1	1:Y:683:GLU:OE2	2.33	0.61
1:1:238:ARG:NH1	1:1:683:GLU:OE2	2.33	0.61
1:4:610:ASP:OD1	1:4:728:THR:OG1	2.19	0.61
1:G:610:ASP:OD1	1:G:728:THR:OG1	2.19	0.61
1:N:610:ASP:OD1	1:N:728:THR:OG1	2.19	0.61
1:V:238:ARG:NH1	1:V:683:GLU:OE2	2.33	0.61
1:E:610:ASP:OD1	1:E:728:THR:OG1	2.19	0.61
1:W:610:ASP:OD1	1:W:728:THR:OG1	2.19	0.61
1:C:238:ARG:NH1	1:C:683:GLU:OE2	2.33	0.61
1:F:610:ASP:OD1	1:F:728:THR:OG1	2.19	0.61
1:O:610:ASP:OD1	1:O:728:THR:OG1	2.19	0.61
1:T:610:ASP:OD1	1:T:728:THR:OG1	2.19	0.61
1:X:610:ASP:OD1	1:X:728:THR:OG1	2.19	0.61
1:Z:610:ASP:OD1	1:Z:728:THR:OG1	2.19	0.61
1:0:238:ARG:NH1	1:0:683:GLU:OE2	2.33	0.61
1:H:610:ASP:OD1	1:H:728:THR:OG1	2.19	0.61
1:I:610:ASP:OD1	1:I:728:THR:OG1	2.19	0.61
1:J:610:ASP:OD1	1:J:728:THR:OG1	2.19	0.61
1:L:610:ASP:OD1	1:L:728:THR:OG1	2.19	0.61
1:U:610:ASP:OD1	1:U:728:THR:OG1	2.19	0.61
1:V:610:ASP:OD1	1:V:728:THR:OG1	2.19	0.61
1:C:610:ASP:OD1	1:C:728:THR:OG1	2.19	0.61
1:P:610:ASP:OD1	1:P:728:THR:OG1	2.19	0.61
1:4:238:ARG:NH1	1:4:683:GLU:OE2	2.33	0.60
1:F:238:ARG:NH1	1:F:683:GLU:OE2	2.33	0.60
1:K:610:ASP:OD1	1:K:728:THR:OG1	2.19	0.60
1:Y:610:ASP:OD1	1:Y:728:THR:OG1	2.19	0.60
1:2:610:ASP:OD1	1:2:728:THR:OG1	2.19	0.60
1:D:610:ASP:OD1	1:D:728:THR:OG1	2.19	0.60
1:R:610:ASP:OD1	1:R:728:THR:OG1	2.19	0.60
1:S:610:ASP:OD1	1:S:728:THR:OG1	2.19	0.60
1:0:610:ASP:OD1	1:0:728:THR:OG1	2.19	0.60
1:5:610:ASP:OD1	1:5:728:THR:OG1	2.19	0.60
1:A:610:ASP:OD1	1:A:728:THR:OG1	2.19	0.60
1:B:610:ASP:OD1	1:B:728:THR:OG1	2.19	0.60
1:M:610:ASP:OD1	1:M:728:THR:OG1	2.19	0.60
1:1:610:ASP:OD1	1:1:728:THR:OG1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:610:ASP:OD1	1:3:728:THR:OG1	2.19	0.60
1:7:610:ASP:OD1	1:7:728:THR:OG1	2.19	0.60
1:Q:610:ASP:OD1	1:Q:728:THR:OG1	2.19	0.60
1:6:610:ASP:OD1	1:6:728:THR:OG1	2.19	0.59
1:M:452:SER:N	1:M:455:THR:O	2.38	0.55
1:H:452:SER:N	1:H:455:THR:O	2.38	0.55
1:D:452:SER:N	1:D:455:THR:O	2.38	0.55
1:L:452:SER:N	1:L:455:THR:O	2.38	0.55
1:Y:452:SER:N	1:Y:455:THR:O	2.38	0.55
1:F:452:SER:N	1:F:455:THR:O	2.38	0.55
1:I:452:SER:N	1:I:455:THR:O	2.38	0.55
1:I:396:GLU:OE2	1:I:649:LYS:NZ	2.37	0.55
1:Q:452:SER:N	1:Q:455:THR:O	2.38	0.55
1:T:452:SER:N	1:T:455:THR:O	2.38	0.55
1:C:452:SER:N	1:C:455:THR:O	2.38	0.54
1:B:452:SER:N	1:B:455:THR:O	2.38	0.54
1:P:452:SER:N	1:P:455:THR:O	2.38	0.54
1:6:452:SER:N	1:6:455:THR:O	2.38	0.54
1:O:452:SER:N	1:O:455:THR:O	2.38	0.54
1:S:452:SER:N	1:S:455:THR:O	2.38	0.54
1:V:452:SER:N	1:V:455:THR:O	2.38	0.54
1:Z:452:SER:N	1:Z:455:THR:O	2.38	0.54
1:0:396:GLU:OE2	1:0:649:LYS:NZ	2.37	0.54
1:V:434:MET:SD	1:V:434:MET:N	2.76	0.54
1:N:452:SER:N	1:N:455:THR:O	2.38	0.54
1:W:396:GLU:OE2	1:W:649:LYS:NZ	2.37	0.54
1:B:434:MET:N	1:B:434:MET:SD	2.76	0.53
1:N:434:MET:N	1:N:434:MET:SD	2.76	0.53
1:P:396:GLU:OE2	1:P:649:LYS:NZ	2.37	0.53
1:U:452:SER:N	1:U:455:THR:O	2.38	0.53
1:Z:396:GLU:OE2	1:Z:649:LYS:NZ	2.37	0.53
1:V:620:LYS:HB2	1:V:642:PRO:HG3	1.91	0.53
1:X:452:SER:N	1:X:455:THR:O	2.38	0.53
1:C:620:LYS:HB2	1:C:642:PRO:HG3	1.91	0.53
1:K:620:LYS:HB2	1:K:642:PRO:HG3	1.91	0.53
1:M:620:LYS:HB2	1:M:642:PRO:HG3	1.91	0.53
1:R:620:LYS:HB2	1:R:642:PRO:HG3	1.91	0.53
1:3:452:SER:N	1:3:455:THR:O	2.38	0.53
1:4:620:LYS:HB2	1:4:642:PRO:HG3	1.91	0.53
1:B:620:LYS:HB2	1:B:642:PRO:HG3	1.91	0.53
1:G:620:LYS:HB2	1:G:642:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:620:LYS:HB2	1:J:642:PRO:HG3	1.91	0.53
1:O:396:GLU:OE2	1:O:649:LYS:NZ	2.37	0.53
1:T:620:LYS:HB2	1:T:642:PRO:HG3	1.91	0.53
1:U:396:GLU:OE2	1:U:649:LYS:NZ	2.37	0.53
1:X:620:LYS:HB2	1:X:642:PRO:HG3	1.91	0.53
1:3:620:LYS:HB2	1:3:642:PRO:HG3	1.91	0.53
1:5:620:LYS:HB2	1:5:642:PRO:HG3	1.91	0.53
1:A:452:SER:N	1:A:455:THR:O	2.38	0.53
1:Q:620:LYS:HB2	1:Q:642:PRO:HG3	1.91	0.53
1:S:620:LYS:HB2	1:S:642:PRO:HG3	1.91	0.53
1:U:620:LYS:HB2	1:U:642:PRO:HG3	1.91	0.53
1:1:396:GLU:OE2	1:1:649:LYS:NZ	2.37	0.53
1:A:620:LYS:HB2	1:A:642:PRO:HG3	1.91	0.53
1:E:620:LYS:HB2	1:E:642:PRO:HG3	1.91	0.53
1:D:620:LYS:HB2	1:D:642:PRO:HG3	1.91	0.53
1:G:452:SER:N	1:G:455:THR:O	2.38	0.53
1:N:620:LYS:HB2	1:N:642:PRO:HG3	1.91	0.53
1:P:620:LYS:HB2	1:P:642:PRO:HG3	1.91	0.53
1:Y:620:LYS:HB2	1:Y:642:PRO:HG3	1.91	0.53
1:F:620:LYS:HB2	1:F:642:PRO:HG3	1.91	0.53
1:O:620:LYS:HB2	1:O:642:PRO:HG3	1.91	0.53
1:W:620:LYS:HB2	1:W:642:PRO:HG3	1.91	0.53
1:Y:396:GLU:OE2	1:Y:649:LYS:NZ	2.37	0.53
1:0:620:LYS:HB2	1:0:642:PRO:HG3	1.91	0.52
1:6:620:LYS:HB2	1:6:642:PRO:HG3	1.91	0.52
1:H:620:LYS:HB2	1:H:642:PRO:HG3	1.91	0.52
1:S:434:MET:N	1:S:434:MET:SD	2.76	0.52
1:Z:620:LYS:HB2	1:Z:642:PRO:HG3	1.91	0.52
1:4:452:SER:N	1:4:455:THR:O	2.38	0.52
1:G:434:MET:N	1:G:434:MET:SD	2.76	0.52
1:K:396:GLU:OE2	1:K:649:LYS:NZ	2.37	0.52
1:M:434:MET:SD	1:M:434:MET:N	2.76	0.52
1:S:396:GLU:OE2	1:S:649:LYS:NZ	2.37	0.52
1:W:434:MET:N	1:W:434:MET:SD	2.76	0.52
1:D:396:GLU:OE2	1:D:649:LYS:NZ	2.37	0.52
1:1:620:LYS:HB2	1:1:642:PRO:HG3	1.91	0.52
1:2:620:LYS:HB2	1:2:642:PRO:HG3	1.91	0.52
1:V:396:GLU:OE2	1:V:649:LYS:NZ	2.37	0.52
1:5:452:SER:N	1:5:455:THR:O	2.38	0.52
1:7:396:GLU:OE2	1:7:649:LYS:NZ	2.37	0.52
1:I:620:LYS:HB2	1:I:642:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:434:MET:SD	1:L:434:MET:N	2.76	0.52
1:P:434:MET:SD	1:P:434:MET:N	2.76	0.52
1:Q:396:GLU:OE2	1:Q:649:LYS:NZ	2.37	0.52
1:7:620:LYS:HB2	1:7:642:PRO:HG3	1.91	0.52
1:E:452:SER:N	1:E:455:THR:O	2.38	0.52
1:L:620:LYS:HB2	1:L:642:PRO:HG3	1.91	0.52
1:K:397:TYR:OH	1:Q:295:ASP:OD2	66.93	0.52
1:R:452:SER:N	1:R:455:THR:O	2.38	0.51
1:R:397:TYR:OH	1:J:295:ASP:OD2	63.79	0.51
1:T:295:ASP:OD2	1:H:397:TYR:OH	178.93	0.51
1:M:396:GLU:OE2	1:M:649:LYS:NZ	2.37	0.51
1:S:397:TYR:OH	1:Y:295:ASP:OD2	2.28	0.51
1:5:396:GLU:OE2	1:5:649:LYS:NZ	2.37	0.51
1:R:396:GLU:OE2	1:R:649:LYS:NZ	2.37	0.51
1:7:327:ASP:OD1	1:7:327:ASP:N	2.44	0.51
1:3:396:GLU:OE2	1:3:649:LYS:NZ	2.37	0.51
1:7:452:SER:N	1:7:455:THR:O	2.38	0.51
1:O:327:ASP:N	1:O:327:ASP:OD1	2.44	0.51
1:O:295:ASP:OD2	1:P:397:TYR:OH	2.29	0.51
1:K:397:TYR:OH	1:C:295:ASP:OD2	2.28	0.51
1:Z:327:ASP:OD1	1:Z:327:ASP:N	2.44	0.51
1:0:434:MET:SD	1:0:434:MET:N	2.76	0.51
1:1:327:ASP:OD1	1:1:327:ASP:N	2.44	0.51
1:J:396:GLU:OE2	1:J:649:LYS:NZ	2.37	0.51
1:K:327:ASP:OD1	1:K:327:ASP:N	2.44	0.51
1:L:327:ASP:OD1	1:L:327:ASP:N	2.44	0.51
1:M:327:ASP:N	1:M:327:ASP:OD1	2.44	0.51
1:P:327:ASP:OD1	1:P:327:ASP:N	2.44	0.51
1:A:295:ASP:OD2	1:Z:397:TYR:OH	95.26	0.51
1:6:327:ASP:N	1:6:327:ASP:OD1	2.44	0.50
1:D:327:ASP:N	1:D:327:ASP:OD1	2.44	0.50
1:E:327:ASP:OD1	1:E:327:ASP:N	2.44	0.50
1:F:396:GLU:OE2	1:F:649:LYS:NZ	2.37	0.50
1:I:327:ASP:OD1	1:I:327:ASP:N	2.44	0.50
1:T:396:GLU:OE2	1:T:649:LYS:NZ	2.37	0.50
1:3:327:ASP:OD1	1:3:327:ASP:N	2.44	0.50
1:J:452:SER:N	1:J:455:THR:O	2.38	0.50
1:N:327:ASP:OD1	1:N:327:ASP:N	2.44	0.50
1:N:397:TYR:OH	1:S:295:ASP:OD2	105.07	0.50
1:S:327:ASP:OD1	1:S:327:ASP:N	2.44	0.50
1:T:327:ASP:N	1:T:327:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:327:ASP:OD1	1:Y:327:ASP:N	2.44	0.50
1:2:413:TYR:OH	1:2:641:HIS:O	2.28	0.50
1:G:327:ASP:N	1:G:327:ASP:OD1	2.44	0.50
1:O:528:ASP:N	1:O:528:ASP:OD1	2.45	0.50
1:S:413:TYR:OH	1:S:641:HIS:O	2.28	0.50
1:W:327:ASP:OD1	1:W:327:ASP:N	2.44	0.50
1:D:295:ASP:OD2	1:3:397:TYR:OH	179.76	0.50
1:3:528:ASP:OD1	1:3:528:ASP:N	2.45	0.50
1:B:396:GLU:OE2	1:B:649:LYS:NZ	2.37	0.50
1:E:252:TYR:OH	1:E:372:VAL:O	2.26	0.50
1:E:397:TYR:OH	1:I:295:ASP:OD2	119.00	0.50
1:N:396:GLU:OE2	1:N:649:LYS:NZ	2.37	0.50
1:T:528:ASP:OD1	1:T:528:ASP:N	2.45	0.50
1:C:327:ASP:OD1	1:C:327:ASP:N	2.44	0.50
1:S:528:ASP:N	1:S:528:ASP:OD1	2.45	0.50
1:F:327:ASP:OD1	1:F:327:ASP:N	2.44	0.50
1:V:397:TYR:OH	1:G:295:ASP:OD2	180.25	0.50
1:O:387:VAL:O	1:O:390:SER:OG	2.30	0.50
1:V:429:SER:OG	1:V:431:ASP:OD1	2.24	0.50
1:3:485:GLN:HA	1:3:506:THR:HG21	1.94	0.50
1:7:387:VAL:O	1:7:390:SER:OG	2.30	0.50
1:H:327:ASP:OD1	1:H:327:ASP:N	2.44	0.50
1:J:327:ASP:N	1:J:327:ASP:OD1	2.44	0.50
1:M:528:ASP:OD1	1:M:528:ASP:N	2.45	0.50
1:Q:387:VAL:O	1:Q:390:SER:OG	2.30	0.50
1:T:485:GLN:HA	1:T:506:THR:HG21	1.94	0.50
1:Q:397:TYR:OH	1:X:295:ASP:OD2	112.99	0.50
1:A:396:GLU:OE2	1:A:649:LYS:NZ	2.37	0.50
1:I:252:TYR:OH	1:I:372:VAL:O	2.26	0.50
1:M:485:GLN:HA	1:M:506:THR:HG21	1.94	0.50
1:Q:327:ASP:N	1:Q:327:ASP:OD1	2.44	0.50
1:U:485:GLN:HA	1:U:506:THR:HG21	1.94	0.50
1:1:295:ASP:OD2	1:2:397:TYR:OH	2.30	0.50
1:2:452:SER:N	1:2:455:THR:O	2.38	0.50
1:3:380:LEU:HD12	1:3:389:ARG:HB3	1.94	0.50
1:5:485:GLN:HA	1:5:506:THR:HG21	1.94	0.50
1:7:380:LEU:HD12	1:7:389:ARG:HB3	1.94	0.50
1:A:485:GLN:HA	1:A:506:THR:HG21	1.94	0.50
1:B:252:TYR:OH	1:B:372:VAL:O	2.26	0.50
1:F:485:GLN:HA	1:F:506:THR:HG21	1.94	0.50
1:H:387:VAL:O	1:H:390:SER:OG	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:380:LEU:HD12	1:L:389:ARG:HB3	1.94	0.50
1:P:380:LEU:HD12	1:P:389:ARG:HB3	1.94	0.50
1:Q:528:ASP:N	1:Q:528:ASP:OD1	2.45	0.50
1:R:485:GLN:HA	1:R:506:THR:HG21	1.94	0.50
1:M:295:ASP:OD2	1:T:397:TYR:OH	146.00	0.50
1:U:380:LEU:HD12	1:U:389:ARG:HB3	1.94	0.50
1:U:387:VAL:O	1:U:390:SER:OG	2.30	0.50
1:Z:380:LEU:HD12	1:Z:389:ARG:HB3	1.94	0.50
1:O:452:SER:N	1:O:455:THR:O	2.38	0.49
1:2:380:LEU:HD12	1:2:389:ARG:HB3	1.94	0.49
1:2:396:GLU:OE2	1:2:649:LYS:NZ	2.37	0.49
1:O:295:ASP:OD2	1:7:397:TYR:OH	2.29	0.49
1:7:528:ASP:N	1:7:528:ASP:OD1	2.45	0.49
1:A:380:LEU:HD12	1:A:389:ARG:HB3	1.94	0.49
1:B:387:VAL:O	1:B:390:SER:OG	2.30	0.49
1:M:295:ASP:OD2	1:B:397:TYR:OH	73.01	0.49
1:C:485:GLN:HA	1:C:506:THR:HG21	1.94	0.49
1:D:387:VAL:O	1:D:390:SER:OG	2.30	0.49
1:D:485:GLN:HA	1:D:506:THR:HG21	1.94	0.49
1:E:485:GLN:HA	1:E:506:THR:HG21	1.94	0.49
1:H:485:GLN:HA	1:H:506:THR:HG21	1.94	0.49
1:I:387:VAL:O	1:I:390:SER:OG	2.30	0.49
1:H:295:ASP:OD2	1:I:397:TYR:OH	2.30	0.49
1:I:485:GLN:HA	1:I:506:THR:HG21	1.94	0.49
1:L:396:GLU:OE2	1:L:649:LYS:NZ	2.37	0.49
1:L:485:GLN:HA	1:L:506:THR:HG21	1.94	0.49
1:N:387:VAL:O	1:N:390:SER:OG	2.30	0.49
1:O:380:LEU:HD12	1:O:389:ARG:HB3	1.94	0.49
1:Q:380:LEU:HD12	1:Q:389:ARG:HB3	1.94	0.49
1:R:528:ASP:OD1	1:R:528:ASP:N	2.45	0.49
1:S:380:LEU:HD12	1:S:389:ARG:HB3	1.94	0.49
1:T:380:LEU:HD12	1:T:389:ARG:HB3	1.94	0.49
1:U:295:ASP:OD2	1:V:397:TYR:OH	2.29	0.49
1:V:327:ASP:N	1:V:327:ASP:OD1	2.44	0.49
1:V:380:LEU:HD12	1:V:389:ARG:HB3	1.94	0.49
1:A:397:TYR:OH	1:W:295:ASP:OD2	183.16	0.49
1:X:327:ASP:OD1	1:X:327:ASP:N	2.44	0.49
1:X:387:VAL:O	1:X:390:SER:OG	2.30	0.49
1:X:485:GLN:HA	1:X:506:THR:HG21	1.94	0.49
1:Y:485:GLN:HA	1:Y:506:THR:HG21	1.94	0.49
1:6:380:LEU:HD12	1:6:389:ARG:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:295:ASP:OD2	1:6:397:TYR:OH	2.30	0.49
1:A:528:ASP:OD1	1:A:528:ASP:N	2.45	0.49
1:B:295:ASP:OD2	1:C:397:TYR:OH	146.82	0.49
1:C:380:LEU:HD12	1:C:389:ARG:HB3	1.94	0.49
1:D:528:ASP:OD1	1:D:528:ASP:N	2.45	0.49
1:F:380:LEU:HD12	1:F:389:ARG:HB3	1.94	0.49
1:U:397:TYR:OH	1:G:295:ASP:OD2	189.23	0.49
1:I:380:LEU:HD12	1:I:389:ARG:HB3	1.94	0.49
1:K:387:VAL:O	1:K:390:SER:OG	2.30	0.49
1:L:528:ASP:N	1:L:528:ASP:OD1	2.45	0.49
1:Q:295:ASP:OD2	1:J:397:TYR:OH	2.30	0.49
1:R:387:VAL:O	1:R:390:SER:OG	2.30	0.49
1:Z:485:GLN:HA	1:Z:506:THR:HG21	1.94	0.49
1:1:380:LEU:HD12	1:1:389:ARG:HB3	1.94	0.49
1:1:528:ASP:N	1:1:528:ASP:OD1	2.45	0.49
1:4:387:VAL:O	1:4:390:SER:OG	2.30	0.49
1:5:380:LEU:HD12	1:5:389:ARG:HB3	1.94	0.49
1:C:528:ASP:OD1	1:C:528:ASP:N	2.45	0.49
1:E:380:LEU:HD12	1:E:389:ARG:HB3	1.94	0.49
1:G:387:VAL:O	1:G:390:SER:OG	2.30	0.49
1:H:380:LEU:HD12	1:H:389:ARG:HB3	1.94	0.49
1:J:485:GLN:HA	1:J:506:THR:HG21	1.94	0.49
1:K:485:GLN:HA	1:K:506:THR:HG21	1.94	0.49
1:N:380:LEU:HD12	1:N:389:ARG:HB3	1.94	0.49
1:V:252:TYR:OH	1:V:372:VAL:O	2.26	0.49
1:V:387:VAL:O	1:V:390:SER:OG	2.30	0.49
1:4:327:ASP:OD1	1:4:327:ASP:N	2.44	0.49
1:B:485:GLN:HA	1:B:506:THR:HG21	1.94	0.49
1:L:295:ASP:OD2	1:F:397:TYR:OH	99.82	0.49
1:M:387:VAL:O	1:M:390:SER:OG	2.30	0.49
1:N:485:GLN:HA	1:N:506:THR:HG21	1.94	0.49
1:O:485:GLN:HA	1:O:506:THR:HG21	1.94	0.49
1:V:485:GLN:HA	1:V:506:THR:HG21	1.94	0.49
1:W:452:SER:N	1:W:455:THR:O	2.38	0.49
1:W:485:GLN:HA	1:W:506:THR:HG21	1.94	0.49
1:X:380:LEU:HD12	1:X:389:ARG:HB3	1.94	0.49
1:Y:380:LEU:HD12	1:Y:389:ARG:HB3	1.94	0.49
1:Y:528:ASP:OD1	1:Y:528:ASP:N	2.45	0.49
1:Z:387:VAL:O	1:Z:390:SER:OG	2.30	0.49
1:O:387:VAL:O	1:O:390:SER:OG	2.30	0.49
1:A:387:VAL:O	1:A:390:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TYR:OH	1:5:295:ASP:OD2	146.48	0.49
1:F:387:VAL:O	1:F:390:SER:OG	2.30	0.49
1:B:295:ASP:OD2	1:G:397:TYR:OH	188.49	0.49
1:G:485:GLN:HA	1:G:506:THR:HG21	1.94	0.49
1:G:528:ASP:N	1:G:528:ASP:OD1	2.45	0.49
1:D:397:TYR:OH	1:J:295:ASP:OD2	2.29	0.49
1:K:452:SER:N	1:K:455:THR:O	2.38	0.49
1:L:295:ASP:OD2	1:U:397:TYR:OH	163.78	0.49
1:P:295:ASP:OD2	1:Y:397:TYR:OH	2.30	0.49
1:P:387:VAL:O	1:P:390:SER:OG	2.30	0.49
1:Q:485:GLN:HA	1:Q:506:THR:HG21	1.94	0.49
1:R:380:LEU:HD12	1:R:389:ARG:HB3	1.94	0.49
1:S:387:VAL:O	1:S:390:SER:OG	2.30	0.49
1:U:295:ASP:OD2	1:H:397:TYR:OH	167.14	0.49
1:W:387:VAL:O	1:W:390:SER:OG	2.30	0.49
1:Z:397:TYR:OH	1:E:295:ASP:OD2	105.04	0.49
1:2:528:ASP:OD1	1:2:528:ASP:N	2.45	0.49
1:4:528:ASP:N	1:4:528:ASP:OD1	2.45	0.49
1:A:434:MET:SD	1:A:434:MET:N	2.76	0.49
1:K:380:LEU:HD12	1:K:389:ARG:HB3	1.94	0.49
1:M:397:TYR:OH	1:F:295:ASP:OD2	180.23	0.49
1:T:387:VAL:O	1:T:390:SER:OG	2.30	0.49
1:U:434:MET:N	1:U:434:MET:SD	2.76	0.49
1:A:295:ASP:OD2	1:X:397:TYR:OH	146.12	0.49
1:I:528:ASP:OD1	1:I:528:ASP:N	2.45	0.49
1:J:380:LEU:HD12	1:J:389:ARG:HB3	1.94	0.49
1:L:387:VAL:O	1:L:390:SER:OG	2.30	0.49
1:W:528:ASP:OD1	1:W:528:ASP:N	2.45	0.49
1:X:397:TYR:OH	1:3:295:ASP:OD2	157.38	0.49
1:3:387:VAL:O	1:3:390:SER:OG	2.30	0.49
1:6:528:ASP:N	1:6:528:ASP:OD1	2.45	0.49
1:7:429:SER:OG	1:7:431:ASP:OD1	2.24	0.49
1:A:327:ASP:OD1	1:A:327:ASP:N	2.44	0.49
1:E:528:ASP:OD1	1:E:528:ASP:N	2.45	0.49
1:J:387:VAL:O	1:J:390:SER:OG	2.30	0.49
1:B:327:ASP:N	1:B:327:ASP:OD1	2.44	0.49
1:B:380:LEU:HD12	1:B:389:ARG:HB3	1.94	0.49
1:C:387:VAL:O	1:C:390:SER:OG	2.30	0.49
1:C:397:TYR:OH	1:7:295:ASP:OD2	2.30	0.49
1:D:380:LEU:HD12	1:D:389:ARG:HB3	1.94	0.49
1:E:295:ASP:OD2	1:5:397:TYR:OH	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:VAL:O	1:E:390:SER:OG	2.30	0.49
1:O:397:TYR:OH	1:F:295:ASP:OD2	2.30	0.49
1:J:528:ASP:N	1:J:528:ASP:OD1	2.45	0.49
1:U:327:ASP:OD1	1:U:327:ASP:N	2.44	0.49
1:Y:387:VAL:O	1:Y:390:SER:OG	2.30	0.49
1:V:295:ASP:OD2	1:4:397:TYR:OH	2.31	0.49
1:5:327:ASP:N	1:5:327:ASP:OD1	2.44	0.49
1:G:396:GLU:OE2	1:G:649:LYS:NZ	2.37	0.49
1:L:397:TYR:OH	1:C:295:ASP:OD2	112.98	0.49
1:M:252:TYR:OH	1:M:372:VAL:O	2.26	0.49
1:M:397:TYR:OH	1:R:295:ASP:OD2	179.81	0.49
1:P:485:GLN:HA	1:P:506:THR:HG21	1.94	0.49
1:P:498:SER:O	1:R:448:THR:OG1	2.26	0.49
1:P:528:ASP:OD1	1:P:528:ASP:N	2.45	0.49
1:R:327:ASP:OD1	1:R:327:ASP:N	2.44	0.49
1:V:528:ASP:N	1:V:528:ASP:OD1	2.45	0.49
1:X:528:ASP:OD1	1:X:528:ASP:N	2.45	0.49
1:O:485:GLN:HA	1:O:506:THR:HG21	1.94	0.48
1:B:485:GLN:HE21	1:B:485:GLN:HB3	1.47	0.48
1:F:735:LEU:HD22	1:G:622:PRO:HB3	1.97	0.48
1:K:528:ASP:OD1	1:K:528:ASP:N	2.45	0.48
1:S:485:GLN:HA	1:S:506:THR:HG21	1.94	0.48
1:V:295:ASP:OD2	1:W:397:TYR:OH	28.86	0.48
1:U:735:LEU:HD22	1:V:622:PRO:HB3	50.26	0.48
1:3:413:TYR:OH	1:3:641:HIS:O	2.28	0.48
1:4:485:GLN:HA	1:4:506:THR:HG21	1.94	0.48
1:B:528:ASP:N	1:B:528:ASP:OD1	2.45	0.48
1:H:528:ASP:N	1:H:528:ASP:OD1	2.45	0.48
1:S:252:TYR:OH	1:S:372:VAL:O	2.26	0.48
1:U:528:ASP:N	1:U:528:ASP:OD1	2.45	0.48
1:B:397:TYR:OH	1:4:295:ASP:OD2	2.30	0.48
1:X:295:ASP:OD2	1:I:397:TYR:OH	159.32	0.48
1:U:413:TYR:OH	1:U:641:HIS:O	2.28	0.48
1:O:327:ASP:OD1	1:O:327:ASP:N	2.44	0.48
1:1:397:TYR:OH	1:6:295:ASP:OD2	2.30	0.48
1:1:485:GLN:HA	1:1:506:THR:HG21	1.94	0.48
1:F:434:MET:SD	1:F:434:MET:N	2.76	0.48
1:K:413:TYR:OH	1:K:641:HIS:O	2.28	0.48
1:Y:434:MET:SD	1:Y:434:MET:N	2.76	0.48
1:W:735:LEU:HD22	1:Y:622:PRO:HB3	1.95	0.48
1:C:396:GLU:OE2	1:C:649:LYS:NZ	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:257:TYR:OH	1:N:396:GLU:OE1	2.28	0.48
1:T:413:TYR:OH	1:T:641:HIS:O	2.28	0.48
1:X:413:TYR:OH	1:X:641:HIS:O	2.28	0.48
1:Z:295:ASP:OD2	1:G:397:TYR:OH	114.64	0.48
1:2:485:GLN:HA	1:2:506:THR:HG21	1.94	0.48
1:7:485:GLN:HA	1:7:506:THR:HG21	1.94	0.48
1:F:528:ASP:N	1:F:528:ASP:OD1	2.45	0.48
1:N:295:ASP:OD2	1:O:397:TYR:OH	28.87	0.48
1:N:528:ASP:OD1	1:N:528:ASP:N	2.45	0.48
1:W:380:LEU:HD12	1:W:389:ARG:HB3	1.94	0.48
1:T:295:ASP:OD2	1:W:397:TYR:OH	119.01	0.48
1:A:622:PRO:HB3	1:Z:735:LEU:HD22	139.23	0.48
1:D:257:TYR:OH	1:D:396:GLU:OE1	2.28	0.48
1:H:295:ASP:OD2	1:J:397:TYR:OH	66.93	0.48
1:M:380:LEU:HD12	1:M:389:ARG:HB3	1.94	0.48
1:M:485:GLN:HB3	1:M:485:GLN:HE21	1.47	0.48
1:M:622:PRO:HB3	1:B:735:LEU:HD22	1.95	0.48
1:Z:528:ASP:N	1:Z:528:ASP:OD1	2.45	0.48
1:O:380:LEU:HD12	1:O:389:ARG:HB3	1.94	0.48
1:4:380:LEU:HD12	1:4:389:ARG:HB3	1.94	0.48
1:6:735:LEU:HD22	1:7:622:PRO:HB3	1.96	0.48
1:G:380:LEU:HD12	1:G:389:ARG:HB3	1.94	0.48
1:I:735:LEU:HD22	1:J:622:PRO:HB3	1.96	0.48
1:T:622:PRO:HB3	1:I:735:LEU:HD22	166.88	0.48
1:T:735:LEU:HD22	1:U:622:PRO:HB3	1.96	0.48
1:3:657:PRO:HB3	1:3:666:PHE:CZ	2.46	0.48
1:5:387:VAL:O	1:5:390:SER:OG	2.30	0.48
1:D:434:MET:SD	1:D:434:MET:N	2.76	0.48
1:G:413:TYR:OH	1:G:641:HIS:O	2.28	0.48
1:K:434:MET:SD	1:K:434:MET:N	2.76	0.48
1:O:252:TYR:OH	1:O:372:VAL:O	2.26	0.48
1:T:397:TYR:OH	1:D:295:ASP:OD2	159.33	0.48
1:X:485:GLN:HE21	1:X:485:GLN:HB3	1.47	0.48
1:Z:252:TYR:OH	1:Z:372:VAL:O	2.26	0.48
1:Z:448:THR:OG1	1:O:498:SER:O	156.84	0.48
1:E:397:TYR:OH	1:2:295:ASP:OD2	153.62	0.48
1:A:622:PRO:HB3	1:3:735:LEU:HD22	1.96	0.48
1:K:295:ASP:OD2	1:F:397:TYR:OH	2.31	0.48
1:P:735:LEU:HD22	1:Q:622:PRO:HB3	1.98	0.48
1:Q:413:TYR:OH	1:Q:641:HIS:O	2.28	0.48
1:T:657:PRO:HB3	1:T:666:PHE:CZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:622:PRO:HB3	1:Y:735:LEU:HD22	31.73	0.48
1:W:413:TYR:OH	1:W:641:HIS:O	2.28	0.48
1:Z:622:PRO:HB3	1:1:735:LEU:HD22	115.44	0.48
1:A:657:PRO:HB3	1:A:666:PHE:CZ	2.46	0.47
1:B:413:TYR:OH	1:B:641:HIS:O	2.28	0.47
1:H:434:MET:SD	1:H:434:MET:N	2.76	0.47
1:H:413:TYR:OH	1:H:641:HIS:O	2.28	0.47
1:I:434:MET:SD	1:I:434:MET:N	2.76	0.47
1:M:413:TYR:OH	1:M:641:HIS:O	2.28	0.47
1:N:413:TYR:OH	1:N:641:HIS:O	2.28	0.47
1:Q:448:THR:OG1	1:R:498:SER:O	2.38	0.47
1:Q:397:TYR:OH	1:W:295:ASP:OD2	2.31	0.47
1:O:528:ASP:OD1	1:O:528:ASP:N	2.45	0.47
1:6:387:VAL:O	1:6:390:SER:OG	2.30	0.47
1:P:413:TYR:OH	1:P:641:HIS:O	2.28	0.47
1:P:622:PRO:HB3	1:R:735:LEU:HD22	2.00	0.47
1:V:735:LEU:HD22	1:W:622:PRO:HB3	1.96	0.47
1:J:413:TYR:OH	1:J:641:HIS:O	2.28	0.47
1:1:387:VAL:O	1:1:390:SER:OG	2.30	0.47
1:6:485:GLN:HA	1:6:506:THR:HG21	1.94	0.47
1:C:657:PRO:HB3	1:C:666:PHE:CZ	2.46	0.47
1:L:252:TYR:OH	1:L:372:VAL:O	2.26	0.47
1:U:657:PRO:HB3	1:U:666:PHE:CZ	2.46	0.47
1:6:413:TYR:OH	1:6:641:HIS:O	2.28	0.47
1:A:252:TYR:OH	1:A:372:VAL:O	2.26	0.47
1:K:295:ASP:OD2	1:D:397:TYR:OH	63.74	0.47
1:M:657:PRO:HB3	1:M:666:PHE:CZ	2.46	0.47
1:5:735:LEU:HD22	1:6:622:PRO:HB3	1.96	0.47
1:D:413:TYR:OH	1:D:641:HIS:O	2.28	0.47
1:J:657:PRO:HB3	1:J:666:PHE:CZ	2.46	0.47
1:X:657:PRO:HB3	1:X:666:PHE:CZ	2.46	0.47
1:2:327:ASP:OD1	1:2:327:ASP:N	2.44	0.47
1:2:387:VAL:O	1:2:390:SER:OG	2.30	0.47
1:T:735:LEU:HD22	1:4:622:PRO:HB3	95.57	0.47
1:7:434:MET:N	1:7:434:MET:SD	2.76	0.47
1:D:614:GLN:OE1	1:D:614:GLN:N	2.48	0.47
1:D:657:PRO:HB3	1:D:666:PHE:CZ	2.46	0.47
1:U:485:GLN:HE21	1:U:485:GLN:HB3	1.47	0.47
1:1:452:SER:N	1:1:455:THR:O	2.38	0.47
1:6:614:GLN:OE1	1:6:614:GLN:N	2.48	0.47
1:E:396:GLU:OE2	1:E:649:LYS:NZ	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:TYR:OH	1:E:641:HIS:O	2.28	0.47
1:H:396:GLU:OE2	1:H:649:LYS:NZ	2.37	0.47
1:H:657:PRO:HB3	1:H:666:PHE:CZ	2.46	0.47
1:R:397:TYR:OH	1:I:295:ASP:OD2	2.33	0.47
1:K:614:GLN:OE1	1:K:614:GLN:N	2.48	0.47
1:T:252:TYR:OH	1:T:372:VAL:O	2.26	0.47
1:O:735:LEU:HD22	1:I:622:PRO:HB3	1.96	0.47
1:2:614:GLN:OE1	1:2:614:GLN:N	2.48	0.47
1:C:622:PRO:HB3	1:E:735:LEU:HD22	1.97	0.47
1:D:252:TYR:OH	1:D:372:VAL:O	2.26	0.47
1:4:735:LEU:HD22	1:I:622:PRO:HB3	142.23	0.47
1:K:622:PRO:HB3	1:J:735:LEU:HD22	1.96	0.47
1:L:735:LEU:HD22	1:N:622:PRO:HB3	1.96	0.47
1:M:735:LEU:HD22	1:N:622:PRO:HB3	203.24	0.47
1:P:614:GLN:N	1:P:614:GLN:OE1	2.48	0.47
1:Q:434:MET:N	1:Q:434:MET:SD	2.76	0.47
1:S:448:THR:OG1	1:U:498:SER:O	44.34	0.47
1:O:485:GLN:HE21	1:O:485:GLN:HB3	1.47	0.47
1:1:657:PRO:HB3	1:1:666:PHE:CZ	2.46	0.47
1:S:614:GLN:N	1:S:614:GLN:OE1	2.48	0.47
1:4:314:LYS:HG3	1:4:410:THR:HG22	1.97	0.47
1:6:396:GLU:OE2	1:6:649:LYS:NZ	2.37	0.47
1:G:314:LYS:HG3	1:G:410:THR:HG22	1.97	0.47
1:L:622:PRO:HB3	1:O:735:LEU:HD22	1.97	0.47
1:N:735:LEU:HD22	1:O:622:PRO:HB3	1.96	0.47
1:R:485:GLN:HE21	1:R:485:GLN:HB3	1.47	0.47
1:X:396:GLU:OE2	1:X:649:LYS:NZ	2.37	0.47
1:Z:314:LYS:HG3	1:Z:410:THR:HG22	1.97	0.47
1:V:314:LYS:HG3	1:V:410:THR:HG22	1.98	0.46
1:5:528:ASP:OD1	1:5:528:ASP:N	2.45	0.46
1:A:735:LEU:HD22	1:2:622:PRO:HB3	1.96	0.46
1:G:614:GLN:OE1	1:G:614:GLN:N	2.48	0.46
1:N:252:TYR:OH	1:N:372:VAL:O	2.26	0.46
1:Q:485:GLN:HE21	1:Q:485:GLN:HB3	1.47	0.46
1:S:622:PRO:HB3	1:V:735:LEU:HD22	78.66	0.46
1:Y:614:GLN:N	1:Y:614:GLN:OE1	2.48	0.46
1:Y:657:PRO:HB3	1:Y:666:PHE:CZ	2.46	0.46
1:1:614:GLN:N	1:1:614:GLN:OE1	2.48	0.46
1:7:614:GLN:N	1:7:614:GLN:OE1	2.48	0.46
1:D:314:LYS:HG3	1:D:410:THR:HG22	1.98	0.46
1:D:735:LEU:HD22	1:E:622:PRO:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:314:LYS:HG3	1:K:410:THR:HG22	1.97	0.46
1:M:314:LYS:HG3	1:M:410:THR:HG22	1.97	0.46
1:Q:614:GLN:N	1:Q:614:GLN:OE1	2.48	0.46
1:S:735:LEU:HD22	1:U:622:PRO:HB3	31.72	0.46
1:U:614:GLN:OE1	1:U:614:GLN:N	2.48	0.46
1:V:498:SER:O	1:Y:448:THR:OG1	2.29	0.46
1:W:614:GLN:OE1	1:W:614:GLN:N	2.48	0.46
1:X:614:GLN:OE1	1:X:614:GLN:N	2.48	0.46
1:M:735:LEU:HD22	1:X:622:PRO:HB3	1.97	0.46
1:B:622:PRO:HB3	1:X:735:LEU:HD22	1.97	0.46
1:X:735:LEU:HD22	1:Y:622:PRO:HB3	119.20	0.46
1:G:735:LEU:HD22	1:H:622:PRO:HB3	1.98	0.46
1:K:657:PRO:HB3	1:K:666:PHE:CZ	2.46	0.46
1:I:614:GLN:OE1	1:I:614:GLN:N	2.48	0.46
1:J:485:GLN:HB3	1:J:485:GLN:HE21	1.47	0.46
1:N:614:GLN:OE1	1:N:614:GLN:N	2.48	0.46
1:S:735:LEU:HD22	1:T:622:PRO:HB3	1.97	0.46
1:S:622:PRO:HB3	1:U:735:LEU:HD22	1.97	0.46
1:C:735:LEU:HD22	1:D:622:PRO:HB3	1.96	0.46
1:E:314:LYS:HG3	1:E:410:THR:HG22	1.97	0.46
1:E:614:GLN:N	1:E:614:GLN:OE1	2.48	0.46
1:F:622:PRO:HB3	1:H:735:LEU:HD22	1.98	0.46
1:H:614:GLN:OE1	1:H:614:GLN:N	2.48	0.46
1:N:314:LYS:HG3	1:N:410:THR:HG22	1.98	0.46
1:O:657:PRO:HB3	1:O:666:PHE:CZ	2.46	0.46
1:R:657:PRO:HB3	1:R:666:PHE:CZ	2.46	0.46
1:W:735:LEU:HD22	1:X:622:PRO:HB3	141.75	0.46
1:2:314:LYS:HG3	1:2:410:THR:HG22	1.98	0.46
1:5:314:LYS:HG3	1:5:410:THR:HG22	1.97	0.46
1:5:657:PRO:HB3	1:5:666:PHE:CZ	2.46	0.46
1:A:735:LEU:HD22	1:B:622:PRO:HB3	175.13	0.46
1:E:485:GLN:HE21	1:E:485:GLN:HB3	1.47	0.46
1:S:314:LYS:HG3	1:S:410:THR:HG22	1.98	0.46
1:W:485:GLN:HB3	1:W:485:GLN:HE21	1.47	0.46
1:X:252:TYR:OH	1:X:372:VAL:O	2.26	0.46
1:Y:314:LYS:HG3	1:Y:410:THR:HG22	1.97	0.46
1:F:314:LYS:HG3	1:F:410:THR:HG22	1.97	0.46
1:M:498:SER:O	1:O:448:THR:OG1	260.85	0.46
1:M:614:GLN:N	1:M:614:GLN:OE1	2.48	0.46
1:R:314:LYS:HG3	1:R:410:THR:HG22	1.97	0.46
1:T:485:GLN:HB3	1:T:485:GLN:HE21	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:622:PRO:HB3	1:7:735:LEU:HD22	1.97	0.46
1:C:314:LYS:HG3	1:C:410:THR:HG22	1.97	0.46
1:F:413:TYR:OH	1:F:641:HIS:O	2.28	0.46
1:T:314:LYS:HG3	1:T:410:THR:HG22	1.97	0.46
1:V:614:GLN:OE1	1:V:614:GLN:N	2.48	0.46
1:V:622:PRO:HB3	1:Y:735:LEU:HD22	1.97	0.46
1:3:314:LYS:HG3	1:3:410:THR:HG22	1.98	0.46
1:5:252:TYR:OH	1:5:372:VAL:O	2.26	0.46
1:B:614:GLN:OE1	1:B:614:GLN:N	2.48	0.46
1:J:314:LYS:HG3	1:J:410:THR:HG22	1.97	0.46
1:L:614:GLN:N	1:L:614:GLN:OE1	2.48	0.46
1:R:614:GLN:N	1:R:614:GLN:OE1	2.48	0.46
1:0:314:LYS:HG3	1:0:410:THR:HG22	1.97	0.45
1:0:614:GLN:OE1	1:0:614:GLN:N	2.48	0.45
1:2:485:GLN:HE21	1:2:485:GLN:HB3	1.47	0.45
1:4:614:GLN:OE1	1:4:614:GLN:N	2.48	0.45
1:5:413:TYR:OH	1:5:641:HIS:O	2.28	0.45
1:A:309:LYS:HD3	1:A:685:GLU:HB2	1.99	0.45
1:A:314:LYS:HG3	1:A:410:THR:HG22	1.97	0.45
1:A:485:GLN:HE21	1:A:485:GLN:HB3	1.47	0.45
1:A:614:GLN:OE1	1:A:614:GLN:N	2.48	0.45
1:J:614:GLN:N	1:J:614:GLN:OE1	2.48	0.45
1:K:448:THR:OG1	1:L:498:SER:O	116.63	0.45
1:L:735:LEU:HD22	1:J:622:PRO:HB3	125.96	0.45
1:Q:314:LYS:HG3	1:Q:410:THR:HG22	1.98	0.45
1:Q:735:LEU:HD22	1:R:622:PRO:HB3	1.97	0.45
1:U:314:LYS:HG3	1:U:410:THR:HG22	1.97	0.45
1:Y:413:TYR:OH	1:Y:641:HIS:O	2.28	0.45
1:2:309:LYS:HD3	1:2:685:GLU:HB2	1.99	0.45
1:5:614:GLN:N	1:5:614:GLN:OE1	2.48	0.45
1:A:413:TYR:OH	1:A:641:HIS:O	2.28	0.45
1:B:314:LYS:HG3	1:B:410:THR:HG22	1.97	0.45
1:F:437:LEU:HB2	1:F:438:ILE:HD12	1.99	0.45
1:F:657:PRO:HB3	1:F:666:PHE:CZ	2.46	0.45
1:4:448:THR:OG1	1:I:498:SER:O	164.07	0.45
1:M:622:PRO:HB3	1:O:735:LEU:HD22	196.14	0.45
1:O:257:TYR:OH	1:O:396:GLU:OE1	2.28	0.45
1:U:309:LYS:HD3	1:U:685:GLU:HB2	1.99	0.45
1:F:485:GLN:HE21	1:F:485:GLN:HB3	1.47	0.45
1:H:314:LYS:HG3	1:H:410:THR:HG22	1.97	0.45
1:N:485:GLN:HE21	1:N:485:GLN:HB3	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:413:TYR:OH	1:R:641:HIS:O	2.28	0.45
1:S:309:LYS:HD3	1:S:685:GLU:HB2	1.99	0.45
1:Y:437:LEU:HB2	1:Y:438:ILE:HD12	1.99	0.45
1:Z:735:LEU:HD22	1:O:622:PRO:HB3	121.03	0.45
1:7:314:LYS:HG3	1:7:410:THR:HG22	1.98	0.45
1:H:309:LYS:HD3	1:H:685:GLU:HB2	1.99	0.45
1:I:314:LYS:HG3	1:I:410:THR:HG22	1.97	0.45
1:V:309:LYS:HD3	1:V:685:GLU:HB2	1.99	0.45
1:W:314:LYS:HG3	1:W:410:THR:HG22	1.98	0.45
1:W:498:SER:O	1:Y:448:THR:OG1	44.34	0.45
1:X:314:LYS:HG3	1:X:410:THR:HG22	1.97	0.45
1:0:413:TYR:OH	1:0:641:HIS:O	2.28	0.45
1:2:735:LEU:HD22	1:3:622:PRO:HB3	1.98	0.45
1:B:309:LYS:HD3	1:B:685:GLU:HB2	1.99	0.45
1:C:614:GLN:OE1	1:C:614:GLN:N	2.48	0.45
1:H:252:TYR:OH	1:H:372:VAL:O	2.26	0.45
1:H:718:GLY:HA2	1:J:257:TYR:O	77.82	0.45
1:L:437:LEU:HB2	1:L:438:ILE:HD12	1.99	0.45
1:O:314:LYS:HG3	1:O:410:THR:HG22	1.97	0.45
1:O:614:GLN:OE1	1:O:614:GLN:N	2.48	0.45
1:W:309:LYS:HD3	1:W:685:GLU:HB2	1.99	0.45
1:X:309:LYS:HD3	1:X:685:GLU:HB2	1.99	0.45
1:Z:309:LYS:HD3	1:Z:685:GLU:HB2	1.99	0.45
1:1:314:LYS:HG3	1:1:410:THR:HG22	1.97	0.45
1:1:309:LYS:HD3	1:1:685:GLU:HB2	1.99	0.45
1:2:437:LEU:HB2	1:2:438:ILE:HD12	1.99	0.45
1:7:309:LYS:HD3	1:7:685:GLU:HB2	1.99	0.45
1:C:309:LYS:HD3	1:C:685:GLU:HB2	1.99	0.45
1:F:257:TYR:OH	1:F:396:GLU:OE1	2.28	0.45
1:G:448:THR:OG1	1:H:498:SER:O	2.31	0.45
1:I:657:PRO:HB3	1:I:666:PHE:CZ	2.46	0.45
1:I:309:LYS:HD3	1:I:685:GLU:HB2	1.99	0.45
1:J:309:LYS:HD3	1:J:685:GLU:HB2	1.99	0.45
1:K:735:LEU:HD22	1:I:622:PRO:HB3	1.97	0.45
1:M:309:LYS:HD3	1:M:685:GLU:HB2	1.99	0.45
1:O:309:LYS:HD3	1:O:685:GLU:HB2	1.99	0.45
1:S:437:LEU:HB2	1:S:438:ILE:HD12	1.99	0.45
1:S:485:GLN:HB3	1:S:485:GLN:HE21	1.47	0.45
1:T:257:TYR:OH	1:T:396:GLU:OE1	2.28	0.45
1:V:437:LEU:HB2	1:V:438:ILE:HD12	1.99	0.45
1:Y:309:LYS:HD3	1:Y:685:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:309:LYS:HD3	1:0:685:GLU:HB2	1.99	0.45
1:1:413:TYR:OH	1:1:641:HIS:O	2.28	0.45
1:B:437:LEU:HB2	1:B:438:ILE:HD12	1.99	0.45
1:D:309:LYS:HD3	1:D:685:GLU:HB2	1.99	0.45
1:E:309:LYS:HD3	1:E:685:GLU:HB2	1.99	0.45
1:F:309:LYS:HD3	1:F:685:GLU:HB2	1.99	0.45
1:P:437:LEU:HB2	1:P:438:ILE:HD12	1.99	0.45
1:Q:309:LYS:HD3	1:Q:685:GLU:HB2	1.99	0.45
1:4:437:LEU:HB2	1:4:438:ILE:HD12	1.99	0.45
1:C:498:SER:O	1:E:448:THR:OG1	2.32	0.45
1:G:309:LYS:HD3	1:G:685:GLU:HB2	1.99	0.45
1:L:657:PRO:HB3	1:L:666:PHE:CZ	2.46	0.45
1:T:309:LYS:HD3	1:T:685:GLU:HB2	1.99	0.45
1:Z:657:PRO:HB3	1:Z:666:PHE:CZ	2.46	0.45
1:0:657:PRO:HB3	1:0:666:PHE:CZ	2.46	0.45
1:6:314:LYS:HG3	1:6:410:THR:HG22	1.98	0.45
1:C:437:LEU:HB2	1:C:438:ILE:HD12	1.99	0.45
1:G:437:LEU:HB2	1:G:438:ILE:HD12	1.99	0.45
1:J:437:LEU:HB2	1:J:438:ILE:HD12	1.99	0.45
1:L:314:LYS:HG3	1:L:410:THR:HG22	1.97	0.45
1:N:309:LYS:HD3	1:N:685:GLU:HB2	1.99	0.45
1:O:437:LEU:HB2	1:O:438:ILE:HD12	1.99	0.45
1:Q:252:TYR:OH	1:Q:372:VAL:O	2.26	0.45
1:Z:437:LEU:HB2	1:Z:438:ILE:HD12	1.99	0.45
1:3:252:TYR:OH	1:3:372:VAL:O	2.26	0.45
1:L:485:GLN:HE21	1:L:485:GLN:HB3	1.47	0.45
1:P:314:LYS:HG3	1:P:410:THR:HG22	1.98	0.45
1:Q:657:PRO:HB3	1:Q:666:PHE:CZ	2.46	0.45
1:L:397:TYR:OH	1:R:295:ASP:OD2	2.34	0.45
1:T:614:GLN:N	1:T:614:GLN:OE1	2.48	0.45
1:U:437:LEU:HB2	1:U:438:ILE:HD12	1.99	0.45
1:6:657:PRO:HB3	1:6:666:PHE:CZ	2.46	0.44
1:F:614:GLN:N	1:F:614:GLN:OE1	2.48	0.44
1:H:485:GLN:HE21	1:H:485:GLN:HB3	1.47	0.44
1:Q:437:LEU:HB2	1:Q:438:ILE:HD12	1.99	0.44
1:V:657:PRO:HB3	1:V:666:PHE:CZ	2.46	0.44
1:X:429:SER:OG	1:X:431:ASP:OD1	2.24	0.44
1:X:437:LEU:HB2	1:X:438:ILE:HD12	1.99	0.44
1:X:448:THR:OG1	1:Y:498:SER:O	147.74	0.44
1:3:437:LEU:HB2	1:3:438:ILE:HD12	1.99	0.44
1:4:396:GLU:OE2	1:4:649:LYS:NZ	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HB2	1:A:438:ILE:HD12	1.99	0.44
1:E:434:MET:N	1:E:434:MET:SD	2.76	0.44
1:H:229:HIS:O	1:H:244:THR:OG1	2.30	0.44
1:H:257:TYR:OH	1:H:396:GLU:OE1	2.28	0.44
1:P:309:LYS:HD3	1:P:685:GLU:HB2	1.99	0.44
1:P:657:PRO:HB3	1:P:666:PHE:CZ	2.46	0.44
1:W:657:PRO:HB3	1:W:666:PHE:CZ	2.46	0.44
1:1:465:ALA:HB1	1:1:473:GLN:HG2	2.00	0.44
1:6:309:LYS:HD3	1:6:685:GLU:HB2	1.99	0.44
1:D:448:THR:OG1	1:E:498:SER:O	2.29	0.44
1:H:465:ALA:HB1	1:H:473:GLN:HG2	2.00	0.44
1:J:252:TYR:OH	1:J:372:VAL:O	2.26	0.44
1:K:485:GLN:HB3	1:K:485:GLN:HE21	1.47	0.44
1:S:429:SER:OG	1:S:431:ASP:OD1	2.24	0.44
1:V:465:ALA:HB1	1:V:473:GLN:HG2	2.00	0.44
1:V:448:THR:OG1	1:W:498:SER:O	2.31	0.44
1:X:465:ALA:HB1	1:X:473:GLN:HG2	2.00	0.44
1:A:465:ALA:HB1	1:A:473:GLN:HG2	2.00	0.44
1:B:465:ALA:HB1	1:B:473:GLN:HG2	2.00	0.44
1:G:257:TYR:OH	1:G:396:GLU:OE1	2.28	0.44
1:I:429:SER:OG	1:I:431:ASP:OD1	2.24	0.44
1:K:448:THR:OG1	1:I:498:SER:O	2.29	0.44
1:T:437:LEU:HB2	1:T:438:ILE:HD12	1.99	0.44
1:Y:465:ALA:HB1	1:Y:473:GLN:HG2	2.00	0.44
1:2:429:SER:OG	1:2:431:ASP:OD1	2.24	0.44
1:T:448:THR:OG1	1:4:498:SER:O	116.62	0.44
1:5:309:LYS:HD3	1:5:685:GLU:HB2	1.99	0.44
1:E:437:LEU:HB2	1:E:438:ILE:HD12	1.99	0.44
1:E:465:ALA:HB1	1:E:473:GLN:HG2	2.00	0.44
1:F:465:ALA:HB1	1:F:473:GLN:HG2	2.00	0.44
1:G:252:TYR:OH	1:G:372:VAL:O	2.26	0.44
1:H:437:LEU:HB2	1:H:438:ILE:HD12	1.99	0.44
1:I:465:ALA:HB1	1:I:473:GLN:HG2	2.00	0.44
1:L:465:ALA:HB1	1:L:473:GLN:HG2	2.00	0.44
1:L:309:LYS:HD3	1:L:685:GLU:HB2	1.99	0.44
1:N:437:LEU:HB2	1:N:438:ILE:HD12	1.99	0.44
1:X:434:MET:SD	1:X:434:MET:N	2.76	0.44
1:E:429:SER:OG	1:E:431:ASP:OD1	2.24	0.44
1:I:437:LEU:HB2	1:I:438:ILE:HD12	1.99	0.44
1:K:309:LYS:HD3	1:K:685:GLU:HB2	1.99	0.44
1:M:437:LEU:HB2	1:M:438:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:309:LYS:HD3	1:R:685:GLU:HB2	1.99	0.44
1:6:437:LEU:HB2	1:6:438:ILE:HD12	1.99	0.44
1:D:437:LEU:HB2	1:D:438:ILE:HD12	1.99	0.44
1:P:252:TYR:OH	1:P:372:VAL:O	2.26	0.44
1:R:437:LEU:HB2	1:R:438:ILE:HD12	1.99	0.44
1:U:465:ALA:HB1	1:U:473:GLN:HG2	2.00	0.44
1:W:252:TYR:OH	1:W:372:VAL:O	2.26	0.44
1:B:448:THR:OG1	1:Z:498:SER:O	101.21	0.44
1:4:257:TYR:OH	1:4:396:GLU:OE1	2.28	0.44
1:5:437:LEU:HB2	1:5:438:ILE:HD12	1.99	0.44
1:7:469:ASP:OD1	1:7:469:ASP:N	2.51	0.44
1:C:465:ALA:HB1	1:C:473:GLN:HG2	2.00	0.44
1:I:485:GLN:HB3	1:I:485:GLN:HE21	1.47	0.44
1:L:257:TYR:OH	1:L:396:GLU:OE1	2.28	0.44
1:T:465:ALA:HB1	1:T:473:GLN:HG2	2.00	0.44
1:B:735:LEU:HD22	1:Z:622:PRO:HB3	88.38	0.44
1:D:469:ASP:OD1	1:D:469:ASP:N	2.51	0.44
1:K:469:ASP:N	1:K:469:ASP:OD1	2.51	0.44
1:M:465:ALA:HB1	1:M:473:GLN:HG2	2.00	0.44
1:O:465:ALA:HB1	1:O:473:GLN:HG2	2.00	0.44
1:P:485:GLN:HE21	1:P:485:GLN:HB3	1.47	0.44
1:Q:469:ASP:OD1	1:Q:469:ASP:N	2.51	0.44
1:O:696:PRO:HD3	1:R:293:PRO:HB2	2.00	0.44
1:V:469:ASP:N	1:V:469:ASP:OD1	2.51	0.44
1:Z:469:ASP:OD1	1:Z:469:ASP:N	2.51	0.44
1:0:437:LEU:HB2	1:0:438:ILE:HD12	1.99	0.43
1:3:309:LYS:HD3	1:3:685:GLU:HB2	1.99	0.43
1:D:465:ALA:HB1	1:D:473:GLN:HG2	2.00	0.43
1:G:429:SER:OG	1:G:431:ASP:OD1	2.24	0.43
1:H:469:ASP:N	1:H:469:ASP:OD1	2.51	0.43
1:N:465:ALA:HB1	1:N:473:GLN:HG2	2.00	0.43
1:R:465:ALA:HB1	1:R:473:GLN:HG2	2.00	0.43
1:S:465:ALA:HB1	1:S:473:GLN:HG2	2.00	0.43
1:W:437:LEU:HB2	1:W:438:ILE:HD12	1.99	0.43
1:7:437:LEU:HB2	1:7:438:ILE:HD12	1.99	0.43
1:A:257:TYR:OH	1:A:396:GLU:OE1	2.28	0.43
1:C:229:HIS:O	1:C:244:THR:OG1	2.30	0.43
1:G:465:ALA:HB1	1:G:473:GLN:HG2	2.00	0.43
1:J:465:ALA:HB1	1:J:473:GLN:HG2	2.00	0.43
1:I:448:THR:OG1	1:J:498:SER:O	2.33	0.43
1:K:465:ALA:HB1	1:K:473:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:469:ASP:OD1	1:L:469:ASP:N	2.51	0.43
1:P:465:ALA:HB1	1:P:473:GLN:HG2	2.00	0.43
1:Z:465:ALA:HB1	1:Z:473:GLN:HG2	2.00	0.43
1:1:437:LEU:HB2	1:1:438:ILE:HD12	1.99	0.43
1:B:257:TYR:OH	1:B:396:GLU:OE1	2.28	0.43
1:B:469:ASP:N	1:B:469:ASP:OD1	2.51	0.43
1:C:469:ASP:OD1	1:C:469:ASP:N	2.51	0.43
1:M:257:TYR:O	1:F:718:GLY:HA2	202.52	0.43
1:O:469:ASP:OD1	1:O:469:ASP:N	2.51	0.43
1:W:465:ALA:HB1	1:W:473:GLN:HG2	2.00	0.43
1:W:537:SER:OG	1:W:537:SER:O	2.36	0.43
1:X:469:ASP:OD1	1:X:469:ASP:N	2.51	0.43
1:6:465:ALA:HB1	1:6:473:GLN:HG2	2.00	0.43
1:A:469:ASP:OD1	1:A:469:ASP:N	2.51	0.43
1:F:469:ASP:N	1:F:469:ASP:OD1	2.51	0.43
1:U:469:ASP:N	1:U:469:ASP:OD1	2.51	0.43
1:W:469:ASP:OD1	1:W:469:ASP:N	2.51	0.43
1:Z:614:GLN:OE1	1:Z:614:GLN:N	2.48	0.43
1:0:469:ASP:OD1	1:0:469:ASP:N	2.51	0.43
1:4:469:ASP:OD1	1:4:469:ASP:N	2.51	0.43
1:E:657:PRO:HB3	1:E:666:PHE:CZ	2.46	0.43
1:G:469:ASP:N	1:G:469:ASP:OD1	2.51	0.43
1:G:657:PRO:HB3	1:G:666:PHE:CZ	2.46	0.43
1:I:469:ASP:OD1	1:I:469:ASP:N	2.51	0.43
1:K:735:LEU:HD22	1:L:622:PRO:HB3	95.57	0.43
1:T:469:ASP:OD1	1:T:469:ASP:N	2.51	0.43
1:3:469:ASP:N	1:3:469:ASP:OD1	2.51	0.43
1:4:309:LYS:HD3	1:4:685:GLU:HB2	1.99	0.43
1:A:448:THR:OG1	1:B:498:SER:O	214.49	0.43
1:E:229:HIS:O	1:E:244:THR:OG1	2.30	0.43
1:M:448:THR:OG1	1:N:498:SER:O	252.49	0.43
1:O:229:HIS:O	1:O:244:THR:OG1	2.30	0.43
1:2:465:ALA:HB1	1:2:473:GLN:HG2	2.00	0.43
1:G:379:THR:OG1	1:G:380:LEU:N	2.52	0.43
1:N:229:HIS:O	1:N:244:THR:OG1	2.30	0.43
1:N:657:PRO:HB3	1:N:666:PHE:CZ	2.46	0.43
1:O:718:GLY:HA2	1:P:257:TYR:O	2.19	0.43
1:3:465:ALA:HB1	1:3:473:GLN:HG2	2.00	0.43
1:3:614:GLN:OE1	1:3:614:GLN:N	2.48	0.43
1:4:379:THR:OG1	1:4:380:LEU:N	2.52	0.43
1:4:657:PRO:HB3	1:4:666:PHE:CZ	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:THR:OG1	1:B:380:LEU:N	2.52	0.43
1:K:437:LEU:HB2	1:K:438:ILE:HD12	1.99	0.43
1:M:379:THR:OG1	1:M:380:LEU:N	2.52	0.43
1:N:379:THR:OG1	1:N:380:LEU:N	2.52	0.43
1:V:379:THR:OG1	1:V:380:LEU:N	2.52	0.43
1:1:434:MET:SD	1:1:434:MET:N	2.76	0.43
1:5:465:ALA:HB1	1:5:473:GLN:HG2	2.00	0.43
1:0:718:GLY:HA2	1:7:257:TYR:O	2.18	0.43
1:D:485:GLN:HE21	1:D:485:GLN:HB3	1.47	0.43
1:K:498:SER:O	1:J:448:THR:OG1	2.33	0.43
1:L:229:HIS:O	1:L:244:THR:OG1	2.30	0.43
1:R:469:ASP:OD1	1:R:469:ASP:N	2.51	0.43
1:P:270:ASN:ND2	1:R:471:ARG:H	2.17	0.43
1:S:379:THR:OG1	1:S:380:LEU:N	2.52	0.43
1:Z:498:SER:O	1:1:448:THR:OG1	153.57	0.43
1:4:465:ALA:HB1	1:4:473:GLN:HG2	2.00	0.43
1:A:257:TYR:O	1:5:718:GLY:HA2	175.18	0.43
1:D:229:HIS:O	1:D:244:THR:OG1	2.30	0.43
1:F:379:THR:OG1	1:F:380:LEU:N	2.52	0.43
1:F:498:SER:O	1:H:448:THR:OG1	2.31	0.43
1:X:518:ASN:HA	1:X:519:PRO:HA	1.91	0.43
1:Y:379:THR:OG1	1:Y:380:LEU:N	2.52	0.43
1:4:434:MET:SD	1:4:434:MET:N	2.76	0.42
1:7:465:ALA:HB1	1:7:473:GLN:HG2	2.00	0.42
1:A:379:THR:OG1	1:A:380:LEU:N	2.52	0.42
1:B:657:PRO:HB3	1:B:666:PHE:CZ	2.46	0.42
1:E:379:THR:OG1	1:E:380:LEU:N	2.52	0.42
1:I:379:THR:OG1	1:I:380:LEU:N	2.52	0.42
1:L:379:THR:OG1	1:L:380:LEU:N	2.52	0.42
1:P:379:THR:OG1	1:P:380:LEU:N	2.52	0.42
1:Q:465:ALA:HB1	1:Q:473:GLN:HG2	2.00	0.42
1:L:653:VAL:HG11	1:R:321:LYS:HE3	2.01	0.42
1:U:379:THR:OG1	1:U:380:LEU:N	2.52	0.42
1:5:469:ASP:OD1	1:5:469:ASP:N	2.51	0.42
1:B:537:SER:OG	1:B:537:SER:O	2.36	0.42
1:C:379:THR:OG1	1:C:380:LEU:N	2.52	0.42
1:I:537:SER:OG	1:I:537:SER:O	2.36	0.42
1:M:469:ASP:OD1	1:M:469:ASP:N	2.51	0.42
1:S:498:SER:O	1:V:448:THR:OG1	113.90	0.42
1:S:657:PRO:HB3	1:S:666:PHE:CZ	2.46	0.42
1:W:379:THR:OG1	1:W:380:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:HIS:O	1:O:244:THR:OG1	2.30	0.42
1:C:537:SER:OG	1:C:537:SER:O	2.37	0.42
1:D:379:THR:OG1	1:D:380:LEU:N	2.52	0.42
1:E:537:SER:OG	1:E:537:SER:O	2.37	0.42
1:L:293:PRO:HB2	1:H:696:PRO:HD3	105.65	0.42
1:I:413:TYR:OH	1:I:641:HIS:O	2.28	0.42
1:K:379:THR:OG1	1:K:380:LEU:N	2.52	0.42
1:X:379:THR:OG1	1:X:380:LEU:N	2.52	0.42
1:Z:718:GLY:HA2	1:6:257:TYR:O	2.20	0.42
1:O:379:THR:OG1	1:O:380:LEU:N	2.52	0.42
1:2:657:PRO:HB3	1:2:666:PHE:CZ	2.46	0.42
1:A:429:SER:OG	1:A:431:ASP:OD1	2.24	0.42
1:H:379:THR:OG1	1:H:380:LEU:N	2.52	0.42
1:J:379:THR:OG1	1:J:380:LEU:N	2.52	0.42
1:J:537:SER:OG	1:J:537:SER:O	2.37	0.42
1:O:413:TYR:OH	1:O:641:HIS:O	2.28	0.42
1:V:537:SER:OG	1:V:537:SER:O	2.37	0.42
1:Z:485:GLN:HB3	1:Z:485:GLN:HE21	1.47	0.42
1:1:469:ASP:N	1:1:469:ASP:OD1	2.51	0.42
1:6:379:THR:OG1	1:6:380:LEU:N	2.52	0.42
1:O:537:SER:OG	1:O:537:SER:O	2.37	0.42
1:Y:469:ASP:OD1	1:Y:469:ASP:N	2.51	0.42
1:A:718:GLY:HA2	1:Z:257:TYR:O	116.87	0.42
1:1:379:THR:OG1	1:1:380:LEU:N	2.52	0.42
1:E:718:GLY:HA2	1:5:257:TYR:O	2.19	0.42
1:G:471:ARG:H	1:H:270:ASN:ND2	2.21	0.42
1:H:518:ASN:HA	1:H:519:PRO:HA	1.91	0.42
1:L:448:THR:OG1	1:N:498:SER:O	2.32	0.42
1:Q:379:THR:OG1	1:Q:380:LEU:N	2.52	0.42
1:P:448:THR:OG1	1:Q:498:SER:O	2.32	0.42
1:W:229:HIS:O	1:W:244:THR:OG1	2.30	0.42
1:X:257:TYR:O	1:3:718:GLY:HA2	189.29	0.42
1:O:465:ALA:HB1	1:O:473:GLN:HG2	2.00	0.42
1:5:229:HIS:O	1:5:244:THR:OG1	2.30	0.42
1:K:257:TYR:O	1:C:718:GLY:HA2	2.19	0.42
1:D:537:SER:OG	1:D:537:SER:O	2.37	0.42
1:N:718:GLY:HA2	1:O:257:TYR:O	54.91	0.42
1:Z:537:SER:O	1:Z:537:SER:OG	2.36	0.42
1:C:518:ASN:HA	1:C:519:PRO:HA	1.91	0.42
1:K:537:SER:O	1:K:537:SER:OG	2.37	0.42
1:N:469:ASP:N	1:N:469:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:718:GLY:HA2	1:Y:257:TYR:O	2.20	0.42
1:U:252:TYR:OH	1:U:372:VAL:O	2.26	0.42
1:U:429:SER:OG	1:U:431:ASP:OD1	2.24	0.42
1:Z:379:THR:OG1	1:Z:380:LEU:N	2.52	0.42
1:Z:413:TYR:OH	1:Z:641:HIS:O	2.28	0.42
1:3:379:THR:OG1	1:3:380:LEU:N	2.52	0.42
1:4:429:SER:OG	1:4:431:ASP:OD1	2.24	0.42
1:C:434:MET:SD	1:C:434:MET:N	2.76	0.42
1:B:718:GLY:HA2	1:G:257:TYR:O	224.09	0.42
1:J:257:TYR:OH	1:J:396:GLU:OE1	2.28	0.42
1:O:379:THR:OG1	1:O:380:LEU:N	2.52	0.42
1:O:434:MET:N	1:O:434:MET:SD	2.76	0.42
1:R:252:TYR:OH	1:R:372:VAL:O	2.26	0.42
1:F:448:THR:OG1	1:G:498:SER:O	2.34	0.42
1:H:537:SER:O	1:H:537:SER:OG	2.37	0.42
1:O:485:GLN:HE21	1:O:485:GLN:HB3	1.47	0.42
1:R:229:HIS:O	1:R:244:THR:OG1	2.30	0.42
1:T:379:THR:OG1	1:T:380:LEU:N	2.52	0.42
1:X:537:SER:OG	1:X:537:SER:O	2.37	0.42
1:Q:257:TYR:O	1:X:718:GLY:HA2	130.90	0.42
1:1:718:GLY:HA2	1:2:257:TYR:O	2.20	0.41
1:5:379:THR:OG1	1:5:380:LEU:N	2.52	0.41
1:5:448:THR:OG1	1:6:498:SER:O	2.33	0.41
1:C:448:THR:OG1	1:D:498:SER:O	2.34	0.41
1:G:485:GLN:HE21	1:G:485:GLN:HB3	1.47	0.41
1:M:257:TYR:O	1:R:718:GLY:HA2	217.63	0.41
1:O:518:ASN:HA	1:O:519:PRO:HA	1.91	0.41
1:U:718:GLY:HA2	1:H:257:TYR:O	195.02	0.41
1:Q:257:TYR:O	1:W:718:GLY:HA2	2.19	0.41
1:J:518:ASN:HA	1:J:519:PRO:HA	1.91	0.41
1:L:718:GLY:HA2	1:U:257:TYR:O	193.97	0.41
1:R:379:THR:OG1	1:R:380:LEU:N	2.52	0.41
1:T:257:TYR:O	1:D:718:GLY:HA2	181.45	0.41
1:B:498:SER:O	1:X:448:THR:OG1	2.30	0.41
1:C:257:TYR:OH	1:C:396:GLU:OE1	2.28	0.41
1:K:429:SER:OG	1:K:431:ASP:OD1	2.24	0.41
1:P:229:HIS:O	1:P:244:THR:OG1	2.30	0.41
1:6:229:HIS:O	1:6:244:THR:OG1	2.30	0.41
1:X:718:GLY:HA2	1:I:257:TYR:O	181.44	0.41
1:U:537:SER:O	1:U:537:SER:OG	2.37	0.41
1:7:657:PRO:HB3	1:7:666:PHE:CZ	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:GLN:HB3	1:C:485:GLN:HE21	1.47	0.41
1:K:471:ARG:H	1:L:270:ASN:ND2	96.75	0.41
1:L:257:TYR:O	1:C:718:GLY:HA2	130.89	0.41
1:U:363:PRO:HG3	1:U:370:PHE:HB3	2.03	0.41
1:V:363:PRO:HG3	1:V:370:PHE:HB3	2.03	0.41
1:X:363:PRO:HG3	1:X:370:PHE:HB3	2.03	0.41
1:A:537:SER:OG	1:A:537:SER:O	2.37	0.41
1:H:363:PRO:HG3	1:H:370:PHE:HB3	2.03	0.41
1:P:363:PRO:HG3	1:P:370:PHE:HB3	2.03	0.41
1:T:695:ASN:OD1	1:T:695:ASN:N	2.54	0.41
1:V:485:GLN:HE21	1:V:485:GLN:HB3	1.47	0.41
1:Y:257:TYR:OH	1:Y:396:GLU:OE1	2.28	0.41
1:2:379:THR:OG1	1:2:380:LEU:N	2.52	0.41
1:7:379:THR:OG1	1:7:380:LEU:N	2.52	0.41
1:B:363:PRO:HG3	1:B:370:PHE:HB3	2.03	0.41
1:D:363:PRO:HG3	1:D:370:PHE:HB3	2.03	0.41
1:E:257:TYR:OH	1:E:396:GLU:OE1	2.28	0.41
1:H:429:SER:OG	1:H:431:ASP:OD1	2.24	0.41
1:L:363:PRO:HG3	1:L:370:PHE:HB3	2.03	0.41
1:L:718:GLY:HA2	1:F:257:TYR:O	112.55	0.41
1:N:363:PRO:HG3	1:N:370:PHE:HB3	2.03	0.41
1:O:695:ASN:N	1:O:695:ASN:OD1	2.54	0.41
1:P:518:ASN:HA	1:P:519:PRO:HA	1.91	0.41
1:Z:695:ASN:N	1:Z:695:ASN:OD1	2.54	0.41
1:1:257:TYR:O	1:6:718:GLY:HA2	2.20	0.41
1:5:695:ASN:OD1	1:5:695:ASN:N	2.54	0.41
1:E:363:PRO:HG3	1:E:370:PHE:HB3	2.03	0.41
1:G:363:PRO:HG3	1:G:370:PHE:HB3	2.03	0.41
1:K:518:ASN:HA	1:K:519:PRO:HA	1.91	0.41
1:M:363:PRO:HG3	1:M:370:PHE:HB3	2.03	0.41
1:M:695:ASN:OD1	1:M:695:ASN:N	2.54	0.41
1:O:363:PRO:HG3	1:O:370:PHE:HB3	2.03	0.41
1:R:429:SER:OG	1:R:431:ASP:OD1	2.24	0.41
1:V:413:TYR:OH	1:V:641:HIS:O	2.28	0.41
1:W:363:PRO:HG3	1:W:370:PHE:HB3	2.03	0.41
1:Y:252:TYR:OH	1:Y:372:VAL:O	2.26	0.41
1:S:257:TYR:O	1:Y:718:GLY:HA2	2.22	0.41
1:Z:434:MET:SD	1:Z:434:MET:N	2.76	0.41
1:U:257:TYR:O	1:G:718:GLY:HA2	221.64	0.41
1:V:257:TYR:O	1:G:718:GLY:HA2	216.02	0.41
1:I:257:TYR:OH	1:I:396:GLU:OE1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:469:ASP:N	1:P:469:ASP:OD1	2.51	0.41
1:Q:293:PRO:HB2	1:I:696:PRO:HD3	2.03	0.41
1:R:695:ASN:N	1:R:695:ASN:OD1	2.54	0.41
1:A:257:TYR:O	1:W:718:GLY:HA2	210.52	0.41
1:Z:363:PRO:HG3	1:Z:370:PHE:HB3	2.03	0.41
1:V:718:GLY:HA2	1:4:257:TYR:O	2.20	0.41
1:4:485:GLN:HE21	1:4:485:GLN:HB3	1.47	0.41
1:6:469:ASP:N	1:6:469:ASP:OD1	2.51	0.41
1:B:229:HIS:O	1:B:244:THR:OG1	2.30	0.41
1:M:429:SER:OG	1:M:431:ASP:OD1	2.24	0.41
1:R:257:TYR:O	1:I:718:GLY:HA2	2.21	0.41
1:S:229:HIS:O	1:S:244:THR:OG1	2.30	0.41
1:S:363:PRO:HG3	1:S:370:PHE:HB3	2.03	0.41
1:S:695:ASN:N	1:S:695:ASN:OD1	2.54	0.41
1:U:518:ASN:HA	1:U:519:PRO:HA	1.91	0.41
1:U:718:GLY:HA2	1:V:257:TYR:O	2.21	0.41
1:V:518:ASN:HA	1:V:519:PRO:HA	1.91	0.41
1:Z:257:TYR:O	1:E:718:GLY:HA2	108.79	0.41
1:1:252:TYR:OH	1:1:372:VAL:O	2.26	0.41
1:6:363:PRO:HG3	1:6:370:PHE:HB3	2.03	0.41
1:B:718:GLY:HA2	1:C:257:TYR:O	179.31	0.41
1:J:434:MET:N	1:J:434:MET:SD	2.76	0.41
1:K:363:PRO:HG3	1:K:370:PHE:HB3	2.03	0.41
1:Q:363:PRO:HG3	1:Q:370:PHE:HB3	2.03	0.41
1:3:428:GLN:HB2	1:3:735:LEU:HB2	2.04	0.40
1:4:413:TYR:OH	1:4:641:HIS:O	2.28	0.40
1:0:257:TYR:O	1:F:718:GLY:HA2	2.20	0.40
1:J:695:ASN:OD1	1:J:695:ASN:N	2.54	0.40
1:R:363:PRO:HG3	1:R:370:PHE:HB3	2.03	0.40
1:S:498:SER:O	1:U:448:THR:OG1	2.31	0.40
1:Z:229:HIS:O	1:Z:244:THR:OG1	2.30	0.40
1:A:363:PRO:HG3	1:A:370:PHE:HB3	2.03	0.40
1:D:695:ASN:OD1	1:D:695:ASN:N	2.54	0.40
1:F:363:PRO:HG3	1:F:370:PHE:HB3	2.03	0.40
1:H:428:GLN:HB2	1:H:735:LEU:HB2	2.04	0.40
1:I:363:PRO:HG3	1:I:370:PHE:HB3	2.03	0.40
1:I:428:GLN:HB2	1:I:735:LEU:HB2	2.04	0.40
1:J:363:PRO:HG3	1:J:370:PHE:HB3	2.03	0.40
1:D:257:TYR:O	1:J:718:GLY:HA2	2.21	0.40
1:N:448:THR:OG1	1:O:498:SER:O	2.32	0.40
1:Q:518:ASN:HA	1:Q:519:PRO:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:695:ASN:N	1:Q:695:ASN:OD1	2.54	0.40
1:S:428:GLN:HB2	1:S:735:LEU:HB2	2.04	0.40
1:T:428:GLN:HB2	1:T:735:LEU:HB2	2.04	0.40
1:1:428:GLN:HB2	1:1:735:LEU:HB2	2.04	0.40
1:2:448:THR:OG1	1:3:498:SER:O	2.29	0.40
1:5:363:PRO:HG3	1:5:370:PHE:HB3	2.03	0.40
1:5:434:MET:SD	1:5:434:MET:N	2.76	0.40
1:F:537:SER:OG	1:F:537:SER:O	2.36	0.40
1:L:413:TYR:OH	1:L:641:HIS:O	2.28	0.40
1:M:229:HIS:O	1:M:244:THR:OG1	2.30	0.40
1:M:518:ASN:HA	1:M:519:PRO:HA	1.91	0.40
1:O:428:GLN:HB2	1:O:735:LEU:HB2	2.04	0.40
1:P:428:GLN:HB2	1:P:735:LEU:HB2	2.04	0.40
1:Q:471:ARG:H	1:R:270:ASN:ND2	2.24	0.40
1:R:434:MET:N	1:R:434:MET:SD	2.76	0.40
1:R:518:ASN:HA	1:R:519:PRO:HA	1.91	0.40
1:O:293:PRO:HB2	1:R:696:PRO:HD3	2.08	0.40
1:M:718:GLY:HA2	1:T:257:TYR:O	160.46	0.40
1:U:428:GLN:HB2	1:U:735:LEU:HB2	2.04	0.40
1:V:229:HIS:O	1:V:244:THR:OG1	2.30	0.40
1:V:428:GLN:HB2	1:V:735:LEU:HB2	2.04	0.40
1:Y:537:SER:O	1:Y:537:SER:OG	2.37	0.40
1:Y:428:GLN:HB2	1:Y:735:LEU:HB2	2.04	0.40
1:2:428:GLN:HB2	1:2:735:LEU:HB2	2.04	0.40
1:D:718:GLY:HA2	1:3:257:TYR:O	217.58	0.40
1:4:363:PRO:HG3	1:4:370:PHE:HB3	2.03	0.40
1:4:252:TYR:OH	1:4:372:VAL:O	2.26	0.40
1:B:257:TYR:O	1:4:718:GLY:HA2	2.22	0.40
1:C:428:GLN:HB2	1:C:735:LEU:HB2	2.04	0.40
1:E:428:GLN:HB2	1:E:735:LEU:HB2	2.04	0.40
1:L:518:ASN:HA	1:L:519:PRO:HA	1.91	0.40
1:Q:428:GLN:HB2	1:Q:735:LEU:HB2	2.04	0.40
1:T:448:THR:OG1	1:U:498:SER:O	2.33	0.40
1:W:695:ASN:N	1:W:695:ASN:OD1	2.54	0.40
1:X:428:GLN:HB2	1:X:735:LEU:HB2	2.04	0.40
1:Y:363:PRO:HG3	1:Y:370:PHE:HB3	2.03	0.40
1:Z:428:GLN:HB2	1:Z:735:LEU:HB2	2.04	0.40
1:A:428:GLN:HB2	1:A:735:LEU:HB2	2.04	0.40
1:B:518:ASN:HA	1:B:519:PRO:HA	1.91	0.40
1:C:695:ASN:N	1:C:695:ASN:OD1	2.54	0.40
1:D:518:ASN:HA	1:D:519:PRO:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:LYS:HG2	1:E:321:LYS:HZ3	1.77	0.40
1:G:695:ASN:OD1	1:G:695:ASN:N	2.54	0.40
1:L:428:GLN:HB2	1:L:735:LEU:HB2	2.04	0.40
1:Z:718:GLY:HA2	1:G:257:TYR:O	132.27	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	0	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	1	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	2	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	3	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	4	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	5	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	6	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	7	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	A	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	B	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	C	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	D	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	E	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	F	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	G	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	H	517/735 (70%)	501 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	J	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	K	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	L	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	M	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	N	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	O	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	P	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Q	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	R	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	S	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	T	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	U	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	V	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	W	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	X	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Y	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Z	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	a	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	b	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	c	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	d	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	e	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	f	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	g	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	h	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	i	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	j	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	k	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	l	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	m	517/735 (70%)	501 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	o	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	p	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	q	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	r	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	s	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	t	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	u	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	v	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	w	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	x	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	y	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	z	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
All	All	31020/44100 (70%)	30060 (97%)	960 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	1	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	2	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	3	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	4	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	5	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	6	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	7	458/628 (73%)	439 (96%)	19 (4%)	33	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	B	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	C	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	D	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	E	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	F	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	G	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	H	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	I	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	J	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	K	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	L	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	M	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	N	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	O	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	P	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	Q	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	R	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	S	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	T	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	U	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	V	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	W	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	X	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	Y	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	Z	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	a	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	b	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	c	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	d	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	e	458/628 (73%)	439 (96%)	19 (4%)	33	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	g	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	h	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	i	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	j	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	k	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	l	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	m	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	n	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	o	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	p	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	q	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	r	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	s	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	t	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	u	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	v	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	w	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	x	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	y	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	z	458/628 (73%)	439 (96%)	19 (4%)	33	44
All	All	27480/37680 (73%)	26340 (96%)	1140 (4%)	38	44

All (1140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	A	246	THR
1	A	288	HIS
1	A	309	LYS
1	A	312	ASN
1	A	327	ASP
1	A	382	ASN
1	A	405	THR
1	A	430	LEU

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Mol	Chain	Res	Type
1	A	455	THR
1	A	485	GLN
1	A	531	GLU
1	A	550	THR
1	A	597	THR
1	A	600	VAL
1	A	660	THR
1	A	703	ASN
1	A	716	THR
1	A	735	LEU
1	K	219	ASP
1	K	246	THR
1	K	288	HIS
1	K	309	LYS
1	K	312	ASN
1	K	327	ASP
1	K	382	ASN
1	K	405	THR
1	K	430	LEU
1	K	455	THR
1	K	485	GLN
1	K	531	GLU
1	K	550	THR
1	K	597	THR
1	K	600	VAL
1	K	660	THR
1	K	703	ASN
1	K	716	THR
1	K	735	LEU
1	L	219	ASP
1	L	246	THR
1	L	288	HIS
1	L	309	LYS
1	L	312	ASN
1	L	327	ASP
1	L	382	ASN
1	L	405	THR
1	L	430	LEU
1	L	455	THR
1	L	485	GLN
1	L	531	GLU
1	L	550	THR

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Mol	Chain	Res	Type
1	L	597	THR
1	L	600	VAL
1	L	660	THR
1	L	703	ASN
1	L	716	THR
1	L	735	LEU
1	M	219	ASP
1	M	246	THR
1	M	288	HIS
1	M	309	LYS
1	M	312	ASN
1	M	327	ASP
1	M	382	ASN
1	M	405	THR
1	M	430	LEU
1	M	455	THR
1	M	485	GLN
1	M	531	GLU
1	M	550	THR
1	M	597	THR
1	M	600	VAL
1	M	660	THR
1	M	703	ASN
1	M	716	THR
1	M	735	LEU
1	N	219	ASP
1	N	246	THR
1	N	288	HIS
1	N	309	LYS
1	N	312	ASN
1	N	327	ASP
1	N	382	ASN
1	N	405	THR
1	N	430	LEU
1	N	455	THR
1	N	485	GLN
1	N	531	GLU
1	N	550	THR
1	N	597	THR
1	N	600	VAL
1	N	660	THR
1	N	703	ASN

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Mol	Chain	Res	Type
1	N	716	THR
1	N	735	LEU
1	O	219	ASP
1	O	246	THR
1	O	288	HIS
1	O	309	LYS
1	O	312	ASN
1	O	327	ASP
1	O	382	ASN
1	O	405	THR
1	O	430	LEU
1	O	455	THR
1	O	485	GLN
1	O	531	GLU
1	O	550	THR
1	O	597	THR
1	O	600	VAL
1	O	660	THR
1	O	703	ASN
1	O	716	THR
1	O	735	LEU
1	P	219	ASP
1	P	246	THR
1	P	288	HIS
1	P	309	LYS
1	P	312	ASN
1	P	327	ASP
1	P	382	ASN
1	P	405	THR
1	P	430	LEU
1	P	455	THR
1	P	485	GLN
1	P	531	GLU
1	P	550	THR
1	P	597	THR
1	P	600	VAL
1	P	660	THR
1	P	703	ASN
1	P	716	THR
1	P	735	LEU
1	Q	219	ASP
1	Q	246	THR

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Mol	Chain	Res	Type
1	Q	288	HIS
1	Q	309	LYS
1	Q	312	ASN
1	Q	327	ASP
1	Q	382	ASN
1	Q	405	THR
1	Q	430	LEU
1	Q	455	THR
1	Q	485	GLN
1	Q	531	GLU
1	Q	550	THR
1	Q	597	THR
1	Q	600	VAL
1	Q	660	THR
1	Q	703	ASN
1	Q	716	THR
1	Q	735	LEU
1	R	219	ASP
1	R	246	THR
1	R	288	HIS
1	R	309	LYS
1	R	312	ASN
1	R	327	ASP
1	R	382	ASN
1	R	405	THR
1	R	430	LEU
1	R	455	THR
1	R	485	GLN
1	R	531	GLU
1	R	550	THR
1	R	597	THR
1	R	600	VAL
1	R	660	THR
1	R	703	ASN
1	R	716	THR
1	R	735	LEU
1	S	219	ASP
1	S	246	THR
1	S	288	HIS
1	S	309	LYS
1	S	312	ASN
1	S	327	ASP

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Mol	Chain	Res	Type
1	S	382	ASN
1	S	405	THR
1	S	430	LEU
1	S	455	THR
1	S	485	GLN
1	S	531	GLU
1	S	550	THR
1	S	597	THR
1	S	600	VAL
1	S	660	THR
1	S	703	ASN
1	S	716	THR
1	S	735	LEU
1	T	219	ASP
1	T	246	THR
1	T	288	HIS
1	T	309	LYS
1	T	312	ASN
1	T	327	ASP
1	T	382	ASN
1	T	405	THR
1	T	430	LEU
1	T	455	THR
1	T	485	GLN
1	T	531	GLU
1	T	550	THR
1	T	597	THR
1	T	600	VAL
1	T	660	THR
1	T	703	ASN
1	T	716	THR
1	T	735	LEU
1	B	219	ASP
1	B	246	THR
1	B	288	HIS
1	B	309	LYS
1	B	312	ASN
1	B	327	ASP
1	B	382	ASN
1	B	405	THR
1	B	430	LEU
1	B	455	THR

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Mol	Chain	Res	Type
1	B	485	GLN
1	B	531	GLU
1	B	550	THR
1	B	597	THR
1	B	600	VAL
1	B	660	THR
1	B	703	ASN
1	B	716	THR
1	B	735	LEU
1	U	219	ASP
1	U	246	THR
1	U	288	HIS
1	U	309	LYS
1	U	312	ASN
1	U	327	ASP
1	U	382	ASN
1	U	405	THR
1	U	430	LEU
1	U	455	THR
1	U	485	GLN
1	U	531	GLU
1	U	550	THR
1	U	597	THR
1	U	600	VAL
1	U	660	THR
1	U	703	ASN
1	U	716	THR
1	U	735	LEU
1	V	219	ASP
1	V	246	THR
1	V	288	HIS
1	V	309	LYS
1	V	312	ASN
1	V	327	ASP
1	V	382	ASN
1	V	405	THR
1	V	430	LEU
1	V	455	THR
1	V	485	GLN
1	V	531	GLU
1	V	550	THR
1	V	597	THR

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Mol	Chain	Res	Type
1	V	600	VAL
1	V	660	THR
1	V	703	ASN
1	V	716	THR
1	V	735	LEU
1	W	219	ASP
1	W	246	THR
1	W	288	HIS
1	W	309	LYS
1	W	312	ASN
1	W	327	ASP
1	W	382	ASN
1	W	405	THR
1	W	430	LEU
1	W	455	THR
1	W	485	GLN
1	W	531	GLU
1	W	550	THR
1	W	597	THR
1	W	600	VAL
1	W	660	THR
1	W	703	ASN
1	W	716	THR
1	W	735	LEU
1	X	219	ASP
1	X	246	THR
1	X	288	HIS
1	X	309	LYS
1	X	312	ASN
1	X	327	ASP
1	X	382	ASN
1	X	405	THR
1	X	430	LEU
1	X	455	THR
1	X	485	GLN
1	X	531	GLU
1	X	550	THR
1	X	597	THR
1	X	600	VAL
1	X	660	THR
1	X	703	ASN
1	X	716	THR

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Mol	Chain	Res	Type
1	X	735	LEU
1	Y	219	ASP
1	Y	246	THR
1	Y	288	HIS
1	Y	309	LYS
1	Y	312	ASN
1	Y	327	ASP
1	Y	382	ASN
1	Y	405	THR
1	Y	430	LEU
1	Y	455	THR
1	Y	485	GLN
1	Y	531	GLU
1	Y	550	THR
1	Y	597	THR
1	Y	600	VAL
1	Y	660	THR
1	Y	703	ASN
1	Y	716	THR
1	Y	735	LEU
1	Z	219	ASP
1	Z	246	THR
1	Z	288	HIS
1	Z	309	LYS
1	Z	312	ASN
1	Z	327	ASP
1	Z	382	ASN
1	Z	405	THR
1	Z	430	LEU
1	Z	455	THR
1	Z	485	GLN
1	Z	531	GLU
1	Z	550	THR
1	Z	597	THR
1	Z	600	VAL
1	Z	660	THR
1	Z	703	ASN
1	Z	716	THR
1	Z	735	LEU
1	a	219	ASP
1	a	246	THR
1	a	288	HIS

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Mol	Chain	Res	Type
1	a	309	LYS
1	a	312	ASN
1	a	327	ASP
1	a	382	ASN
1	a	405	THR
1	a	430	LEU
1	a	455	THR
1	a	485	GLN
1	a	531	GLU
1	a	550	THR
1	a	597	THR
1	a	600	VAL
1	a	660	THR
1	a	703	ASN
1	a	716	THR
1	a	735	LEU
1	b	219	ASP
1	b	246	THR
1	b	288	HIS
1	b	309	LYS
1	b	312	ASN
1	b	327	ASP
1	b	382	ASN
1	b	405	THR
1	b	430	LEU
1	b	455	THR
1	b	485	GLN
1	b	531	GLU
1	b	550	THR
1	b	597	THR
1	b	600	VAL
1	b	660	THR
1	b	703	ASN
1	b	716	THR
1	b	735	LEU
1	c	219	ASP
1	c	246	THR
1	c	288	HIS
1	c	309	LYS
1	c	312	ASN
1	c	327	ASP
1	c	382	ASN

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Mol	Chain	Res	Type
1	c	405	THR
1	c	430	LEU
1	c	455	THR
1	c	485	GLN
1	c	531	GLU
1	c	550	THR
1	c	597	THR
1	c	600	VAL
1	c	660	THR
1	c	703	ASN
1	c	716	THR
1	c	735	LEU
1	d	219	ASP
1	d	246	THR
1	d	288	HIS
1	d	309	LYS
1	d	312	ASN
1	d	327	ASP
1	d	382	ASN
1	d	405	THR
1	d	430	LEU
1	d	455	THR
1	d	485	GLN
1	d	531	GLU
1	d	550	THR
1	d	597	THR
1	d	600	VAL
1	d	660	THR
1	d	703	ASN
1	d	716	THR
1	d	735	LEU
1	C	219	ASP
1	C	246	THR
1	C	288	HIS
1	C	309	LYS
1	C	312	ASN
1	C	327	ASP
1	C	382	ASN
1	C	405	THR
1	C	430	LEU
1	C	455	THR
1	C	485	GLN

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Mol	Chain	Res	Type
1	C	531	GLU
1	C	550	THR
1	C	597	THR
1	C	600	VAL
1	C	660	THR
1	C	703	ASN
1	C	716	THR
1	C	735	LEU
1	e	219	ASP
1	e	246	THR
1	e	288	HIS
1	e	309	LYS
1	e	312	ASN
1	e	327	ASP
1	e	382	ASN
1	e	405	THR
1	e	430	LEU
1	e	455	THR
1	e	485	GLN
1	e	531	GLU
1	e	550	THR
1	e	597	THR
1	e	600	VAL
1	e	660	THR
1	e	703	ASN
1	e	716	THR
1	e	735	LEU
1	f	219	ASP
1	f	246	THR
1	f	288	HIS
1	f	309	LYS
1	f	312	ASN
1	f	327	ASP
1	f	382	ASN
1	f	405	THR
1	f	430	LEU
1	f	455	THR
1	f	485	GLN
1	f	531	GLU
1	f	550	THR
1	f	597	THR
1	f	600	VAL

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Mol	Chain	Res	Type
1	f	660	THR
1	f	703	ASN
1	f	716	THR
1	f	735	LEU
1	g	219	ASP
1	g	246	THR
1	g	288	HIS
1	g	309	LYS
1	g	312	ASN
1	g	327	ASP
1	g	382	ASN
1	g	405	THR
1	g	430	LEU
1	g	455	THR
1	g	485	GLN
1	g	531	GLU
1	g	550	THR
1	g	597	THR
1	g	600	VAL
1	g	660	THR
1	g	703	ASN
1	g	716	THR
1	g	735	LEU
1	h	219	ASP
1	h	246	THR
1	h	288	HIS
1	h	309	LYS
1	h	312	ASN
1	h	327	ASP
1	h	382	ASN
1	h	405	THR
1	h	430	LEU
1	h	455	THR
1	h	485	GLN
1	h	531	GLU
1	h	550	THR
1	h	597	THR
1	h	600	VAL
1	h	660	THR
1	h	703	ASN
1	h	716	THR
1	h	735	LEU

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Mol	Chain	Res	Type
1	i	219	ASP
1	i	246	THR
1	i	288	HIS
1	i	309	LYS
1	i	312	ASN
1	i	327	ASP
1	i	382	ASN
1	i	405	THR
1	i	430	LEU
1	i	455	THR
1	i	485	GLN
1	i	531	GLU
1	i	550	THR
1	i	597	THR
1	i	600	VAL
1	i	660	THR
1	i	703	ASN
1	i	716	THR
1	i	735	LEU
1	j	219	ASP
1	j	246	THR
1	j	288	HIS
1	j	309	LYS
1	j	312	ASN
1	j	327	ASP
1	j	382	ASN
1	j	405	THR
1	j	430	LEU
1	j	455	THR
1	j	485	GLN
1	j	531	GLU
1	j	550	THR
1	j	597	THR
1	j	600	VAL
1	j	660	THR
1	j	703	ASN
1	j	716	THR
1	j	735	LEU
1	k	219	ASP
1	k	246	THR
1	k	288	HIS
1	k	309	LYS

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Mol	Chain	Res	Type
1	k	312	ASN
1	k	327	ASP
1	k	382	ASN
1	k	405	THR
1	k	430	LEU
1	k	455	THR
1	k	485	GLN
1	k	531	GLU
1	k	550	THR
1	k	597	THR
1	k	600	VAL
1	k	660	THR
1	k	703	ASN
1	k	716	THR
1	k	735	LEU
1	l	219	ASP
1	l	246	THR
1	l	288	HIS
1	l	309	LYS
1	l	312	ASN
1	l	327	ASP
1	l	382	ASN
1	l	405	THR
1	l	430	LEU
1	l	455	THR
1	l	485	GLN
1	l	531	GLU
1	l	550	THR
1	l	597	THR
1	l	600	VAL
1	l	660	THR
1	l	703	ASN
1	l	716	THR
1	l	735	LEU
1	m	219	ASP
1	m	246	THR
1	m	288	HIS
1	m	309	LYS
1	m	312	ASN
1	m	327	ASP
1	m	382	ASN
1	m	405	THR

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Mol	Chain	Res	Type
1	m	430	LEU
1	m	455	THR
1	m	485	GLN
1	m	531	GLU
1	m	550	THR
1	m	597	THR
1	m	600	VAL
1	m	660	THR
1	m	703	ASN
1	m	716	THR
1	m	735	LEU
1	n	219	ASP
1	n	246	THR
1	n	288	HIS
1	n	309	LYS
1	n	312	ASN
1	n	327	ASP
1	n	382	ASN
1	n	405	THR
1	n	430	LEU
1	n	455	THR
1	n	485	GLN
1	n	531	GLU
1	n	550	THR
1	n	597	THR
1	n	600	VAL
1	n	660	THR
1	n	703	ASN
1	n	716	THR
1	n	735	LEU
1	D	219	ASP
1	D	246	THR
1	D	288	HIS
1	D	309	LYS
1	D	312	ASN
1	D	327	ASP
1	D	382	ASN
1	D	405	THR
1	D	430	LEU
1	D	455	THR
1	D	485	GLN
1	D	531	GLU

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Mol	Chain	Res	Type
1	D	550	THR
1	D	597	THR
1	D	600	VAL
1	D	660	THR
1	D	703	ASN
1	D	716	THR
1	D	735	LEU
1	o	219	ASP
1	o	246	THR
1	o	288	HIS
1	o	309	LYS
1	o	312	ASN
1	o	327	ASP
1	o	382	ASN
1	o	405	THR
1	o	430	LEU
1	o	455	THR
1	o	485	GLN
1	o	531	GLU
1	o	550	THR
1	o	597	THR
1	o	600	VAL
1	o	660	THR
1	o	703	ASN
1	o	716	THR
1	o	735	LEU
1	p	219	ASP
1	p	246	THR
1	p	288	HIS
1	p	309	LYS
1	p	312	ASN
1	p	327	ASP
1	p	382	ASN
1	p	405	THR
1	p	430	LEU
1	p	455	THR
1	p	485	GLN
1	p	531	GLU
1	p	550	THR
1	p	597	THR
1	p	600	VAL
1	p	660	THR

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Mol	Chain	Res	Type
1	p	703	ASN
1	p	716	THR
1	p	735	LEU
1	q	219	ASP
1	q	246	THR
1	q	288	HIS
1	q	309	LYS
1	q	312	ASN
1	q	327	ASP
1	q	382	ASN
1	q	405	THR
1	q	430	LEU
1	q	455	THR
1	q	485	GLN
1	q	531	GLU
1	q	550	THR
1	q	597	THR
1	q	600	VAL
1	q	660	THR
1	q	703	ASN
1	q	716	THR
1	q	735	LEU
1	r	219	ASP
1	r	246	THR
1	r	288	HIS
1	r	309	LYS
1	r	312	ASN
1	r	327	ASP
1	r	382	ASN
1	r	405	THR
1	r	430	LEU
1	r	455	THR
1	r	485	GLN
1	r	531	GLU
1	r	550	THR
1	r	597	THR
1	r	600	VAL
1	r	660	THR
1	r	703	ASN
1	r	716	THR
1	r	735	LEU
1	s	219	ASP

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Mol	Chain	Res	Type
1	s	246	THR
1	s	288	HIS
1	s	309	LYS
1	s	312	ASN
1	s	327	ASP
1	s	382	ASN
1	s	405	THR
1	s	430	LEU
1	s	455	THR
1	s	485	GLN
1	s	531	GLU
1	s	550	THR
1	s	597	THR
1	s	600	VAL
1	s	660	THR
1	s	703	ASN
1	s	716	THR
1	s	735	LEU
1	t	219	ASP
1	t	246	THR
1	t	288	HIS
1	t	309	LYS
1	t	312	ASN
1	t	327	ASP
1	t	382	ASN
1	t	405	THR
1	t	430	LEU
1	t	455	THR
1	t	485	GLN
1	t	531	GLU
1	t	550	THR
1	t	597	THR
1	t	600	VAL
1	t	660	THR
1	t	703	ASN
1	t	716	THR
1	t	735	LEU
1	u	219	ASP
1	u	246	THR
1	u	288	HIS
1	u	309	LYS
1	u	312	ASN

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Mol	Chain	Res	Type
1	u	327	ASP
1	u	382	ASN
1	u	405	THR
1	u	430	LEU
1	u	455	THR
1	u	485	GLN
1	u	531	GLU
1	u	550	THR
1	u	597	THR
1	u	600	VAL
1	u	660	THR
1	u	703	ASN
1	u	716	THR
1	u	735	LEU
1	v	219	ASP
1	v	246	THR
1	v	288	HIS
1	v	309	LYS
1	v	312	ASN
1	v	327	ASP
1	v	382	ASN
1	v	405	THR
1	v	430	LEU
1	v	455	THR
1	v	485	GLN
1	v	531	GLU
1	v	550	THR
1	v	597	THR
1	v	600	VAL
1	v	660	THR
1	v	703	ASN
1	v	716	THR
1	v	735	LEU
1	w	219	ASP
1	w	246	THR
1	w	288	HIS
1	w	309	LYS
1	w	312	ASN
1	w	327	ASP
1	w	382	ASN
1	w	405	THR
1	w	430	LEU

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Mol	Chain	Res	Type
1	w	455	THR
1	w	485	GLN
1	w	531	GLU
1	w	550	THR
1	w	597	THR
1	w	600	VAL
1	w	660	THR
1	w	703	ASN
1	w	716	THR
1	w	735	LEU
1	x	219	ASP
1	x	246	THR
1	x	288	HIS
1	x	309	LYS
1	x	312	ASN
1	x	327	ASP
1	x	382	ASN
1	x	405	THR
1	x	430	LEU
1	x	455	THR
1	x	485	GLN
1	x	531	GLU
1	x	550	THR
1	x	597	THR
1	x	600	VAL
1	x	660	THR
1	x	703	ASN
1	x	716	THR
1	x	735	LEU
1	E	219	ASP
1	E	246	THR
1	E	288	HIS
1	E	309	LYS
1	E	312	ASN
1	E	327	ASP
1	E	382	ASN
1	E	405	THR
1	E	430	LEU
1	E	455	THR
1	E	485	GLN
1	E	531	GLU
1	E	550	THR

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Mol	Chain	Res	Type
1	E	597	THR
1	E	600	VAL
1	E	660	THR
1	E	703	ASN
1	E	716	THR
1	E	735	LEU
1	y	219	ASP
1	y	246	THR
1	y	288	HIS
1	y	309	LYS
1	y	312	ASN
1	y	327	ASP
1	y	382	ASN
1	y	405	THR
1	y	430	LEU
1	y	455	THR
1	y	485	GLN
1	y	531	GLU
1	y	550	THR
1	y	597	THR
1	y	600	VAL
1	y	660	THR
1	y	703	ASN
1	y	716	THR
1	y	735	LEU
1	z	219	ASP
1	z	246	THR
1	z	288	HIS
1	z	309	LYS
1	z	312	ASN
1	z	327	ASP
1	z	382	ASN
1	z	405	THR
1	z	430	LEU
1	z	455	THR
1	z	485	GLN
1	z	531	GLU
1	z	550	THR
1	z	597	THR
1	z	600	VAL
1	z	660	THR
1	z	703	ASN

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Mol	Chain	Res	Type
1	z	716	THR
1	z	735	LEU
1	0	219	ASP
1	0	246	THR
1	0	288	HIS
1	0	309	LYS
1	0	312	ASN
1	0	327	ASP
1	0	382	ASN
1	0	405	THR
1	0	430	LEU
1	0	455	THR
1	0	485	GLN
1	0	531	GLU
1	0	550	THR
1	0	597	THR
1	0	600	VAL
1	0	660	THR
1	0	703	ASN
1	0	716	THR
1	0	735	LEU
1	1	219	ASP
1	1	246	THR
1	1	288	HIS
1	1	309	LYS
1	1	312	ASN
1	1	327	ASP
1	1	382	ASN
1	1	405	THR
1	1	430	LEU
1	1	455	THR
1	1	485	GLN
1	1	531	GLU
1	1	550	THR
1	1	597	THR
1	1	600	VAL
1	1	660	THR
1	1	703	ASN
1	1	716	THR
1	1	735	LEU
1	2	219	ASP
1	2	246	THR

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Mol	Chain	Res	Type
1	2	288	HIS
1	2	309	LYS
1	2	312	ASN
1	2	327	ASP
1	2	382	ASN
1	2	405	THR
1	2	430	LEU
1	2	455	THR
1	2	485	GLN
1	2	531	GLU
1	2	550	THR
1	2	597	THR
1	2	600	VAL
1	2	660	THR
1	2	703	ASN
1	2	716	THR
1	2	735	LEU
1	3	219	ASP
1	3	246	THR
1	3	288	HIS
1	3	309	LYS
1	3	312	ASN
1	3	327	ASP
1	3	382	ASN
1	3	405	THR
1	3	430	LEU
1	3	455	THR
1	3	485	GLN
1	3	531	GLU
1	3	550	THR
1	3	597	THR
1	3	600	VAL
1	3	660	THR
1	3	703	ASN
1	3	716	THR
1	3	735	LEU
1	4	219	ASP
1	4	246	THR
1	4	288	HIS
1	4	309	LYS
1	4	312	ASN
1	4	327	ASP

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Mol	Chain	Res	Type
1	4	382	ASN
1	4	405	THR
1	4	430	LEU
1	4	455	THR
1	4	485	GLN
1	4	531	GLU
1	4	550	THR
1	4	597	THR
1	4	600	VAL
1	4	660	THR
1	4	703	ASN
1	4	716	THR
1	4	735	LEU
1	5	219	ASP
1	5	246	THR
1	5	288	HIS
1	5	309	LYS
1	5	312	ASN
1	5	327	ASP
1	5	382	ASN
1	5	405	THR
1	5	430	LEU
1	5	455	THR
1	5	485	GLN
1	5	531	GLU
1	5	550	THR
1	5	597	THR
1	5	600	VAL
1	5	660	THR
1	5	703	ASN
1	5	716	THR
1	5	735	LEU
1	6	219	ASP
1	6	246	THR
1	6	288	HIS
1	6	309	LYS
1	6	312	ASN
1	6	327	ASP
1	6	382	ASN
1	6	405	THR
1	6	430	LEU
1	6	455	THR

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Mol	Chain	Res	Type
1	6	485	GLN
1	6	531	GLU
1	6	550	THR
1	6	597	THR
1	6	600	VAL
1	6	660	THR
1	6	703	ASN
1	6	716	THR
1	6	735	LEU
1	7	219	ASP
1	7	246	THR
1	7	288	HIS
1	7	309	LYS
1	7	312	ASN
1	7	327	ASP
1	7	382	ASN
1	7	405	THR
1	7	430	LEU
1	7	455	THR
1	7	485	GLN
1	7	531	GLU
1	7	550	THR
1	7	597	THR
1	7	600	VAL
1	7	660	THR
1	7	703	ASN
1	7	716	THR
1	7	735	LEU
1	F	219	ASP
1	F	246	THR
1	F	288	HIS
1	F	309	LYS
1	F	312	ASN
1	F	327	ASP
1	F	382	ASN
1	F	405	THR
1	F	430	LEU
1	F	455	THR
1	F	485	GLN
1	F	531	GLU
1	F	550	THR
1	F	597	THR

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Mol	Chain	Res	Type
1	F	600	VAL
1	F	660	THR
1	F	703	ASN
1	F	716	THR
1	F	735	LEU
1	G	219	ASP
1	G	246	THR
1	G	288	HIS
1	G	309	LYS
1	G	312	ASN
1	G	327	ASP
1	G	382	ASN
1	G	405	THR
1	G	430	LEU
1	G	455	THR
1	G	485	GLN
1	G	531	GLU
1	G	550	THR
1	G	597	THR
1	G	600	VAL
1	G	660	THR
1	G	703	ASN
1	G	716	THR
1	G	735	LEU
1	H	219	ASP
1	H	246	THR
1	H	288	HIS
1	H	309	LYS
1	H	312	ASN
1	H	327	ASP
1	H	382	ASN
1	H	405	THR
1	H	430	LEU
1	H	455	THR
1	H	485	GLN
1	H	531	GLU
1	H	550	THR
1	H	597	THR
1	H	600	VAL
1	H	660	THR
1	H	703	ASN
1	H	716	THR

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Mol	Chain	Res	Type
1	H	735	LEU
1	I	219	ASP
1	I	246	THR
1	I	288	HIS
1	I	309	LYS
1	I	312	ASN
1	I	327	ASP
1	I	382	ASN
1	I	405	THR
1	I	430	LEU
1	I	455	THR
1	I	485	GLN
1	I	531	GLU
1	I	550	THR
1	I	597	THR
1	I	600	VAL
1	I	660	THR
1	I	703	ASN
1	I	716	THR
1	I	735	LEU
1	J	219	ASP
1	J	246	THR
1	J	288	HIS
1	J	309	LYS
1	J	312	ASN
1	J	327	ASP
1	J	382	ASN
1	J	405	THR
1	J	430	LEU
1	J	455	THR
1	J	485	GLN
1	J	531	GLU
1	J	550	THR
1	J	597	THR
1	J	600	VAL
1	J	660	THR
1	J	703	ASN
1	J	716	THR
1	J	735	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (858) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	270	ASN
1	A	303	ASN
1	A	325	GLN
1	A	334	ASN
1	A	359	GLN
1	A	382	ASN
1	A	385	GLN
1	A	485	GLN
1	A	509	HIS
1	A	536	GLN
1	A	589	GLN
1	A	677	GLN
1	A	709	ASN
1	K	259	GLN
1	K	263	GLN
1	K	270	ASN
1	K	303	ASN
1	K	325	GLN
1	K	334	ASN
1	K	359	GLN
1	K	385	GLN
1	K	485	GLN
1	K	509	HIS
1	K	536	GLN
1	K	589	GLN
1	K	677	GLN
1	K	709	ASN
1	L	259	GLN
1	L	263	GLN
1	L	270	ASN
1	L	303	ASN
1	L	325	GLN
1	L	334	ASN
1	L	359	GLN
1	L	385	GLN
1	L	485	GLN
1	L	509	HIS
1	L	536	GLN
1	L	589	GLN
1	L	677	GLN
1	L	709	ASN
1	M	259	GLN

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Mol	Chain	Res	Type
1	M	263	GLN
1	M	270	ASN
1	M	303	ASN
1	M	325	GLN
1	M	334	ASN
1	M	359	GLN
1	M	385	GLN
1	M	485	GLN
1	M	509	HIS
1	M	536	GLN
1	M	589	GLN
1	M	677	GLN
1	M	709	ASN
1	N	259	GLN
1	N	263	GLN
1	N	270	ASN
1	N	303	ASN
1	N	325	GLN
1	N	334	ASN
1	N	359	GLN
1	N	385	GLN
1	N	485	GLN
1	N	509	HIS
1	N	536	GLN
1	N	589	GLN
1	N	677	GLN
1	N	709	ASN
1	O	259	GLN
1	O	263	GLN
1	O	270	ASN
1	O	303	ASN
1	O	325	GLN
1	O	334	ASN
1	O	359	GLN
1	O	385	GLN
1	O	485	GLN
1	O	509	HIS
1	O	536	GLN
1	O	589	GLN
1	O	677	GLN
1	O	709	ASN
1	P	259	GLN

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Mol	Chain	Res	Type
1	P	263	GLN
1	P	270	ASN
1	P	303	ASN
1	P	325	GLN
1	P	334	ASN
1	P	359	GLN
1	P	385	GLN
1	P	485	GLN
1	P	509	HIS
1	P	518	ASN
1	P	536	GLN
1	P	589	GLN
1	P	677	GLN
1	P	709	ASN
1	Q	259	GLN
1	Q	263	GLN
1	Q	270	ASN
1	Q	303	ASN
1	Q	325	GLN
1	Q	334	ASN
1	Q	359	GLN
1	Q	382	ASN
1	Q	385	GLN
1	Q	485	GLN
1	Q	509	HIS
1	Q	536	GLN
1	Q	589	GLN
1	Q	677	GLN
1	Q	709	ASN
1	R	259	GLN
1	R	263	GLN
1	R	270	ASN
1	R	303	ASN
1	R	325	GLN
1	R	334	ASN
1	R	359	GLN
1	R	382	ASN
1	R	385	GLN
1	R	485	GLN
1	R	509	HIS
1	R	536	GLN
1	R	589	GLN

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Mol	Chain	Res	Type
1	R	677	GLN
1	R	709	ASN
1	S	259	GLN
1	S	263	GLN
1	S	270	ASN
1	S	303	ASN
1	S	325	GLN
1	S	334	ASN
1	S	359	GLN
1	S	385	GLN
1	S	485	GLN
1	S	509	HIS
1	S	536	GLN
1	S	589	GLN
1	S	677	GLN
1	S	709	ASN
1	T	259	GLN
1	T	263	GLN
1	T	270	ASN
1	T	303	ASN
1	T	325	GLN
1	T	334	ASN
1	T	359	GLN
1	T	385	GLN
1	T	485	GLN
1	T	509	HIS
1	T	536	GLN
1	T	589	GLN
1	T	677	GLN
1	T	709	ASN
1	B	259	GLN
1	B	263	GLN
1	B	270	ASN
1	B	303	ASN
1	B	325	GLN
1	B	334	ASN
1	B	359	GLN
1	B	385	GLN
1	B	485	GLN
1	B	509	HIS
1	B	536	GLN
1	B	589	GLN

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Mol	Chain	Res	Type
1	B	677	GLN
1	B	709	ASN
1	U	263	GLN
1	U	270	ASN
1	U	303	ASN
1	U	325	GLN
1	U	334	ASN
1	U	359	GLN
1	U	382	ASN
1	U	385	GLN
1	U	485	GLN
1	U	509	HIS
1	U	536	GLN
1	U	589	GLN
1	U	677	GLN
1	U	709	ASN
1	V	259	GLN
1	V	263	GLN
1	V	270	ASN
1	V	303	ASN
1	V	325	GLN
1	V	334	ASN
1	V	359	GLN
1	V	385	GLN
1	V	485	GLN
1	V	509	HIS
1	V	536	GLN
1	V	589	GLN
1	V	677	GLN
1	V	709	ASN
1	W	259	GLN
1	W	263	GLN
1	W	270	ASN
1	W	303	ASN
1	W	325	GLN
1	W	334	ASN
1	W	359	GLN
1	W	382	ASN
1	W	385	GLN
1	W	485	GLN
1	W	509	HIS
1	W	536	GLN

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Mol	Chain	Res	Type
1	W	589	GLN
1	W	677	GLN
1	W	709	ASN
1	X	259	GLN
1	X	263	GLN
1	X	270	ASN
1	X	303	ASN
1	X	325	GLN
1	X	334	ASN
1	X	359	GLN
1	X	385	GLN
1	X	485	GLN
1	X	509	HIS
1	X	536	GLN
1	X	589	GLN
1	X	677	GLN
1	X	709	ASN
1	Y	259	GLN
1	Y	263	GLN
1	Y	270	ASN
1	Y	303	ASN
1	Y	325	GLN
1	Y	334	ASN
1	Y	359	GLN
1	Y	385	GLN
1	Y	485	GLN
1	Y	509	HIS
1	Y	536	GLN
1	Y	589	GLN
1	Y	677	GLN
1	Y	709	ASN
1	Z	259	GLN
1	Z	263	GLN
1	Z	270	ASN
1	Z	303	ASN
1	Z	325	GLN
1	Z	334	ASN
1	Z	359	GLN
1	Z	385	GLN
1	Z	485	GLN
1	Z	509	HIS
1	Z	536	GLN

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Mol	Chain	Res	Type
1	Z	589	GLN
1	Z	677	GLN
1	Z	709	ASN
1	a	259	GLN
1	a	263	GLN
1	a	270	ASN
1	a	303	ASN
1	a	325	GLN
1	a	334	ASN
1	a	359	GLN
1	a	382	ASN
1	a	385	GLN
1	a	485	GLN
1	a	509	HIS
1	a	536	GLN
1	a	589	GLN
1	a	677	GLN
1	a	709	ASN
1	b	259	GLN
1	b	263	GLN
1	b	270	ASN
1	b	303	ASN
1	b	325	GLN
1	b	334	ASN
1	b	359	GLN
1	b	385	GLN
1	b	485	GLN
1	b	509	HIS
1	b	536	GLN
1	b	589	GLN
1	b	677	GLN
1	b	709	ASN
1	c	259	GLN
1	c	263	GLN
1	c	270	ASN
1	c	303	ASN
1	c	325	GLN
1	c	334	ASN
1	c	359	GLN
1	c	385	GLN
1	c	485	GLN
1	c	509	HIS

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Mol	Chain	Res	Type
1	c	536	GLN
1	c	589	GLN
1	c	677	GLN
1	c	709	ASN
1	d	259	GLN
1	d	263	GLN
1	d	270	ASN
1	d	303	ASN
1	d	325	GLN
1	d	334	ASN
1	d	359	GLN
1	d	385	GLN
1	d	485	GLN
1	d	509	HIS
1	d	536	GLN
1	d	589	GLN
1	d	677	GLN
1	d	709	ASN
1	C	259	GLN
1	C	263	GLN
1	C	270	ASN
1	C	303	ASN
1	C	325	GLN
1	C	334	ASN
1	C	359	GLN
1	C	385	GLN
1	C	485	GLN
1	C	509	HIS
1	C	536	GLN
1	C	589	GLN
1	C	677	GLN
1	C	709	ASN
1	e	259	GLN
1	e	263	GLN
1	e	270	ASN
1	e	303	ASN
1	e	325	GLN
1	e	334	ASN
1	e	359	GLN
1	e	385	GLN
1	e	485	GLN
1	e	509	HIS

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Mol	Chain	Res	Type
1	e	536	GLN
1	e	589	GLN
1	e	677	GLN
1	e	709	ASN
1	f	259	GLN
1	f	263	GLN
1	f	270	ASN
1	f	303	ASN
1	f	325	GLN
1	f	334	ASN
1	f	359	GLN
1	f	385	GLN
1	f	485	GLN
1	f	509	HIS
1	f	536	GLN
1	f	589	GLN
1	f	677	GLN
1	f	709	ASN
1	g	259	GLN
1	g	263	GLN
1	g	270	ASN
1	g	303	ASN
1	g	325	GLN
1	g	334	ASN
1	g	359	GLN
1	g	385	GLN
1	g	485	GLN
1	g	509	HIS
1	g	536	GLN
1	g	589	GLN
1	g	677	GLN
1	h	259	GLN
1	h	263	GLN
1	h	270	ASN
1	h	303	ASN
1	h	325	GLN
1	h	334	ASN
1	h	359	GLN
1	h	385	GLN
1	h	485	GLN
1	h	509	HIS
1	h	536	GLN

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Mol	Chain	Res	Type
1	h	589	GLN
1	h	677	GLN
1	h	709	ASN
1	i	259	GLN
1	i	263	GLN
1	i	270	ASN
1	i	303	ASN
1	i	325	GLN
1	i	334	ASN
1	i	359	GLN
1	i	382	ASN
1	i	385	GLN
1	i	485	GLN
1	i	509	HIS
1	i	536	GLN
1	i	589	GLN
1	i	677	GLN
1	i	709	ASN
1	j	259	GLN
1	j	263	GLN
1	j	270	ASN
1	j	303	ASN
1	j	325	GLN
1	j	334	ASN
1	j	359	GLN
1	j	385	GLN
1	j	485	GLN
1	j	509	HIS
1	j	536	GLN
1	j	589	GLN
1	j	677	GLN
1	j	709	ASN
1	k	259	GLN
1	k	263	GLN
1	k	270	ASN
1	k	303	ASN
1	k	325	GLN
1	k	334	ASN
1	k	359	GLN
1	k	385	GLN
1	k	485	GLN
1	k	509	HIS

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Mol	Chain	Res	Type
1	k	536	GLN
1	k	589	GLN
1	k	677	GLN
1	k	709	ASN
1	l	259	GLN
1	l	263	GLN
1	l	270	ASN
1	l	303	ASN
1	l	325	GLN
1	l	334	ASN
1	l	359	GLN
1	l	385	GLN
1	l	485	GLN
1	l	509	HIS
1	l	536	GLN
1	l	589	GLN
1	l	677	GLN
1	l	709	ASN
1	m	259	GLN
1	m	263	GLN
1	m	270	ASN
1	m	303	ASN
1	m	325	GLN
1	m	334	ASN
1	m	359	GLN
1	m	382	ASN
1	m	385	GLN
1	m	485	GLN
1	m	509	HIS
1	m	536	GLN
1	m	589	GLN
1	m	677	GLN
1	m	709	ASN
1	n	259	GLN
1	n	263	GLN
1	n	270	ASN
1	n	303	ASN
1	n	325	GLN
1	n	334	ASN
1	n	359	GLN
1	n	382	ASN
1	n	385	GLN

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Mol	Chain	Res	Type
1	n	485	GLN
1	n	509	HIS
1	n	536	GLN
1	n	589	GLN
1	n	677	GLN
1	n	709	ASN
1	D	259	GLN
1	D	263	GLN
1	D	270	ASN
1	D	303	ASN
1	D	325	GLN
1	D	334	ASN
1	D	359	GLN
1	D	385	GLN
1	D	485	GLN
1	D	509	HIS
1	D	536	GLN
1	D	589	GLN
1	D	677	GLN
1	D	709	ASN
1	o	259	GLN
1	o	263	GLN
1	o	270	ASN
1	o	303	ASN
1	o	325	GLN
1	o	334	ASN
1	o	359	GLN
1	o	382	ASN
1	o	385	GLN
1	o	485	GLN
1	o	509	HIS
1	o	536	GLN
1	o	589	GLN
1	o	677	GLN
1	o	709	ASN
1	p	259	GLN
1	p	263	GLN
1	p	270	ASN
1	p	303	ASN
1	p	325	GLN
1	p	334	ASN
1	p	359	GLN

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Mol	Chain	Res	Type
1	p	385	GLN
1	p	485	GLN
1	p	509	HIS
1	p	536	GLN
1	p	589	GLN
1	p	677	GLN
1	p	709	ASN
1	q	259	GLN
1	q	263	GLN
1	q	270	ASN
1	q	303	ASN
1	q	325	GLN
1	q	334	ASN
1	q	359	GLN
1	q	385	GLN
1	q	485	GLN
1	q	509	HIS
1	q	536	GLN
1	q	589	GLN
1	q	677	GLN
1	q	709	ASN
1	r	259	GLN
1	r	263	GLN
1	r	270	ASN
1	r	303	ASN
1	r	325	GLN
1	r	334	ASN
1	r	359	GLN
1	r	385	GLN
1	r	485	GLN
1	r	509	HIS
1	r	536	GLN
1	r	589	GLN
1	r	677	GLN
1	r	709	ASN
1	s	259	GLN
1	s	263	GLN
1	s	270	ASN
1	s	303	ASN
1	s	325	GLN
1	s	334	ASN
1	s	359	GLN

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Mol	Chain	Res	Type
1	s	385	GLN
1	s	485	GLN
1	s	509	HIS
1	s	536	GLN
1	s	589	GLN
1	s	677	GLN
1	s	709	ASN
1	t	259	GLN
1	t	263	GLN
1	t	270	ASN
1	t	303	ASN
1	t	325	GLN
1	t	334	ASN
1	t	359	GLN
1	t	382	ASN
1	t	385	GLN
1	t	485	GLN
1	t	509	HIS
1	t	536	GLN
1	t	589	GLN
1	t	677	GLN
1	t	709	ASN
1	u	259	GLN
1	u	263	GLN
1	u	270	ASN
1	u	303	ASN
1	u	325	GLN
1	u	334	ASN
1	u	359	GLN
1	u	385	GLN
1	u	485	GLN
1	u	509	HIS
1	u	536	GLN
1	u	589	GLN
1	u	677	GLN
1	u	709	ASN
1	v	259	GLN
1	v	263	GLN
1	v	270	ASN
1	v	303	ASN
1	v	325	GLN
1	v	334	ASN

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Mol	Chain	Res	Type
1	v	359	GLN
1	v	385	GLN
1	v	485	GLN
1	v	509	HIS
1	v	536	GLN
1	v	589	GLN
1	v	677	GLN
1	v	709	ASN
1	w	259	GLN
1	w	263	GLN
1	w	270	ASN
1	w	303	ASN
1	w	325	GLN
1	w	334	ASN
1	w	359	GLN
1	w	385	GLN
1	w	485	GLN
1	w	509	HIS
1	w	536	GLN
1	w	589	GLN
1	w	677	GLN
1	x	259	GLN
1	x	263	GLN
1	x	270	ASN
1	x	303	ASN
1	x	325	GLN
1	x	334	ASN
1	x	359	GLN
1	x	382	ASN
1	x	385	GLN
1	x	485	GLN
1	x	509	HIS
1	x	536	GLN
1	x	589	GLN
1	x	677	GLN
1	x	709	ASN
1	E	259	GLN
1	E	263	GLN
1	E	270	ASN
1	E	303	ASN
1	E	325	GLN
1	E	334	ASN

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Mol	Chain	Res	Type
1	E	359	GLN
1	E	385	GLN
1	E	485	GLN
1	E	509	HIS
1	E	536	GLN
1	E	589	GLN
1	E	677	GLN
1	E	709	ASN
1	y	259	GLN
1	y	263	GLN
1	y	270	ASN
1	y	303	ASN
1	y	325	GLN
1	y	334	ASN
1	y	359	GLN
1	y	385	GLN
1	y	485	GLN
1	y	509	HIS
1	y	536	GLN
1	y	589	GLN
1	y	677	GLN
1	y	709	ASN
1	z	259	GLN
1	z	263	GLN
1	z	270	ASN
1	z	303	ASN
1	z	325	GLN
1	z	334	ASN
1	z	359	GLN
1	z	382	ASN
1	z	385	GLN
1	z	485	GLN
1	z	509	HIS
1	z	536	GLN
1	z	589	GLN
1	z	677	GLN
1	z	709	ASN
1	0	259	GLN
1	0	263	GLN
1	0	270	ASN
1	0	303	ASN
1	0	325	GLN

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Mol	Chain	Res	Type
1	0	334	ASN
1	0	359	GLN
1	0	382	ASN
1	0	385	GLN
1	0	485	GLN
1	0	509	HIS
1	0	518	ASN
1	0	536	GLN
1	0	589	GLN
1	0	677	GLN
1	0	709	ASN
1	1	259	GLN
1	1	263	GLN
1	1	270	ASN
1	1	303	ASN
1	1	325	GLN
1	1	334	ASN
1	1	359	GLN
1	1	382	ASN
1	1	385	GLN
1	1	485	GLN
1	1	509	HIS
1	1	536	GLN
1	1	589	GLN
1	1	677	GLN
1	1	709	ASN
1	2	259	GLN
1	2	263	GLN
1	2	270	ASN
1	2	303	ASN
1	2	325	GLN
1	2	334	ASN
1	2	359	GLN
1	2	385	GLN
1	2	485	GLN
1	2	509	HIS
1	2	536	GLN
1	2	589	GLN
1	2	677	GLN
1	2	709	ASN
1	3	259	GLN
1	3	263	GLN

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Mol	Chain	Res	Type
1	3	270	ASN
1	3	303	ASN
1	3	325	GLN
1	3	334	ASN
1	3	359	GLN
1	3	385	GLN
1	3	485	GLN
1	3	509	HIS
1	3	536	GLN
1	3	589	GLN
1	3	677	GLN
1	3	709	ASN
1	4	259	GLN
1	4	263	GLN
1	4	270	ASN
1	4	303	ASN
1	4	325	GLN
1	4	334	ASN
1	4	359	GLN
1	4	382	ASN
1	4	385	GLN
1	4	485	GLN
1	4	509	HIS
1	4	536	GLN
1	4	589	GLN
1	4	677	GLN
1	4	709	ASN
1	5	259	GLN
1	5	263	GLN
1	5	270	ASN
1	5	303	ASN
1	5	325	GLN
1	5	334	ASN
1	5	359	GLN
1	5	382	ASN
1	5	385	GLN
1	5	485	GLN
1	5	509	HIS
1	5	536	GLN
1	5	589	GLN
1	5	677	GLN
1	5	709	ASN

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Mol	Chain	Res	Type
1	6	259	GLN
1	6	263	GLN
1	6	270	ASN
1	6	303	ASN
1	6	325	GLN
1	6	334	ASN
1	6	359	GLN
1	6	385	GLN
1	6	485	GLN
1	6	509	HIS
1	6	536	GLN
1	6	589	GLN
1	6	677	GLN
1	6	709	ASN
1	7	259	GLN
1	7	263	GLN
1	7	270	ASN
1	7	303	ASN
1	7	325	GLN
1	7	334	ASN
1	7	359	GLN
1	7	382	ASN
1	7	385	GLN
1	7	485	GLN
1	7	509	HIS
1	7	536	GLN
1	7	589	GLN
1	7	677	GLN
1	7	709	ASN
1	F	259	GLN
1	F	263	GLN
1	F	270	ASN
1	F	303	ASN
1	F	325	GLN
1	F	334	ASN
1	F	359	GLN
1	F	385	GLN
1	F	485	GLN
1	F	509	HIS
1	F	536	GLN
1	F	589	GLN
1	F	677	GLN

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Mol	Chain	Res	Type
1	F	709	ASN
1	G	259	GLN
1	G	263	GLN
1	G	270	ASN
1	G	303	ASN
1	G	325	GLN
1	G	334	ASN
1	G	359	GLN
1	G	382	ASN
1	G	385	GLN
1	G	485	GLN
1	G	509	HIS
1	G	536	GLN
1	G	589	GLN
1	G	677	GLN
1	G	709	ASN
1	H	259	GLN
1	H	263	GLN
1	H	270	ASN
1	H	303	ASN
1	H	325	GLN
1	H	334	ASN
1	H	359	GLN
1	H	382	ASN
1	H	385	GLN
1	H	485	GLN
1	H	509	HIS
1	H	536	GLN
1	H	589	GLN
1	H	677	GLN
1	H	709	ASN
1	I	259	GLN
1	I	263	GLN
1	I	270	ASN
1	I	303	ASN
1	I	325	GLN
1	I	334	ASN
1	I	359	GLN
1	I	385	GLN
1	I	485	GLN
1	I	509	HIS
1	I	536	GLN

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Mol	Chain	Res	Type
1	I	589	GLN
1	I	677	GLN
1	I	709	ASN
1	J	259	GLN
1	J	263	GLN
1	J	270	ASN
1	J	303	ASN
1	J	325	GLN
1	J	334	ASN
1	J	359	GLN
1	J	385	GLN
1	J	485	GLN
1	J	509	HIS
1	J	536	GLN
1	J	589	GLN
1	J	677	GLN
1	J	709	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](#)

There are no ligands in this entry.

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.