



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:41 PM UTC

PDB ID : 3HF9 / pdb_00003hf9
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome open-gate mutant modified by inhibitor GL1
Authors : Li, D.; Li, H.
Deposited on : 2009-05-11
Resolution : 2.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

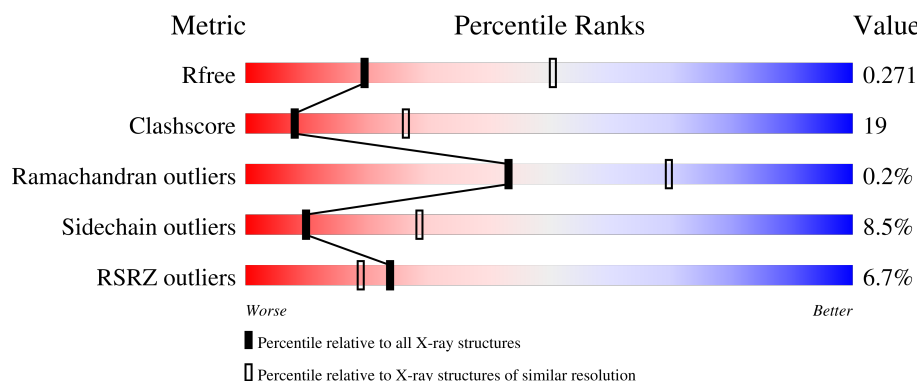
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	240	10% 55% 32% • 12%
1	3	240	4% 58% 25% • 12%
1	A	240	4% 45% 37% 6% 12%
1	B	240	• 50% 30% 8% 12%
1	D	240	31% 42% 39% 7% 12%

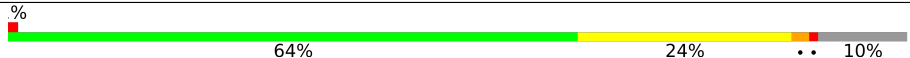
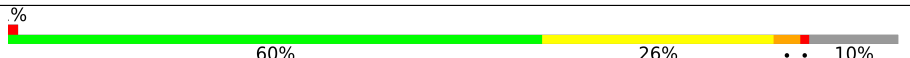
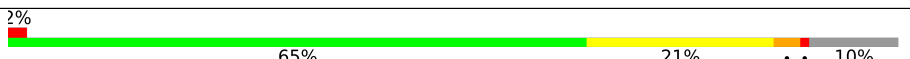
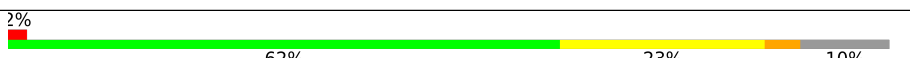
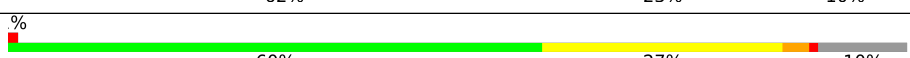
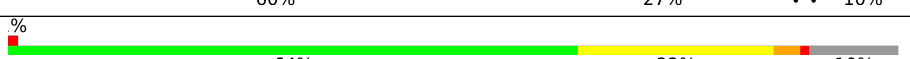
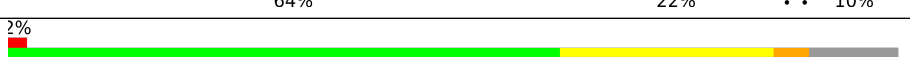
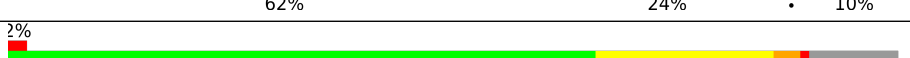
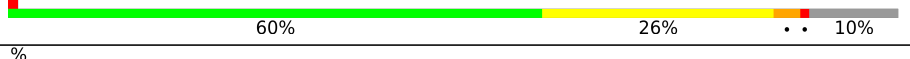
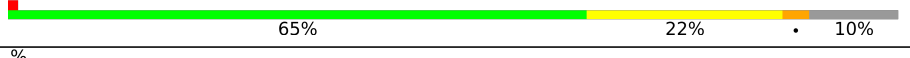
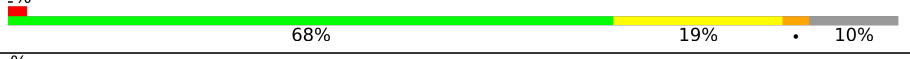
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Mol	Chain	Length	Quality of chain
1	F	240	
1	I	240	
1	K	240	
1	M	240	
1	O	240	
1	Q	240	
1	S	240	
1	U	240	
1	W	240	
1	Y	240	
1	a	240	
1	b	240	
1	d	240	
1	f	240	
1	i	240	
1	k	240	
1	m	240	
1	o	240	
1	q	240	
1	s	240	
1	u	240	
1	w	240	
1	y	240	
2	2	240	
2	4	240	

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Mol	Chain	Length	Quality of chain
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	
2	c	240	
2	e	240	
2	g	240	
2	h	240	
2	j	240	
2	l	240	
2	n	240	
2	p	240	
2	r	240	
2	t	240	
2	v	240	
2	x	240	

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Mol	Chain	Length	Quality of chain
2	z	240	% 62% 25% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OZT	2	1	-	-	X	-
2	OZT	4	301	-	-	X	-
2	OZT	E	1	-	-	X	-
2	OZT	H	1	-	-	X	-
2	OZT	L	1	-	-	X	-
2	OZT	X	1	-	-	X	-
2	OZT	g	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 90443 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome (Alpha subunit) PrcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	B	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	D	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			
1	F	193	Total	C	N	O	S	0	0	0
			1490	939	267	282	2			
1	I	212	Total	C	N	O	S	0	0	0
			1640	1028	300	309	3			
1	K	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	M	205	Total	C	N	O	S	0	0	0
			1589	995	292	299	3			
1	O	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	Q	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	S	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	U	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	W	193	Total	C	N	O	S	0	0	0
			1487	936	267	282	2			
1	Y	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			
1	1	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	a	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	b	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	d	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	f	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	i	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	k	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	m	208	Total	C	N	O	S	0	0	0
			1612	1008	296	305	3			
1	o	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	q	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	s	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	u	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	w	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	y	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	3	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP O33244
B	9	MET	-	initiating methionine	UNP O33244
D	9	MET	-	initiating methionine	UNP O33244
F	9	MET	-	initiating methionine	UNP O33244
I	9	MET	-	initiating methionine	UNP O33244
K	9	MET	-	initiating methionine	UNP O33244
M	9	MET	-	initiating methionine	UNP O33244
O	9	MET	-	initiating methionine	UNP O33244
Q	9	MET	-	initiating methionine	UNP O33244
S	9	MET	-	initiating methionine	UNP O33244
U	9	MET	-	initiating methionine	UNP O33244
W	9	MET	-	initiating methionine	UNP O33244
Y	9	MET	-	initiating methionine	UNP O33244
1	9	MET	-	initiating methionine	UNP O33244
a	309	MET	-	initiating methionine	UNP O33244

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Chain	Residue	Modelled	Actual	Comment	Reference
b	309	MET	-	initiating methionine	UNP O33244
d	309	MET	-	initiating methionine	UNP O33244
f	309	MET	-	initiating methionine	UNP O33244
i	309	MET	-	initiating methionine	UNP O33244
k	309	MET	-	initiating methionine	UNP O33244
m	309	MET	-	initiating methionine	UNP O33244
o	309	MET	-	initiating methionine	UNP O33244
q	309	MET	-	initiating methionine	UNP O33244
s	309	MET	-	initiating methionine	UNP O33244
u	309	MET	-	initiating methionine	UNP O33244
w	309	MET	-	initiating methionine	UNP O33244
y	309	MET	-	initiating methionine	UNP O33244
3	309	MET	-	initiating methionine	UNP O33244

- Molecule 2 is a protein called Proteasome (Beta subunit) PrcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	C	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	E	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	G	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	J	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	L	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	N	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	P	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	R	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	T	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	V	218	Total	C	N	O	S	0	0	0
			1610	1009	277	320	4			
2	X	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	Z	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	h	214	Total	C	N	O	S	0	0	0
			1588	995	273	316	4			
2	c	215	Total	C	N	O	S	0	0	0
			1596	1001	274	317	4			
2	e	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	g	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	j	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	l	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	n	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	p	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	r	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	t	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	v	219	Total	C	N	O	S	0	0	0
			1615	1012	278	321	4			
2	x	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	z	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	4	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	OZT	-	insertion	UNP O33245
H	235	HIS	-	expression tag	UNP O33245
H	236	HIS	-	expression tag	UNP O33245
H	237	HIS	-	expression tag	UNP O33245
H	238	HIS	-	expression tag	UNP O33245
H	239	HIS	-	expression tag	UNP O33245
H	240	HIS	-	expression tag	UNP O33245
C	1	OZT	-	insertion	UNP O33245
C	235	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
C	236	HIS	-	expression tag	UNP O33245
C	237	HIS	-	expression tag	UNP O33245
C	238	HIS	-	expression tag	UNP O33245
C	239	HIS	-	expression tag	UNP O33245
C	240	HIS	-	expression tag	UNP O33245
E	1	OZT	-	insertion	UNP O33245
E	235	HIS	-	expression tag	UNP O33245
E	236	HIS	-	expression tag	UNP O33245
E	237	HIS	-	expression tag	UNP O33245
E	238	HIS	-	expression tag	UNP O33245
E	239	HIS	-	expression tag	UNP O33245
E	240	HIS	-	expression tag	UNP O33245
G	1	OZT	-	insertion	UNP O33245
G	235	HIS	-	expression tag	UNP O33245
G	236	HIS	-	expression tag	UNP O33245
G	237	HIS	-	expression tag	UNP O33245
G	238	HIS	-	expression tag	UNP O33245
G	239	HIS	-	expression tag	UNP O33245
G	240	HIS	-	expression tag	UNP O33245
J	1	OZT	-	insertion	UNP O33245
J	235	HIS	-	expression tag	UNP O33245
J	236	HIS	-	expression tag	UNP O33245
J	237	HIS	-	expression tag	UNP O33245
J	238	HIS	-	expression tag	UNP O33245
J	239	HIS	-	expression tag	UNP O33245
J	240	HIS	-	expression tag	UNP O33245
L	1	OZT	-	insertion	UNP O33245
L	235	HIS	-	expression tag	UNP O33245
L	236	HIS	-	expression tag	UNP O33245
L	237	HIS	-	expression tag	UNP O33245
L	238	HIS	-	expression tag	UNP O33245
L	239	HIS	-	expression tag	UNP O33245
L	240	HIS	-	expression tag	UNP O33245
N	1	OZT	-	insertion	UNP O33245
N	235	HIS	-	expression tag	UNP O33245
N	236	HIS	-	expression tag	UNP O33245
N	237	HIS	-	expression tag	UNP O33245
N	238	HIS	-	expression tag	UNP O33245
N	239	HIS	-	expression tag	UNP O33245
N	240	HIS	-	expression tag	UNP O33245
P	1	OZT	-	insertion	UNP O33245
P	235	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
P	236	HIS	-	expression tag	UNP O33245
P	237	HIS	-	expression tag	UNP O33245
P	238	HIS	-	expression tag	UNP O33245
P	239	HIS	-	expression tag	UNP O33245
P	240	HIS	-	expression tag	UNP O33245
R	1	OZT	-	insertion	UNP O33245
R	235	HIS	-	expression tag	UNP O33245
R	236	HIS	-	expression tag	UNP O33245
R	237	HIS	-	expression tag	UNP O33245
R	238	HIS	-	expression tag	UNP O33245
R	239	HIS	-	expression tag	UNP O33245
R	240	HIS	-	expression tag	UNP O33245
T	1	OZT	-	insertion	UNP O33245
T	235	HIS	-	expression tag	UNP O33245
T	236	HIS	-	expression tag	UNP O33245
T	237	HIS	-	expression tag	UNP O33245
T	238	HIS	-	expression tag	UNP O33245
T	239	HIS	-	expression tag	UNP O33245
T	240	HIS	-	expression tag	UNP O33245
V	1	OZT	-	insertion	UNP O33245
V	235	HIS	-	expression tag	UNP O33245
V	236	HIS	-	expression tag	UNP O33245
V	237	HIS	-	expression tag	UNP O33245
V	238	HIS	-	expression tag	UNP O33245
V	239	HIS	-	expression tag	UNP O33245
V	240	HIS	-	expression tag	UNP O33245
X	1	OZT	-	insertion	UNP O33245
X	235	HIS	-	expression tag	UNP O33245
X	236	HIS	-	expression tag	UNP O33245
X	237	HIS	-	expression tag	UNP O33245
X	238	HIS	-	expression tag	UNP O33245
X	239	HIS	-	expression tag	UNP O33245
X	240	HIS	-	expression tag	UNP O33245
Z	1	OZT	-	insertion	UNP O33245
Z	235	HIS	-	expression tag	UNP O33245
Z	236	HIS	-	expression tag	UNP O33245
Z	237	HIS	-	expression tag	UNP O33245
Z	238	HIS	-	expression tag	UNP O33245
Z	239	HIS	-	expression tag	UNP O33245
Z	240	HIS	-	expression tag	UNP O33245
2	1	OZT	-	insertion	UNP O33245
2	235	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
2	236	HIS	-	expression tag	UNP O33245
2	237	HIS	-	expression tag	UNP O33245
2	238	HIS	-	expression tag	UNP O33245
2	239	HIS	-	expression tag	UNP O33245
2	240	HIS	-	expression tag	UNP O33245
h	301	OZT	-	insertion	UNP O33245
h	535	HIS	-	expression tag	UNP O33245
h	536	HIS	-	expression tag	UNP O33245
h	537	HIS	-	expression tag	UNP O33245
h	538	HIS	-	expression tag	UNP O33245
h	539	HIS	-	expression tag	UNP O33245
h	540	HIS	-	expression tag	UNP O33245
c	301	OZT	-	insertion	UNP O33245
c	535	HIS	-	expression tag	UNP O33245
c	536	HIS	-	expression tag	UNP O33245
c	537	HIS	-	expression tag	UNP O33245
c	538	HIS	-	expression tag	UNP O33245
c	539	HIS	-	expression tag	UNP O33245
c	540	HIS	-	expression tag	UNP O33245
e	301	OZT	-	insertion	UNP O33245
e	535	HIS	-	expression tag	UNP O33245
e	536	HIS	-	expression tag	UNP O33245
e	537	HIS	-	expression tag	UNP O33245
e	538	HIS	-	expression tag	UNP O33245
e	539	HIS	-	expression tag	UNP O33245
e	540	HIS	-	expression tag	UNP O33245
g	301	OZT	-	insertion	UNP O33245
g	535	HIS	-	expression tag	UNP O33245
g	536	HIS	-	expression tag	UNP O33245
g	537	HIS	-	expression tag	UNP O33245
g	538	HIS	-	expression tag	UNP O33245
g	539	HIS	-	expression tag	UNP O33245
g	540	HIS	-	expression tag	UNP O33245
j	301	OZT	-	insertion	UNP O33245
j	535	HIS	-	expression tag	UNP O33245
j	536	HIS	-	expression tag	UNP O33245
j	537	HIS	-	expression tag	UNP O33245
j	538	HIS	-	expression tag	UNP O33245
j	539	HIS	-	expression tag	UNP O33245
j	540	HIS	-	expression tag	UNP O33245
l	301	OZT	-	insertion	UNP O33245
l	535	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
l	536	HIS	-	expression tag	UNP O33245
l	537	HIS	-	expression tag	UNP O33245
l	538	HIS	-	expression tag	UNP O33245
l	539	HIS	-	expression tag	UNP O33245
l	540	HIS	-	expression tag	UNP O33245
n	301	OZT	-	insertion	UNP O33245
n	535	HIS	-	expression tag	UNP O33245
n	536	HIS	-	expression tag	UNP O33245
n	537	HIS	-	expression tag	UNP O33245
n	538	HIS	-	expression tag	UNP O33245
n	539	HIS	-	expression tag	UNP O33245
n	540	HIS	-	expression tag	UNP O33245
p	301	OZT	-	insertion	UNP O33245
p	535	HIS	-	expression tag	UNP O33245
p	536	HIS	-	expression tag	UNP O33245
p	537	HIS	-	expression tag	UNP O33245
p	538	HIS	-	expression tag	UNP O33245
p	539	HIS	-	expression tag	UNP O33245
p	540	HIS	-	expression tag	UNP O33245
r	301	OZT	-	insertion	UNP O33245
r	535	HIS	-	expression tag	UNP O33245
r	536	HIS	-	expression tag	UNP O33245
r	537	HIS	-	expression tag	UNP O33245
r	538	HIS	-	expression tag	UNP O33245
r	539	HIS	-	expression tag	UNP O33245
r	540	HIS	-	expression tag	UNP O33245
t	301	OZT	-	insertion	UNP O33245
t	535	HIS	-	expression tag	UNP O33245
t	536	HIS	-	expression tag	UNP O33245
t	537	HIS	-	expression tag	UNP O33245
t	538	HIS	-	expression tag	UNP O33245
t	539	HIS	-	expression tag	UNP O33245
t	540	HIS	-	expression tag	UNP O33245
v	301	OZT	-	insertion	UNP O33245
v	535	HIS	-	expression tag	UNP O33245
v	536	HIS	-	expression tag	UNP O33245
v	537	HIS	-	expression tag	UNP O33245
v	538	HIS	-	expression tag	UNP O33245
v	539	HIS	-	expression tag	UNP O33245
v	540	HIS	-	expression tag	UNP O33245
x	301	OZT	-	insertion	UNP O33245
x	535	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
x	536	HIS	-	expression tag	UNP O33245
x	537	HIS	-	expression tag	UNP O33245
x	538	HIS	-	expression tag	UNP O33245
x	539	HIS	-	expression tag	UNP O33245
x	540	HIS	-	expression tag	UNP O33245
z	301	OZT	-	insertion	UNP O33245
z	535	HIS	-	expression tag	UNP O33245
z	536	HIS	-	expression tag	UNP O33245
z	537	HIS	-	expression tag	UNP O33245
z	538	HIS	-	expression tag	UNP O33245
z	539	HIS	-	expression tag	UNP O33245
z	540	HIS	-	expression tag	UNP O33245
4	301	OZT	-	insertion	UNP O33245
4	535	HIS	-	expression tag	UNP O33245
4	536	HIS	-	expression tag	UNP O33245
4	537	HIS	-	expression tag	UNP O33245
4	538	HIS	-	expression tag	UNP O33245
4	539	HIS	-	expression tag	UNP O33245
4	540	HIS	-	expression tag	UNP O33245

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	2	Total O 2 2	0	0
3	F	3	Total O 3 3	0	0
3	I	4	Total O 4 4	0	0
3	K	3	Total O 3 3	0	0
3	M	1	Total O 1 1	0	0
3	O	3	Total O 3 3	0	0
3	S	2	Total O 2 2	0	0
3	U	1	Total O 1 1	0	0
3	1	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	a	5	Total O 5 5	0	0
3	b	3	Total O 3 3	0	0
3	d	2	Total O 2 2	0	0
3	f	1	Total O 1 1	0	0
3	i	1	Total O 1 1	0	0
3	k	2	Total O 2 2	0	0
3	o	1	Total O 1 1	0	0
3	q	1	Total O 1 1	0	0
3	s	2	Total O 2 2	0	0
3	u	2	Total O 2 2	0	0
3	w	4	Total O 4 4	0	0
3	y	2	Total O 2 2	0	0
3	3	5	Total O 5 5	0	0
3	H	1	Total O 1 1	0	0
3	E	4	Total O 4 4	0	0
3	G	2	Total O 2 2	0	0
3	J	2	Total O 2 2	0	0
3	L	1	Total O 1 1	0	0
3	N	6	Total O 6 6	0	0
3	P	4	Total O 4 4	0	0
3	R	3	Total O 3 3	0	0

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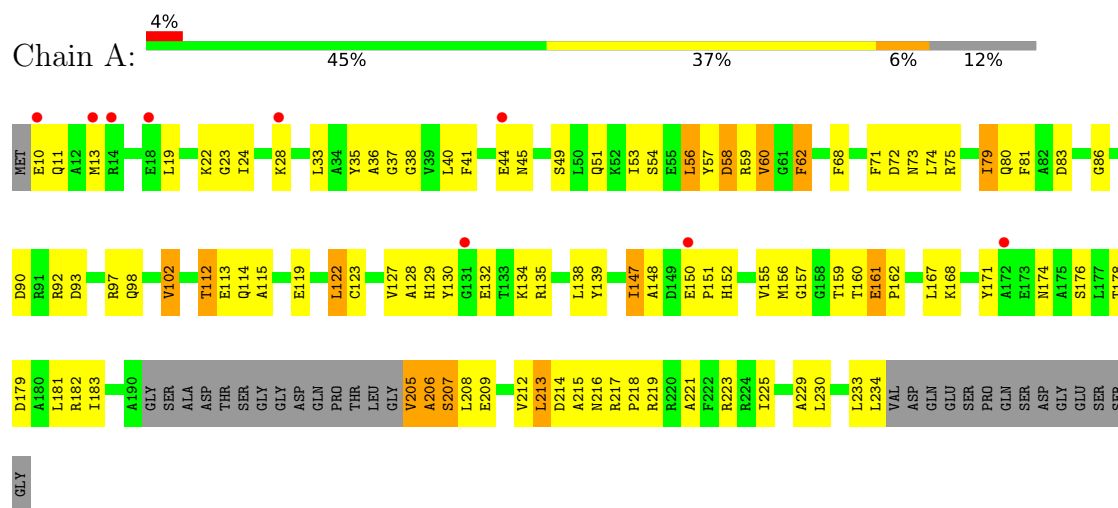
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	T	1	Total O 1 1	0	0
3	V	6	Total O 6 6	0	0
3	X	4	Total O 4 4	0	0
3	2	1	Total O 1 1	0	0
3	h	3	Total O 3 3	0	0
3	c	6	Total O 6 6	0	0
3	e	5	Total O 5 5	0	0
3	g	3	Total O 3 3	0	0
3	j	3	Total O 3 3	0	0
3	l	3	Total O 3 3	0	0
3	n	2	Total O 2 2	0	0
3	p	2	Total O 2 2	0	0
3	r	2	Total O 2 2	0	0
3	t	2	Total O 2 2	0	0
3	v	4	Total O 4 4	0	0
3	x	1	Total O 1 1	0	0
3	z	4	Total O 4 4	0	0
3	4	7	Total O 7 7	0	0

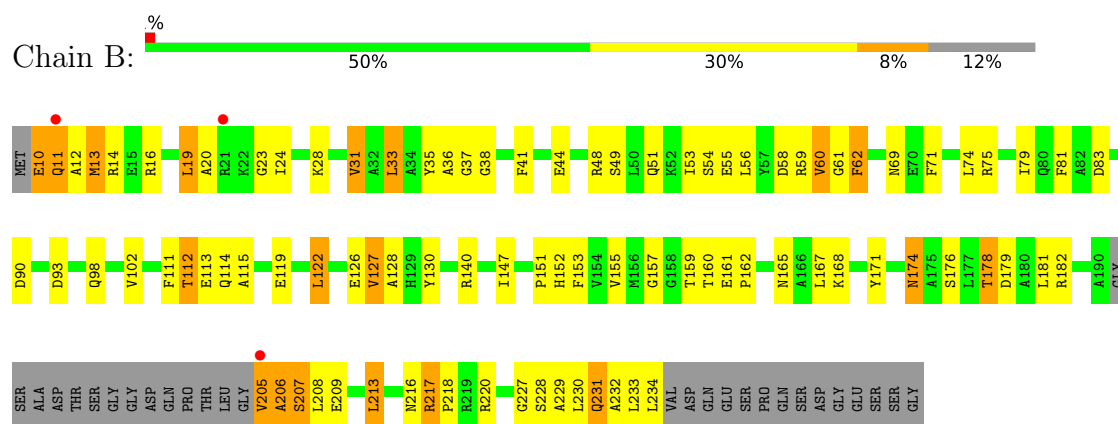
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

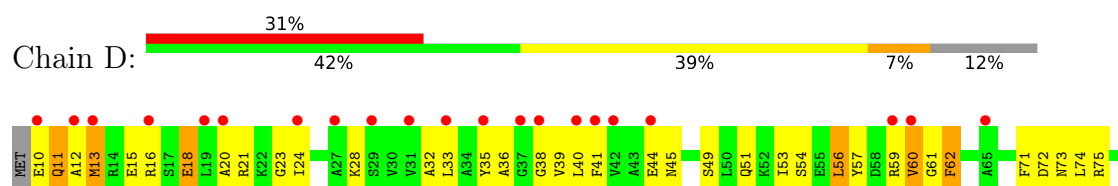
• Molecule 1: Proteasome (Alpha subunit) PrcA

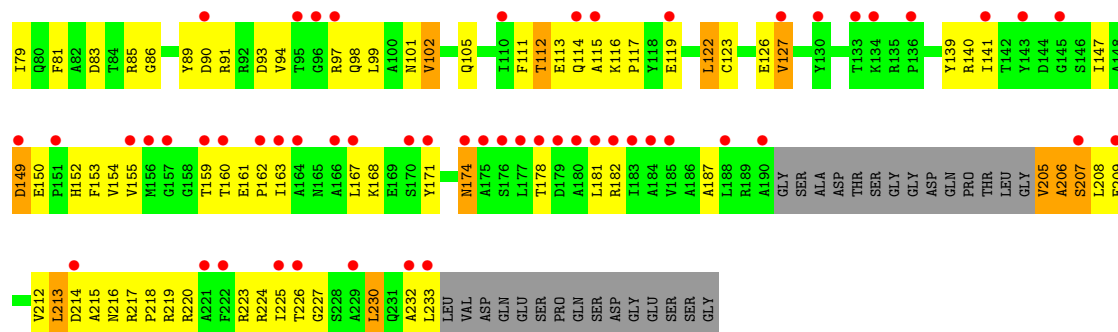


• Molecule 1: Proteasome (Alpha subunit) PrcA

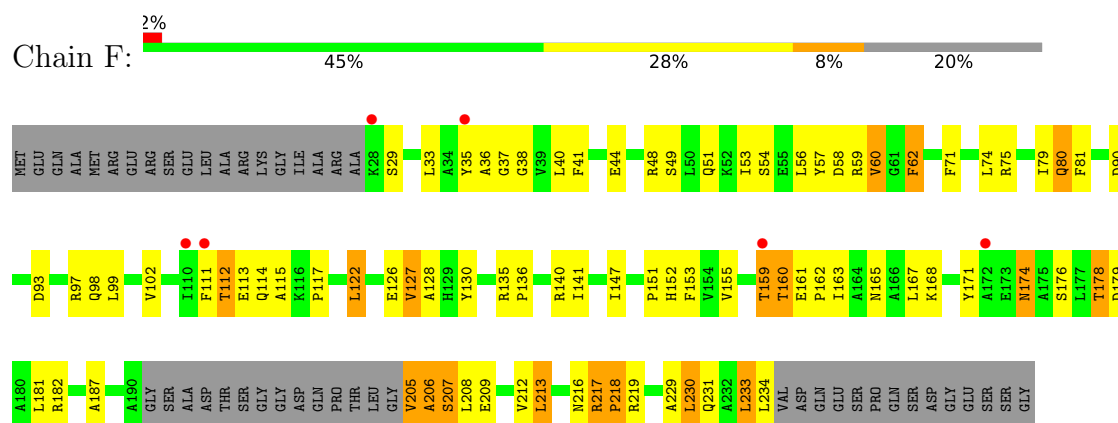


• Molecule 1: Proteasome (Alpha subunit) PrcA

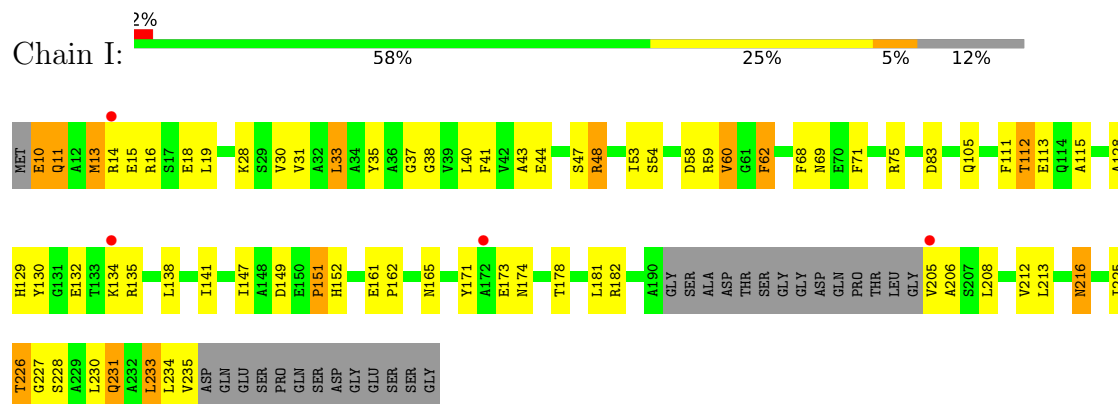




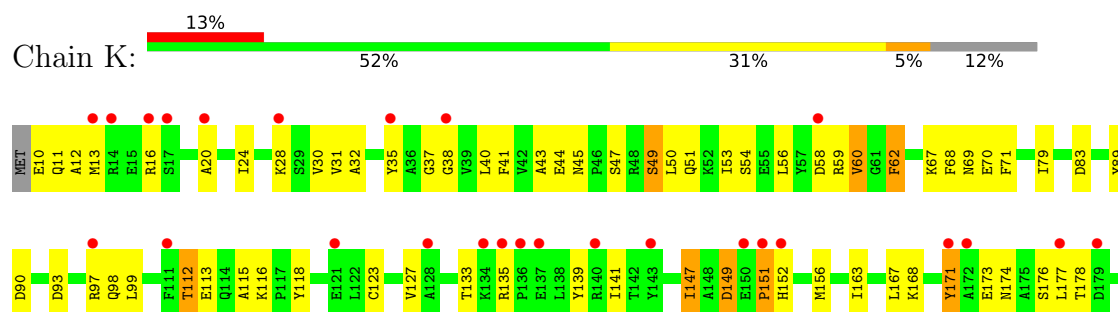
- Molecule 1: Proteasome (Alpha subunit) PrcA



- Molecule 1: Proteasome (Alpha subunit) PrcA

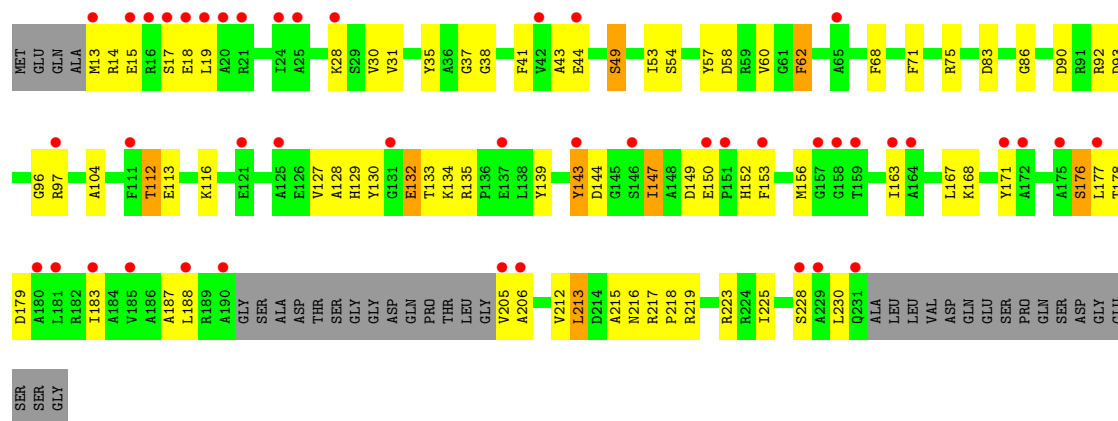


- Molecule 1: Proteasome (Alpha subunit) PrcA

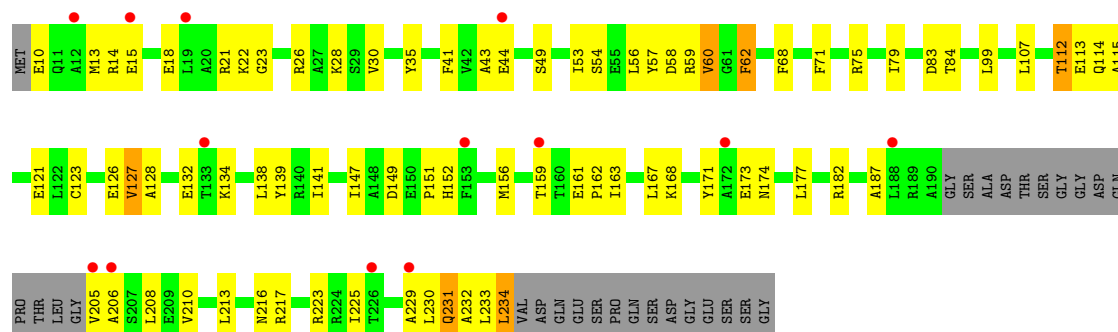




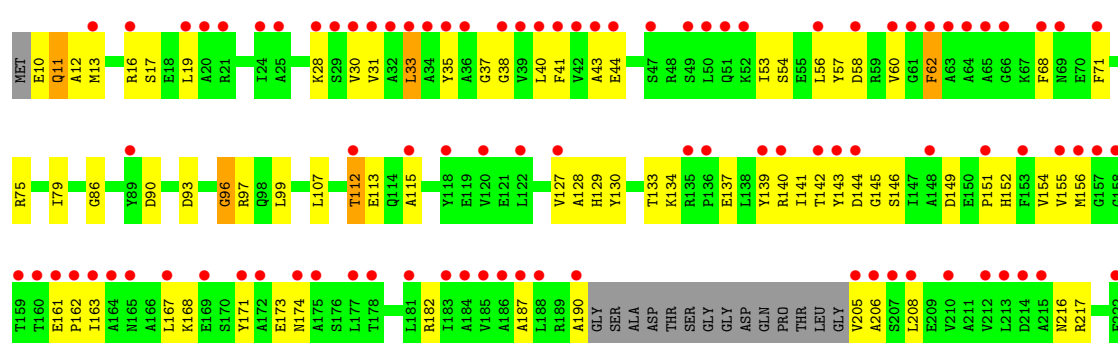
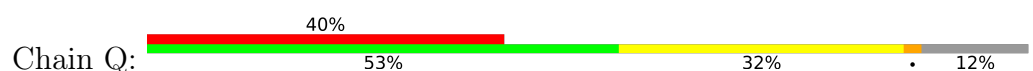
● Molecule 1: Proteasome (Alpha subunit) PrcA

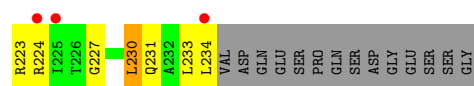


● Molecule 1: Proteasome (Alpha subunit) PrcA

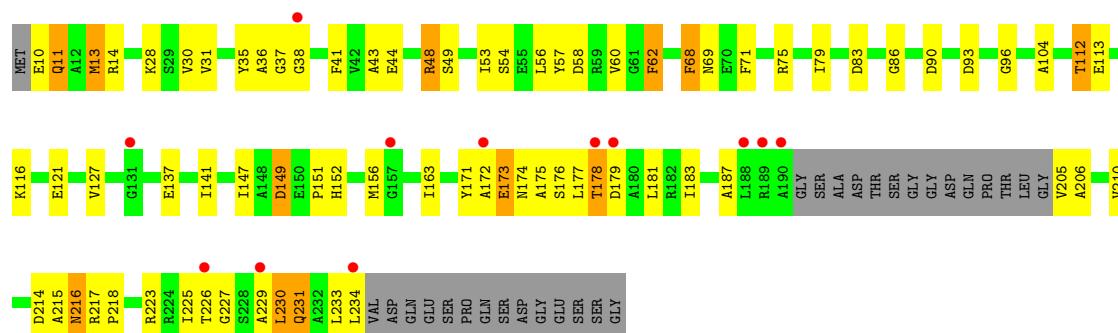


● Molecule 1: Proteasome (Alpha subunit) PrcA

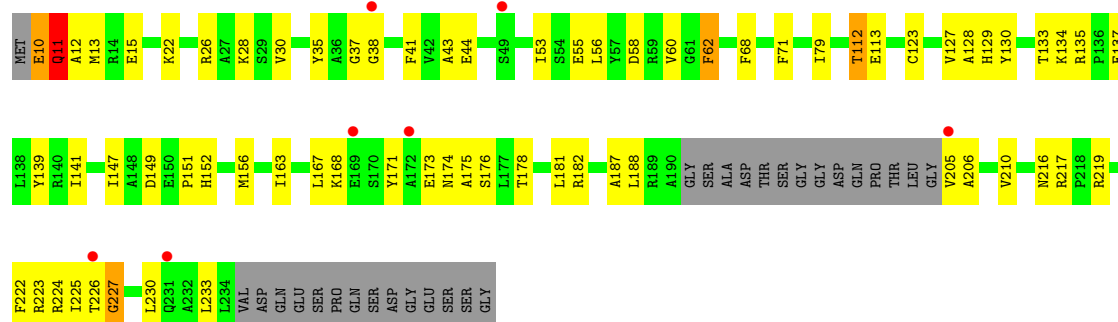




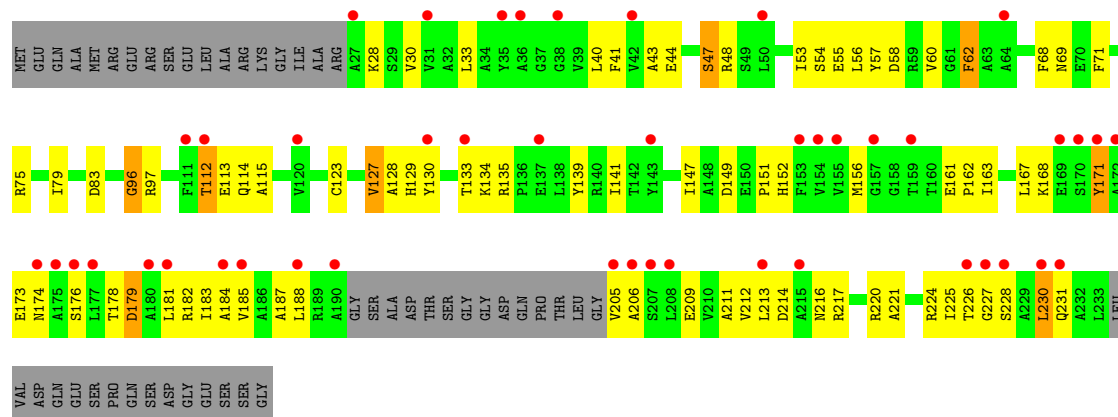
- Molecule 1: Proteasome (Alpha subunit) PrcA



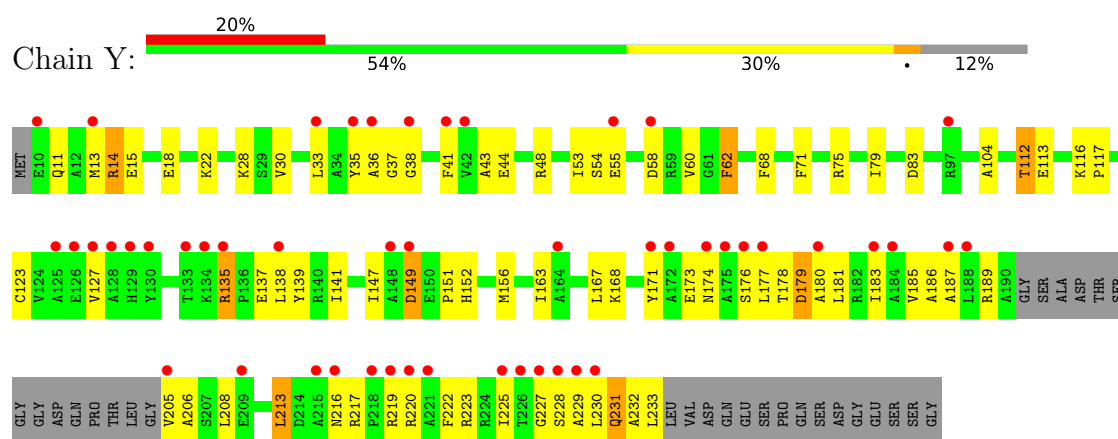
- Molecule 1: Proteasome (Alpha subunit) PrcA



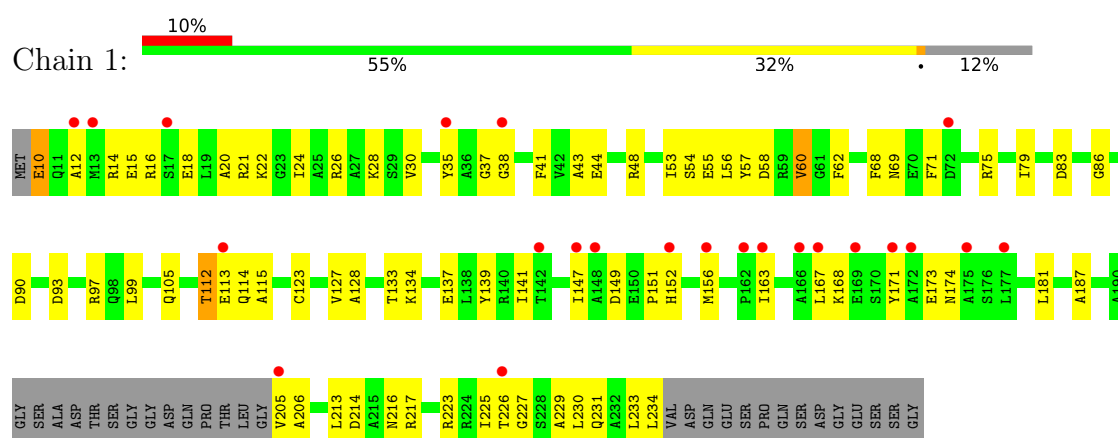
- Molecule 1: Proteasome (Alpha subunit) PrcA



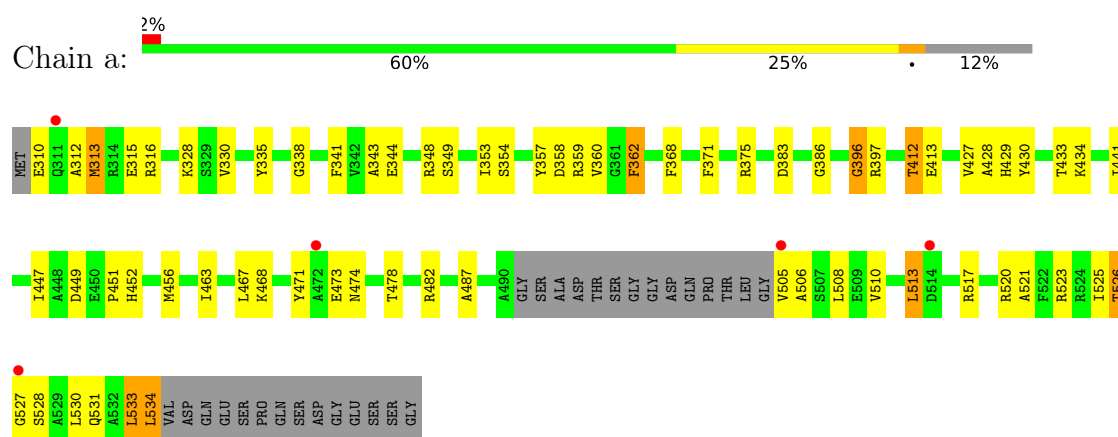
- Molecule 1: Proteasome (Alpha subunit) PrcA



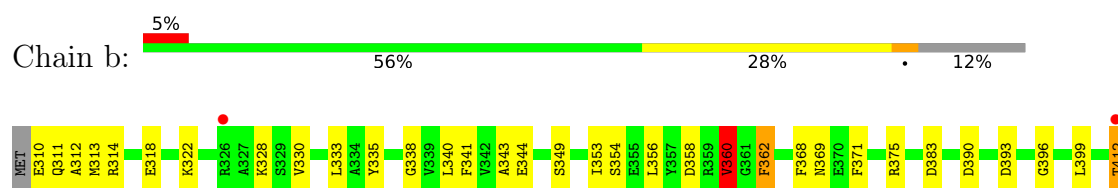
• Molecule 1: Proteasome (Alpha subunit) PrcA



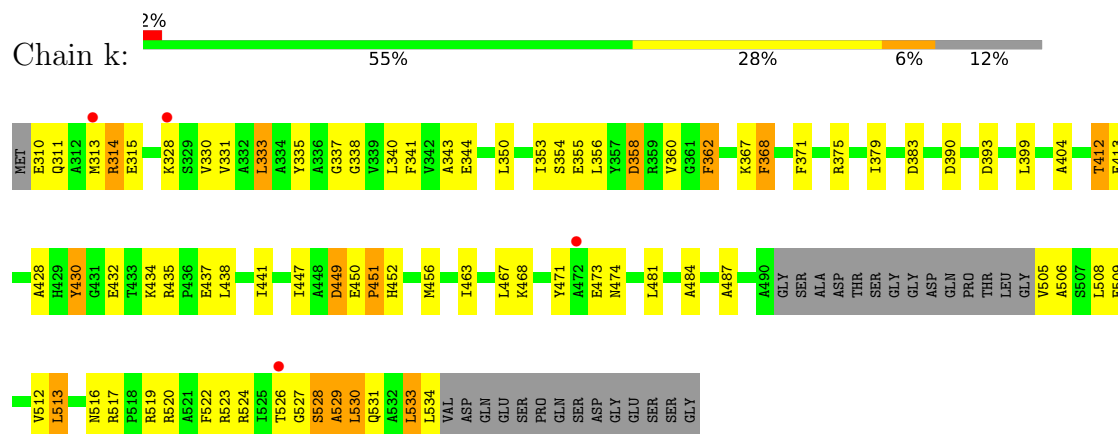
• Molecule 1: Proteasome (Alpha subunit) PrcA



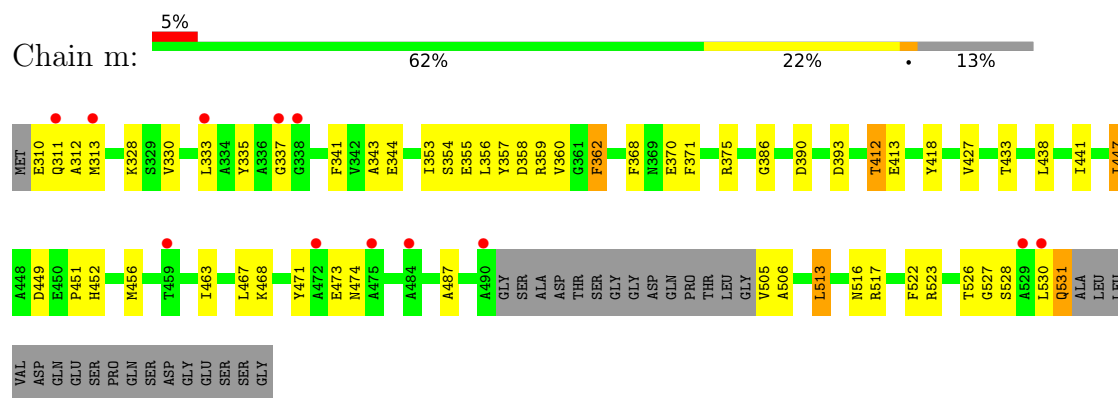
• Molecule 1: Proteasome (Alpha subunit) PrcA



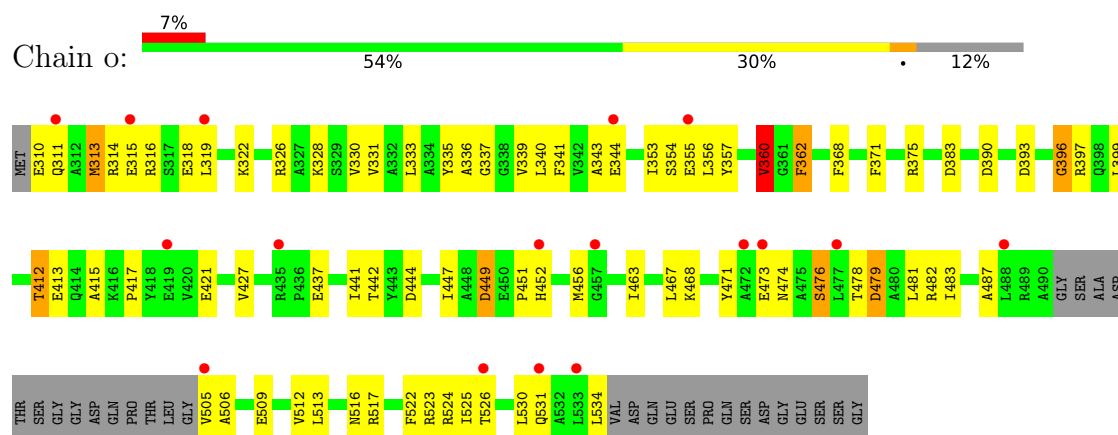
- Molecule 1: Proteasome (Alpha subunit) PrcA



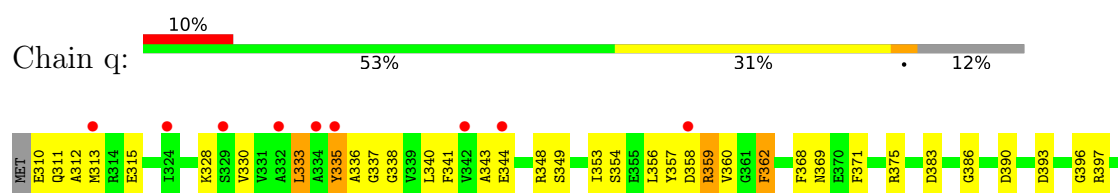
- Molecule 1: Proteasome (Alpha subunit) PrcA

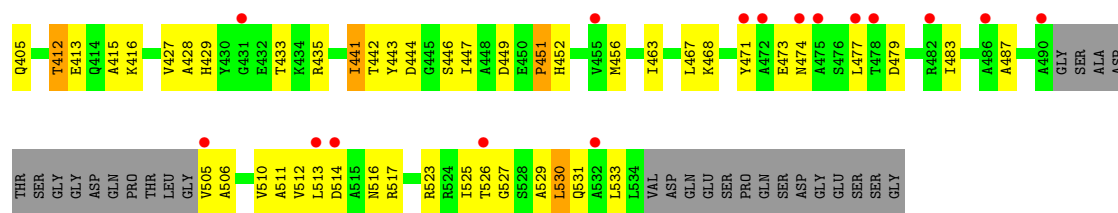


- Molecule 1: Proteasome (Alpha subunit) PrcA

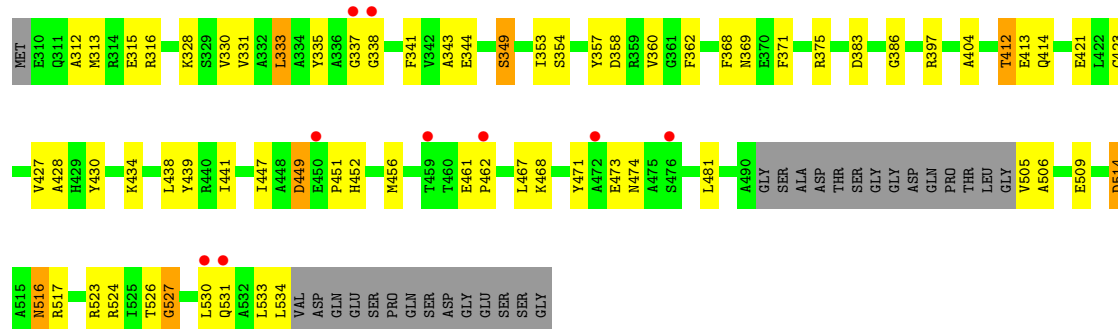


- Molecule 1: Proteasome (Alpha subunit) PrcA

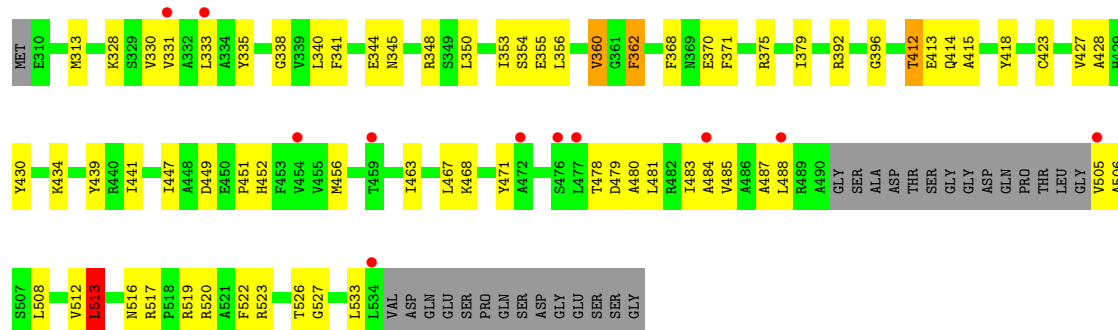




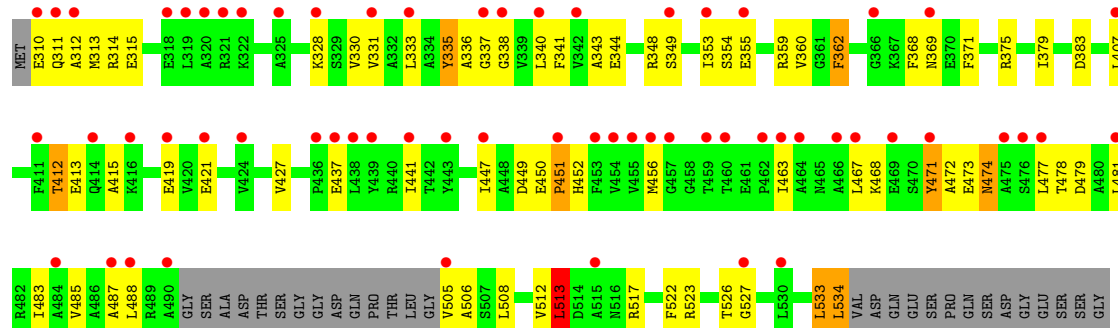
- Molecule 1: Proteasome (Alpha subunit) PrcA



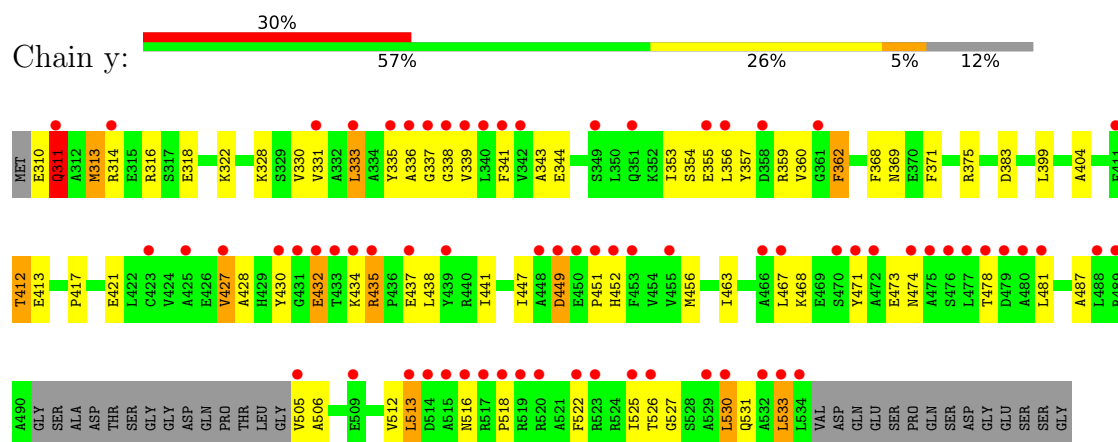
- Molecule 1: Proteasome (Alpha subunit) PrcA



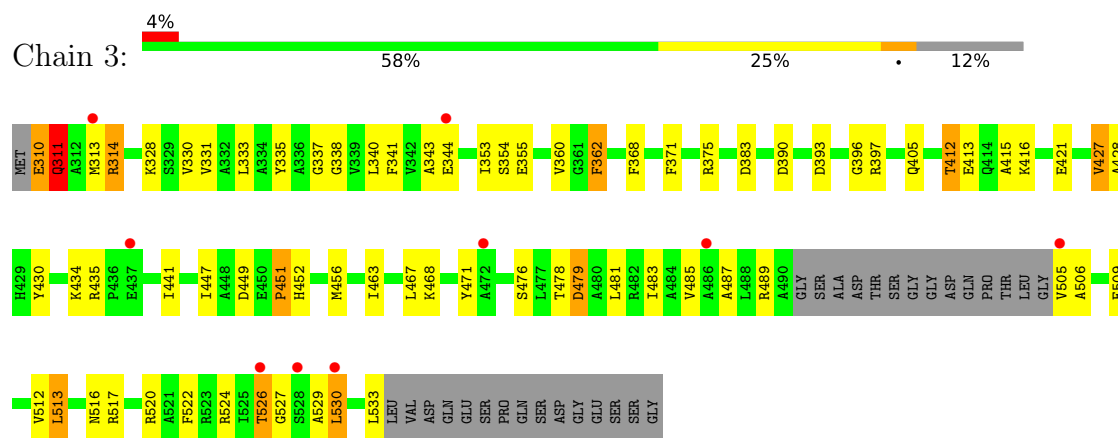
- Molecule 1: Proteasome (Alpha subunit) PrcA



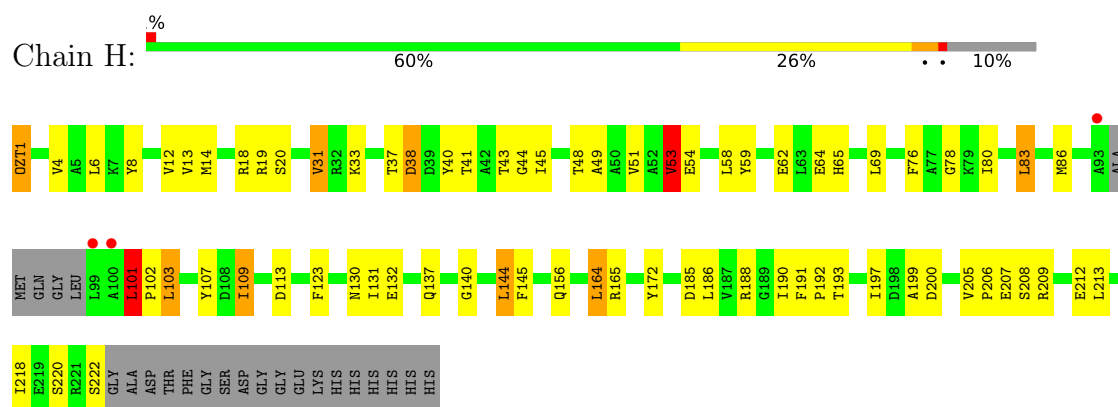
- Molecule 1: Proteasome (Alpha subunit) PrcA



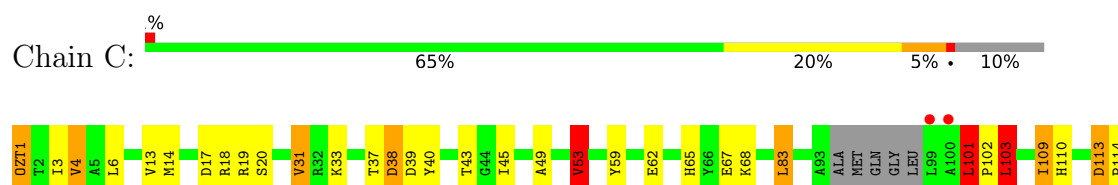
- Molecule 1: Proteasome (Alpha subunit) PrcA

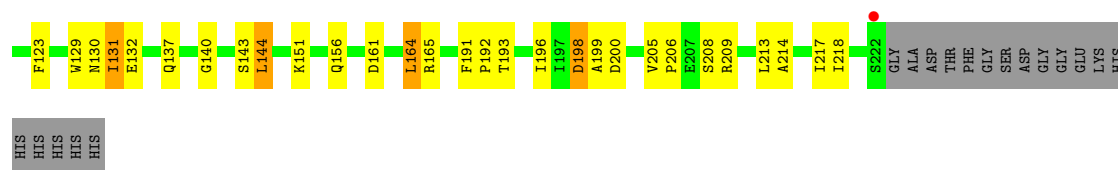


- Molecule 2: Proteasome (Beta subunit) PrcB

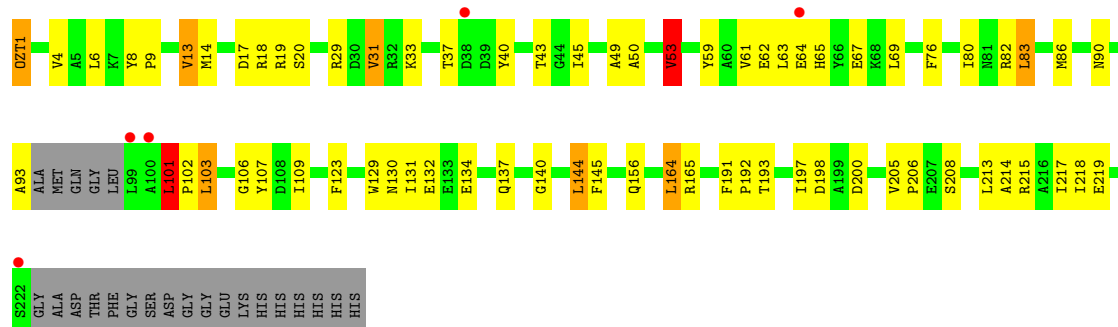


- Molecule 2: Proteasome (Beta subunit) PrcB

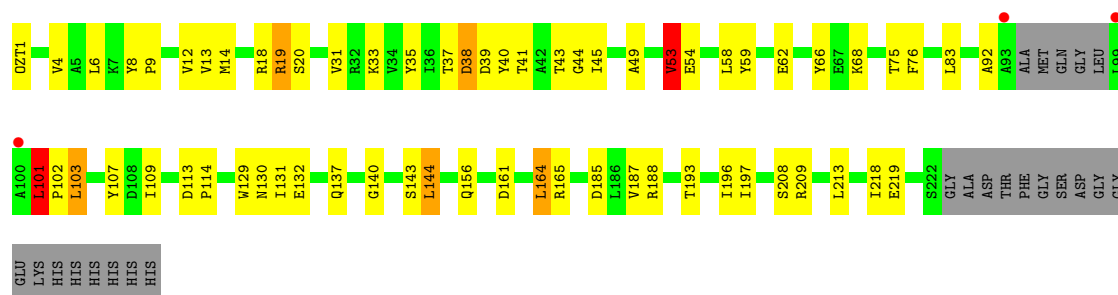




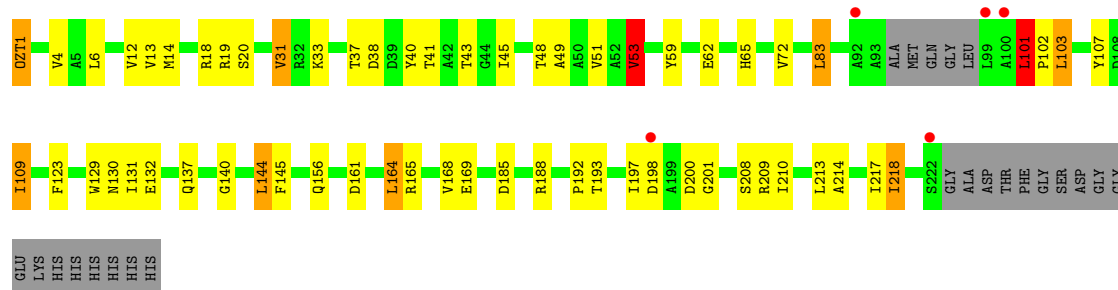
• Molecule 2: Proteasome (Beta subunit) PrcB



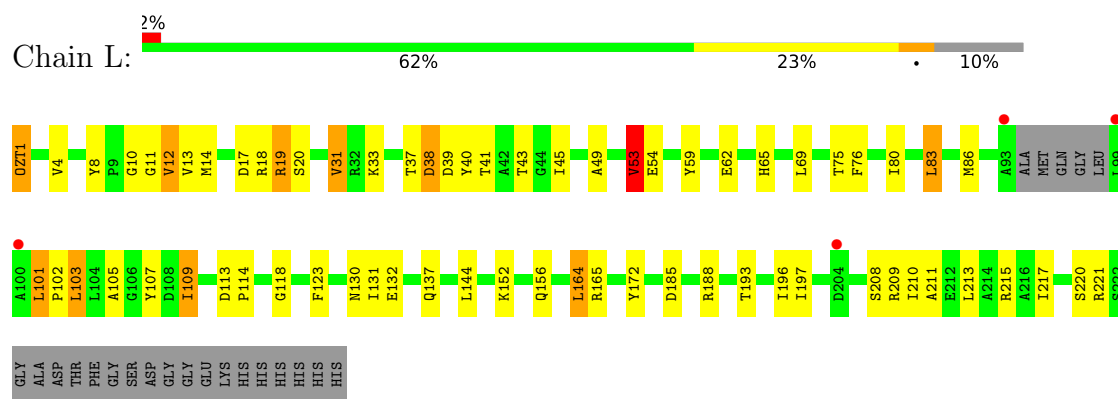
• Molecule 2: Proteasome (Beta subunit) PrcB



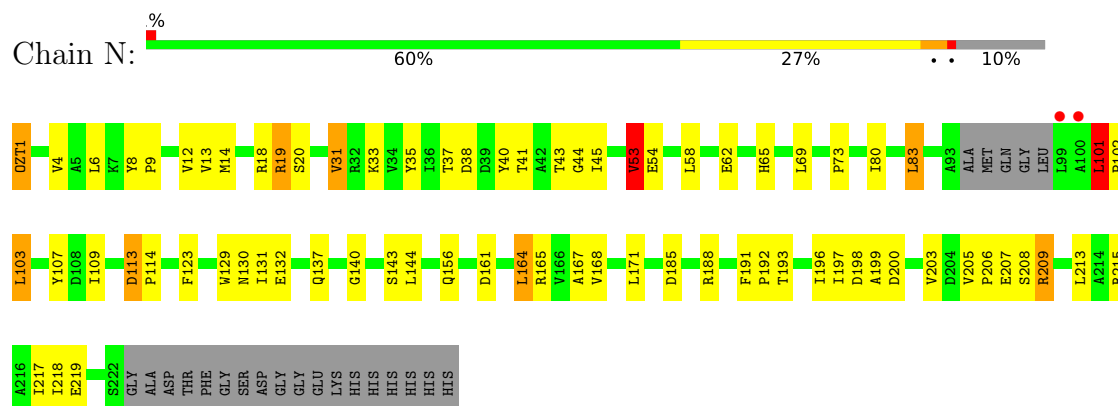
• Molecule 2: Proteasome (Beta subunit) PrcB



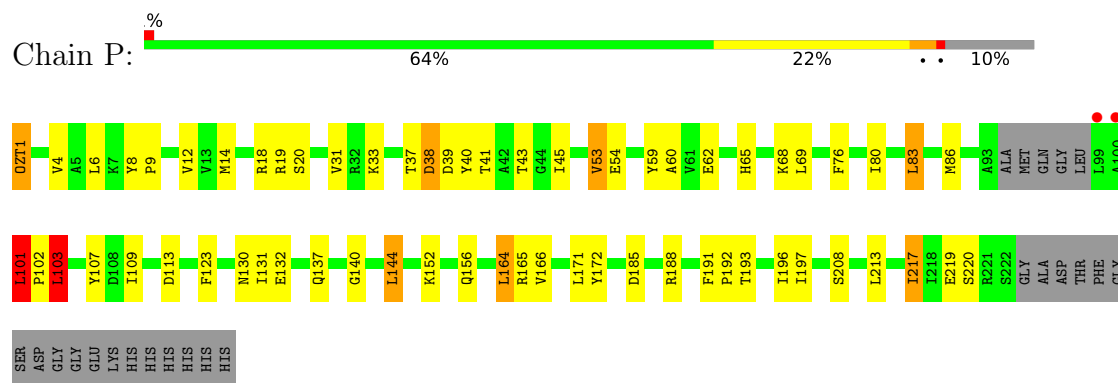
• Molecule 2: Proteasome (Beta subunit) PrcB



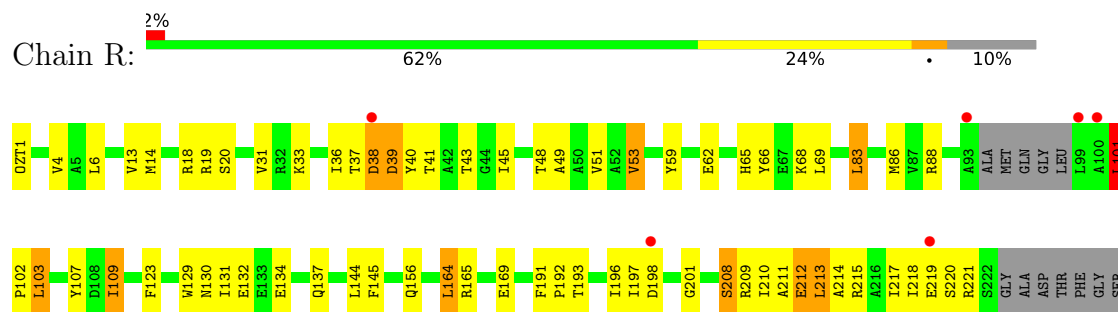
- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB



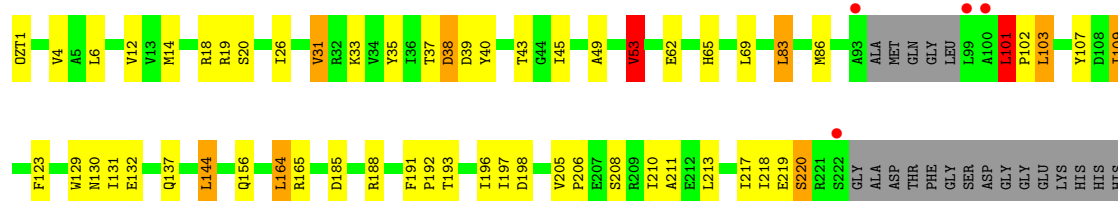
- Molecule 2: Proteasome (Beta subunit) PrcB



ASP
GLY
GLY
GLY
LYS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

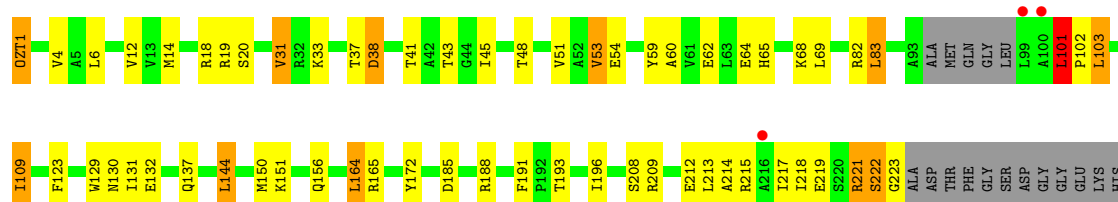
Chain T: 



HIS
HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

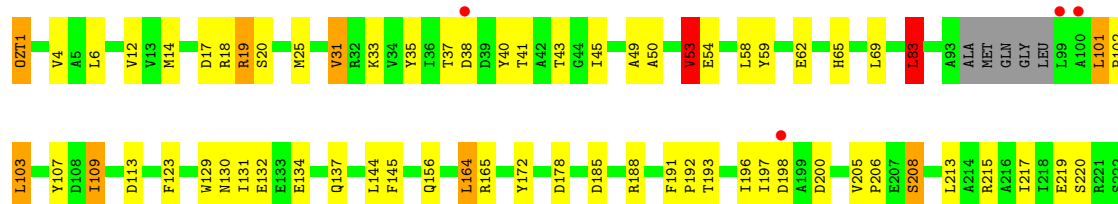
Chain V: 



HIS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

Chain X: 



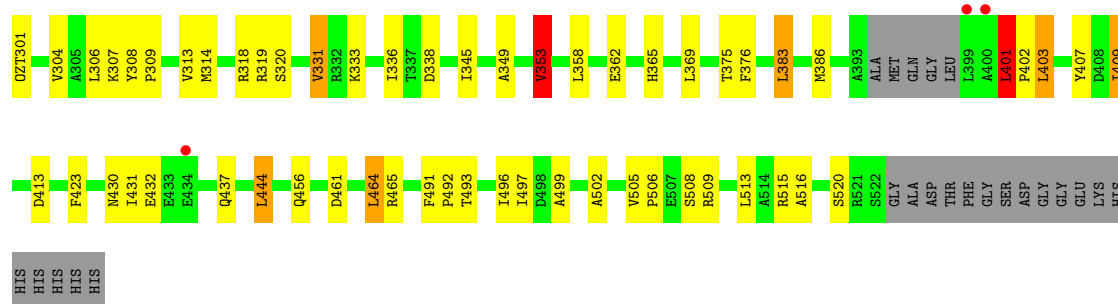
GLY
ALA
ASP
THR
PHE
GLY
SER
ASP
GLY
GLY
GLU
LYS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

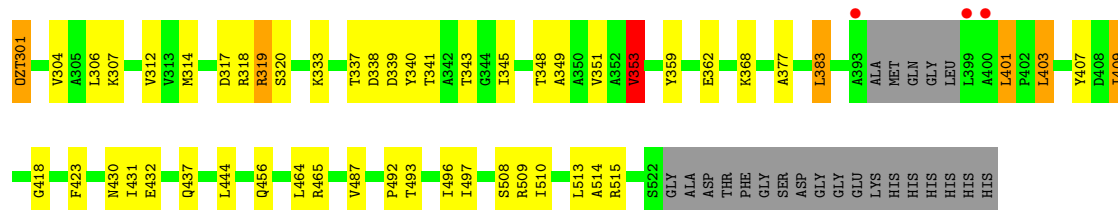
Chain Z: 



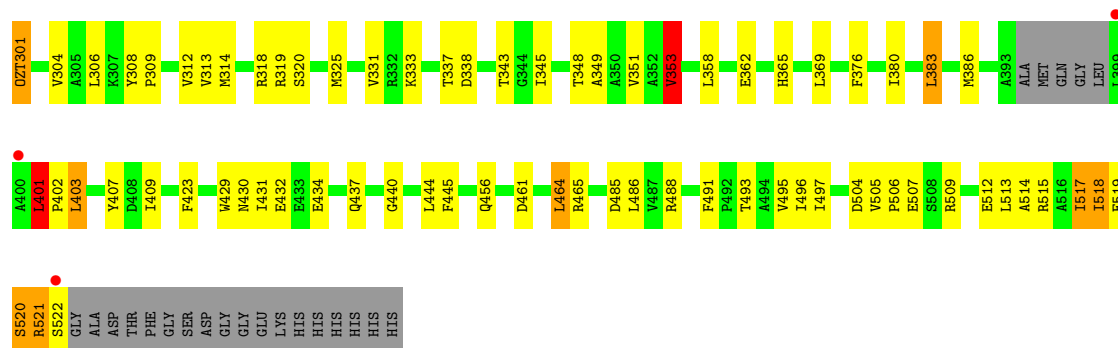




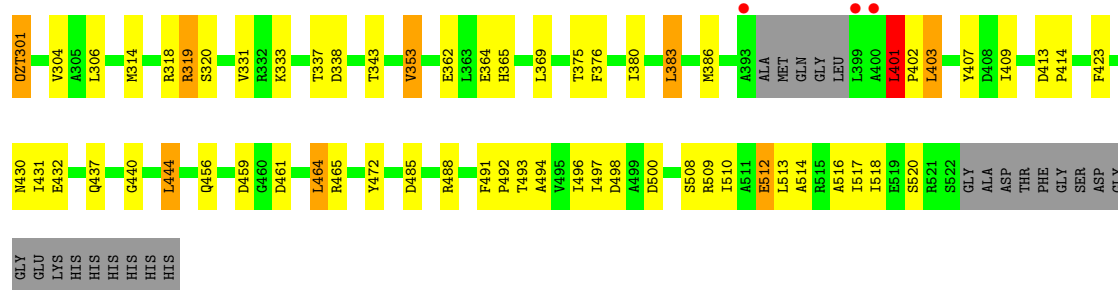
• Molecule 2: Proteasome (Beta subunit) PrcB



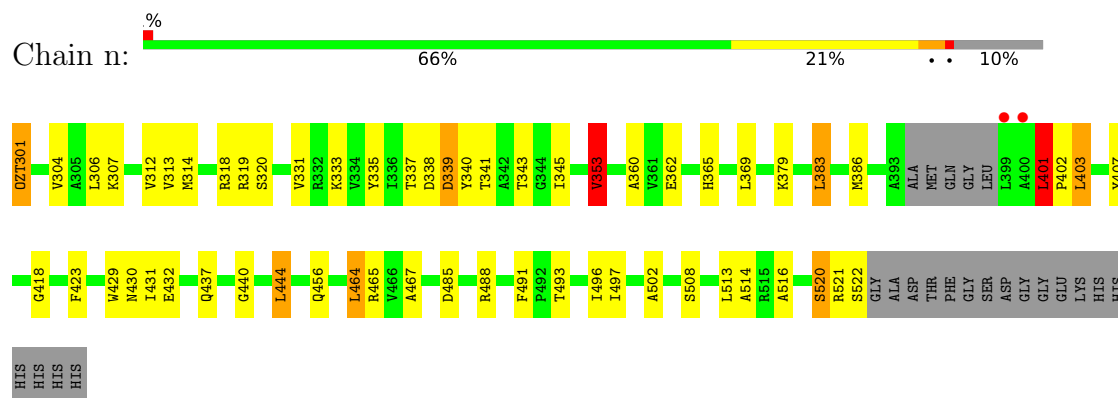
• Molecule 2: Proteasome (Beta subunit) PrcB



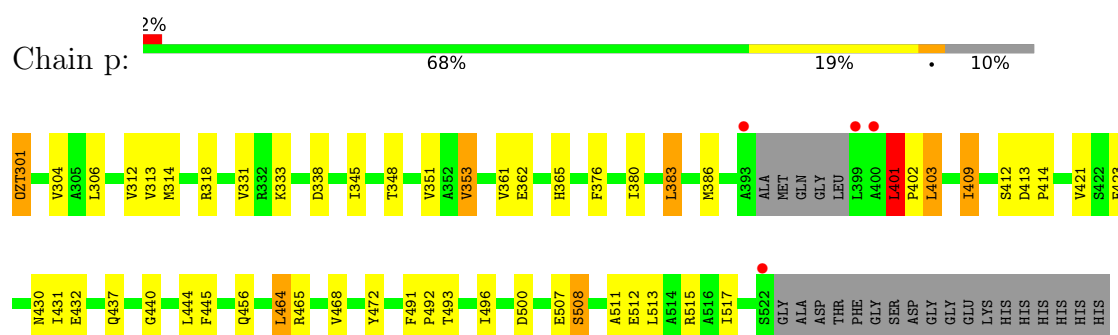
• Molecule 2: Proteasome (Beta subunit) PrcB



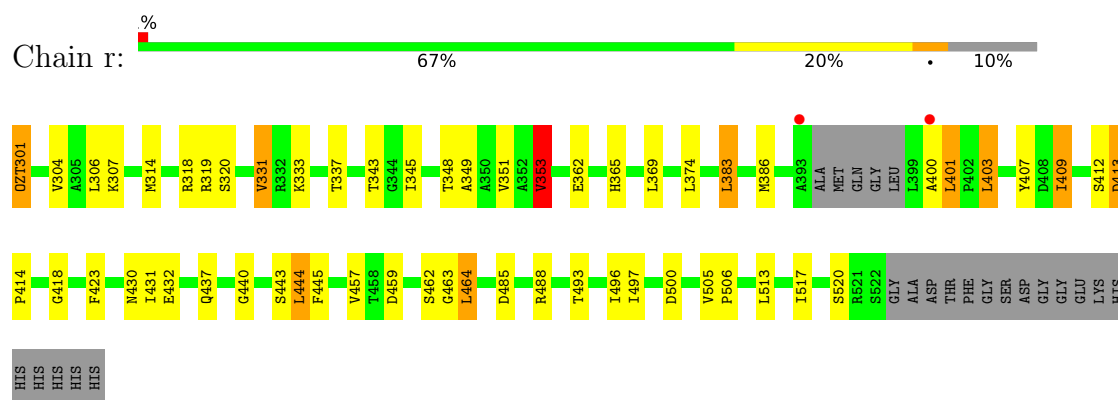
• Molecule 2: Proteasome (Beta subunit) PrcB



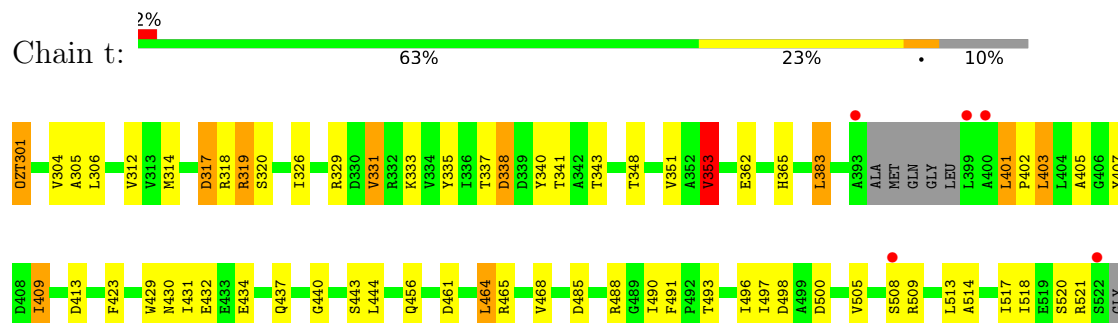
• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB

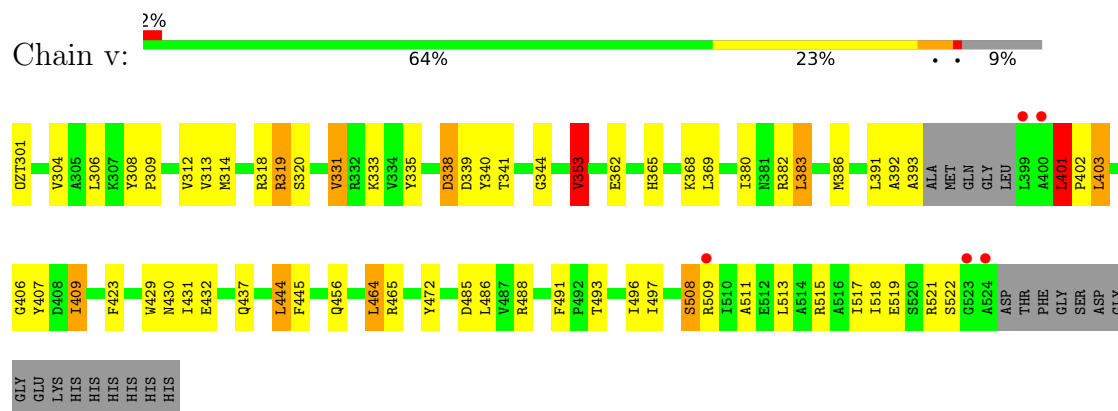


• Molecule 2: Proteasome (Beta subunit) PrcB

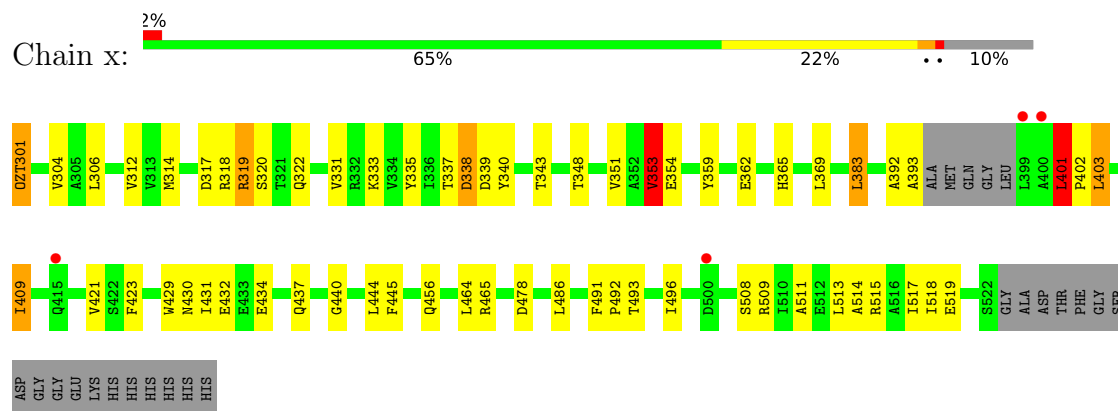


ALA
ASP
THR
PHE
GLY
SER
ASP
GLY
GLY
LYS
LYS
HIS
HIS
HIS
HIS
HIS

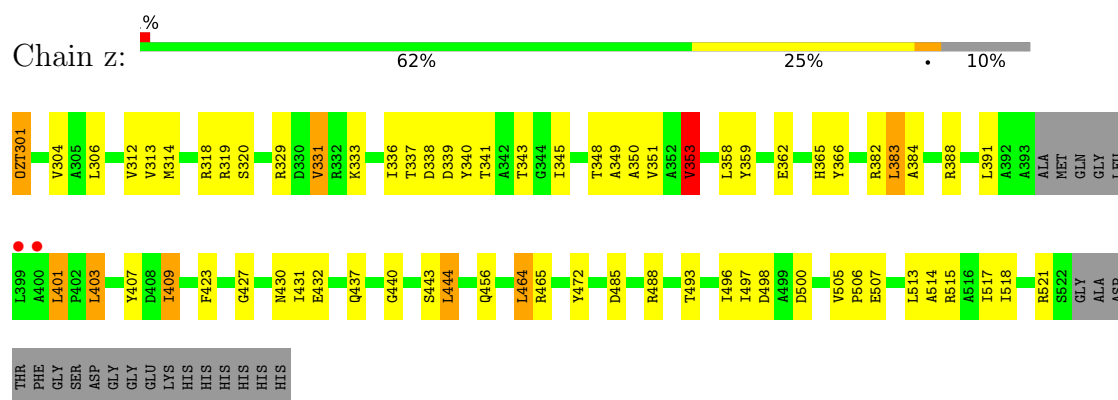
• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB

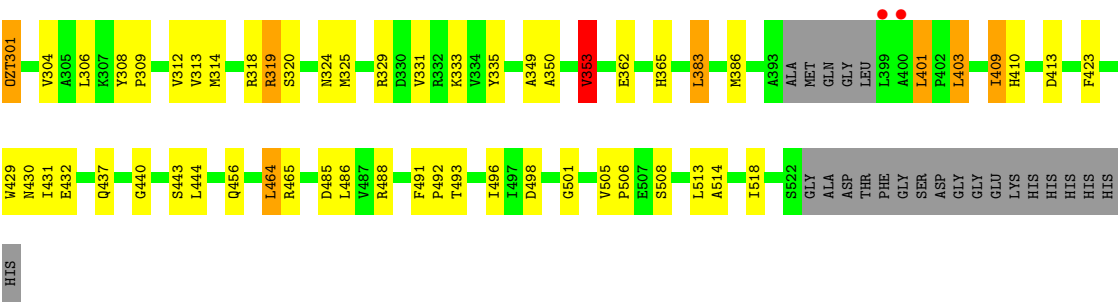


• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB





HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.58Å 209.62Å 284.93Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	25.12 – 2.88 25.12 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.6 (25.12-2.88) 88.5 (25.12-2.88)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.217 , 0.267 0.231 , 0.271	Depositor DCC
R_{free} test set	13598 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	90443	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2193e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OZT

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	1	0.66	0/1657	0.94	3/2238 (0.1%)
1	3	0.66	0/1649	0.95	7/2227 (0.3%)
1	A	0.73	1/1657 (0.1%)	1.04	9/2238 (0.4%)
1	B	0.79	1/1657 (0.1%)	1.07	5/2238 (0.2%)
1	D	0.56	0/1649	0.97	5/2227 (0.2%)
1	F	0.73	0/1514	1.02	3/2050 (0.1%)
1	I	0.65	0/1664	1.00	6/2248 (0.3%)
1	K	0.63	0/1657	1.03	10/2238 (0.4%)
1	M	0.60	0/1613	0.98	7/2178 (0.3%)
1	O	0.68	0/1657	0.96	4/2238 (0.2%)
1	Q	0.56	0/1657	0.94	5/2238 (0.2%)
1	S	0.67	0/1657	0.96	8/2238 (0.4%)
1	U	0.63	0/1657	0.94	3/2238 (0.1%)
1	W	0.54	0/1511	0.96	7/2046 (0.3%)
1	Y	0.62	0/1649	0.97	5/2227 (0.2%)
1	a	0.72	0/1657	0.93	3/2238 (0.1%)
1	b	0.73	0/1657	0.99	6/2238 (0.3%)
1	d	0.58	0/1657	0.93	3/2238 (0.1%)
1	f	0.60	0/1657	0.86	2/2238 (0.1%)
1	i	0.69	0/1657	0.97	2/2238 (0.1%)
1	k	0.64	0/1657	0.99	7/2238 (0.3%)
1	m	0.60	0/1636	0.93	3/2209 (0.1%)
1	o	0.63	0/1657	0.93	4/2238 (0.2%)
1	q	0.59	0/1657	0.93	4/2238 (0.2%)
1	s	0.67	0/1657	0.94	2/2238 (0.1%)
1	u	0.62	0/1657	0.95	3/2238 (0.1%)
1	w	0.57	0/1657	0.93	3/2238 (0.1%)
1	y	0.58	0/1657	0.96	4/2238 (0.2%)
2	2	0.86	0/1620	1.01	4/2196 (0.2%)
2	4	0.85	0/1620	0.99	5/2196 (0.2%)
2	C	0.74	0/1620	0.97	7/2196 (0.3%)
2	E	0.72	0/1620	0.97	4/2196 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	G	0.87	0/1620	0.99	5/2196 (0.2%)
2	H	0.83	1/1620 (0.1%)	1.02	8/2196 (0.4%)
2	J	0.73	1/1620 (0.1%)	0.94	5/2196 (0.2%)
2	L	0.83	0/1620	0.96	5/2196 (0.2%)
2	N	0.93	2/1620 (0.1%)	1.07	8/2196 (0.4%)
2	P	0.99	2/1620 (0.1%)	1.06	9/2196 (0.4%)
2	R	0.70	0/1620	0.95	4/2196 (0.2%)
2	T	0.82	0/1620	1.01	4/2196 (0.2%)
2	V	0.92	1/1624 (0.1%)	1.03	4/2201 (0.2%)
2	X	0.86	0/1620	1.01	7/2196 (0.3%)
2	Z	0.75	0/1620	0.99	7/2196 (0.3%)
2	c	0.77	0/1610	0.99	6/2182 (0.3%)
2	e	0.79	0/1620	1.03	7/2196 (0.3%)
2	g	0.87	1/1620 (0.1%)	0.98	3/2196 (0.1%)
2	h	0.87	0/1602	1.03	7/2171 (0.3%)
2	j	0.76	0/1620	0.96	5/2196 (0.2%)
2	l	0.86	0/1620	1.03	5/2196 (0.2%)
2	n	0.89	2/1620 (0.1%)	1.02	3/2196 (0.1%)
2	p	0.94	1/1620 (0.1%)	1.00	4/2196 (0.2%)
2	r	0.75	0/1620	0.98	6/2196 (0.3%)
2	t	0.79	0/1620	0.94	5/2196 (0.2%)
2	v	0.90	1/1629 (0.1%)	1.04	6/2208 (0.3%)
2	x	0.81	1/1620 (0.1%)	0.99	5/2196 (0.2%)
2	z	0.68	0/1620	0.95	5/2196 (0.2%)
All	All	0.74	15/91370 (0.0%)	0.98	286/123638 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	LYS	C-N	-7.40	1.24	1.33
2	V	60	ALA	CA-CB	-6.23	1.43	1.53
2	p	361	VAL	CA-CB	-6.11	1.46	1.54
2	H	190	ILE	CA-CB	-5.89	1.47	1.54
2	g	377	ALA	CA-CB	-5.74	1.44	1.53
2	N	80	ILE	CA-CB	-5.71	1.47	1.54
2	P	60	ALA	CA-CB	-5.70	1.44	1.53
2	N	167	ALA	CA-CB	-5.62	1.44	1.53
1	B	31	VAL	CA-CB	-5.60	1.47	1.54
2	J	72	VAL	CA-CB	-5.39	1.49	1.55
2	P	166	VAL	CA-CB	-5.22	1.48	1.54
2	x	421	VAL	CA-CB	-5.20	1.48	1.54
2	n	467	ALA	CA-CB	-5.19	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	v	380	ILE	CA-CB	-5.05	1.48	1.54
2	n	360	ALA	CA-CB	-5.02	1.45	1.53

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	GLN	N-CA-C	-12.39	97.26	112.38
2	J	218	ILE	N-CA-C	10.06	120.07	110.42
1	K	226	THR	N-CA-C	10.00	122.18	111.28
1	I	228	SER	N-CA-C	-9.67	100.72	111.07
1	k	528	SER	N-CA-C	-9.59	101.36	112.87
1	B	13	MET	N-CA-C	-8.74	101.75	111.28
1	W	206	ALA	N-CA-C	-8.33	102.13	112.88
2	h	353	VAL	CB-CA-C	-8.21	101.28	111.87
1	d	506	ALA	N-CA-C	-8.21	101.37	112.94
1	a	506	ALA	N-CA-C	-8.20	102.30	112.88
1	3	311	GLN	N-CA-C	-8.15	103.80	112.93
1	k	506	ALA	N-CA-C	-8.10	102.43	112.88
1	y	506	ALA	N-CA-C	-8.08	102.45	112.88
1	Y	206	ALA	N-CA-C	-8.00	102.56	112.88
1	y	526	THR	N-CA-C	7.93	119.93	111.28
1	3	506	ALA	N-CA-C	-7.93	102.65	112.88
1	m	506	ALA	N-CA-C	-7.91	102.68	112.88
2	V	101	LEU	CA-C-N	7.89	128.04	120.31
2	V	101	LEU	C-N-CA	7.89	128.04	120.31
1	b	506	ALA	N-CA-C	-7.87	102.73	112.88
1	Y	231	GLN	N-CA-C	-7.85	102.72	111.28
1	w	506	ALA	N-CA-C	-7.82	102.79	112.88
1	I	206	ALA	N-CA-C	-7.79	102.83	112.88
1	O	206	ALA	N-CA-C	-7.76	102.86	112.88
1	Q	11	GLN	N-CA-C	-7.70	101.89	111.75
1	I	226	THR	N-CA-C	7.70	119.75	111.36
1	S	229	ALA	N-CA-C	-7.68	102.92	111.82
1	o	506	ALA	N-CA-C	-7.66	102.99	112.88
2	v	392	ALA	N-CA-C	-7.60	104.42	112.93
2	N	218	ILE	CB-CA-C	-7.50	102.37	111.97
2	V	53	VAL	CB-CA-C	-7.48	102.22	111.87
1	W	227	GLY	N-CA-C	7.48	122.15	112.13
1	W	226	THR	N-CA-C	7.43	119.46	111.36
2	H	101	LEU	CA-C-N	7.43	127.59	120.31
2	H	101	LEU	C-N-CA	7.43	127.59	120.31
1	1	206	ALA	N-CA-C	-7.36	102.56	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	506	ALA	N-CA-C	-7.35	103.40	112.88
1	i	506	ALA	N-CA-C	-7.35	103.46	113.30
1	s	506	ALA	N-CA-C	-7.31	103.45	112.88
2	T	101	LEU	CA-C-N	7.27	127.22	120.03
2	T	101	LEU	C-N-CA	7.27	127.22	120.03
1	q	506	ALA	N-CA-C	-7.26	103.52	112.88
2	C	53	VAL	CB-CA-C	-7.14	102.65	111.87
1	F	218	PRO	N-CA-C	7.14	123.68	113.47
1	U	206	ALA	N-CA-C	-7.13	103.69	112.88
1	D	206	ALA	N-CA-C	-7.11	102.42	113.02
1	u	513	LEU	N-CA-C	-7.09	96.96	108.52
2	T	53	VAL	CB-CA-C	-7.09	102.73	111.87
1	u	506	ALA	N-CA-C	-7.08	103.75	112.88
1	K	171	TYR	N-CA-C	7.06	120.23	108.73
1	F	206	ALA	N-CA-C	-7.03	102.54	113.02
1	D	226	THR	N-CA-C	7.01	122.00	112.68
2	r	401	LEU	CA-C-N	6.94	126.90	120.03
2	r	401	LEU	C-N-CA	6.94	126.90	120.03
2	h	401	LEU	CA-C-N	6.93	126.89	120.03
2	h	401	LEU	C-N-CA	6.93	126.89	120.03
2	c	413	ASP	CA-C-N	6.93	126.56	119.56
2	c	413	ASP	C-N-CA	6.93	126.56	119.56
1	S	206	ALA	N-CA-C	-6.90	103.98	112.88
2	z	353	VAL	CB-CA-C	-6.90	102.98	112.02
2	E	101	LEU	CA-C-N	6.87	126.83	120.03
2	E	101	LEU	C-N-CA	6.87	126.83	120.03
1	M	206	ALA	N-CA-C	-6.85	104.05	112.88
2	L	53	VAL	CB-CA-C	-6.83	103.06	111.87
2	X	53	VAL	CB-CA-C	-6.81	103.08	111.87
1	y	432	GLU	N-CA-C	6.79	120.51	110.46
1	Q	206	ALA	N-CA-C	-6.79	104.12	112.88
2	z	401	LEU	CA-C-N	6.78	126.96	120.31
2	z	401	LEU	C-N-CA	6.78	126.96	120.31
1	A	206	ALA	N-CA-C	-6.75	102.97	113.02
2	c	331	VAL	N-CA-C	6.73	118.01	108.93
2	P	101	LEU	CA-C-N	6.71	126.89	120.31
2	P	101	LEU	C-N-CA	6.71	126.89	120.31
2	r	331	VAL	N-CA-C	6.71	117.99	108.93
2	t	353	VAL	CB-CA-C	-6.69	103.26	112.02
2	J	101	LEU	CA-C-N	6.68	126.86	120.31
2	J	101	LEU	C-N-CA	6.68	126.86	120.31
2	p	353	VAL	CB-CA-C	-6.67	103.27	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	206	ALA	N-CA-C	-6.63	104.33	112.88
2	n	401	LEU	CA-C-N	6.61	126.79	120.31
2	n	401	LEU	C-N-CA	6.61	126.79	120.31
1	b	527	GLY	N-CA-C	6.60	120.65	112.73
1	s	527	GLY	N-CA-C	6.59	120.15	112.50
2	c	353	VAL	CB-CA-C	-6.56	103.41	111.87
1	k	368	PHE	N-CA-C	6.54	118.41	111.28
2	e	331	VAL	N-CA-C	6.53	117.75	108.93
1	B	206	ALA	N-CA-C	-6.52	103.31	113.02
2	4	353	VAL	CB-CA-C	-6.52	103.46	111.87
2	G	31	VAL	N-CA-C	6.51	117.72	108.93
2	Z	53	VAL	CB-CA-C	-6.50	103.49	111.87
1	M	132	GLU	N-CA-C	6.50	119.32	110.55
2	p	472	TYR	N-CA-C	-6.48	104.30	111.36
1	3	513	LEU	N-CA-C	-6.45	98.21	108.73
2	E	53	VAL	CB-CA-C	-6.44	103.58	112.02
1	K	49	SER	N-CA-C	6.44	118.38	111.36
2	e	353	VAL	CB-CA-C	-6.43	103.62	112.04
1	b	360	VAL	N-CA-C	6.39	117.06	108.11
2	x	401	LEU	CA-C-N	6.37	126.55	120.31
2	x	401	LEU	C-N-CA	6.37	126.55	120.31
2	v	353	VAL	CB-CA-C	-6.36	103.54	111.94
2	G	53	VAL	CB-CA-C	-6.35	103.68	111.87
2	h	472	TYR	N-CA-C	-6.34	104.45	111.36
2	H	113	ASP	CA-C-N	6.34	125.96	119.56
2	H	113	ASP	C-N-CA	6.34	125.96	119.56
2	r	353	VAL	CB-CA-C	-6.34	103.74	112.04
2	j	521	ARG	N-CA-C	-6.32	103.91	113.89
2	x	353	VAL	CB-CA-C	-6.32	103.72	111.87
2	v	401	LEU	CA-C-N	6.31	126.49	120.31
2	v	401	LEU	C-N-CA	6.31	126.49	120.31
2	N	101	LEU	CA-C-N	6.30	126.48	120.31
2	N	101	LEU	C-N-CA	6.30	126.48	120.31
2	R	219	GLU	N-CA-C	-6.29	105.37	114.12
2	l	353	VAL	CB-CA-C	-6.29	103.75	111.87
2	j	401	LEU	CA-C-N	6.29	126.47	120.31
2	j	401	LEU	C-N-CA	6.29	126.47	120.31
2	z	507	GLU	N-CA-C	6.25	118.10	111.28
2	2	53	VAL	CB-CA-C	-6.23	103.83	111.87
2	Z	213	LEU	N-CA-C	6.21	118.56	111.11
1	k	530	LEU	N-CA-C	-6.21	104.52	111.28
2	p	401	LEU	CA-C-N	6.20	126.38	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	p	401	LEU	C-N-CA	6.20	126.38	120.31
1	W	171	TYR	N-CA-C	6.19	119.04	109.07
2	J	53	VAL	CB-CA-C	-6.18	103.94	112.04
1	u	396	GLY	N-CA-C	-6.16	105.36	112.50
1	y	311	GLN	N-CA-C	-6.16	104.57	111.28
2	l	401	LEU	CA-C-N	6.15	126.12	120.03
2	l	401	LEU	C-N-CA	6.15	126.12	120.03
1	i	513	LEU	N-CA-C	-6.14	99.89	108.54
2	e	515	ARG	N-CA-C	-6.13	105.94	113.41
1	S	226	THR	N-CA-C	6.11	117.94	111.28
2	R	220	SER	N-CA-C	-6.10	104.32	110.97
2	2	101	LEU	CA-C-N	6.10	126.29	120.31
2	2	101	LEU	C-N-CA	6.10	126.29	120.31
2	P	217	ILE	CB-CA-C	-6.09	104.06	112.04
2	c	372	VAL	CA-C-N	6.08	126.05	120.03
2	c	372	VAL	C-N-CA	6.08	126.05	120.03
1	U	11	GLN	N-CA-C	-6.08	106.03	113.50
2	g	401	LEU	CA-C-N	6.08	126.04	120.03
2	g	401	LEU	C-N-CA	6.08	126.04	120.03
1	Q	145	GLY	N-CA-C	-6.06	106.88	115.43
2	z	331	VAL	N-CA-C	6.06	117.11	108.93
1	3	416	LYS	CA-C-N	6.05	125.96	119.85
1	3	416	LYS	C-N-CA	6.05	125.96	119.85
1	A	213	LEU	N-CA-C	-6.03	97.88	108.20
1	O	132	GLU	N-CA-C	6.01	118.66	110.55
2	t	331	VAL	N-CA-C	5.99	117.07	107.73
2	H	208	SER	N-CA-C	5.99	118.57	111.33
2	r	413	ASP	CA-C-N	5.98	125.60	119.56
2	r	413	ASP	C-N-CA	5.98	125.60	119.56
1	K	213	LEU	N-CA-C	-5.97	97.99	108.20
1	w	471	TYR	N-CA-C	5.97	118.68	109.07
2	v	508	SER	N-CA-C	5.97	117.45	111.07
2	L	172	TYR	N-CA-C	-5.95	104.71	111.14
1	m	528	SER	N-CA-C	5.94	118.27	111.02
1	Y	213	LEU	N-CA-C	-5.94	97.04	107.73
2	4	401	LEU	CA-C-N	5.94	126.13	120.31
2	4	401	LEU	C-N-CA	5.94	126.13	120.31
2	l	472	TYR	N-CA-C	-5.92	104.75	111.14
2	N	53	VAL	CB-CA-C	-5.89	104.28	111.87
1	S	216	ASN	N-CA-C	5.88	117.69	111.28
1	M	147	ILE	N-CA-C	5.86	116.37	108.17
1	m	513	LEU	N-CA-C	-5.86	98.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	53	VAL	CB-CA-C	-5.84	104.36	112.02
2	j	353	VAL	CB-CA-C	-5.83	104.25	111.94
1	O	213	LEU	N-CA-C	-5.80	96.95	107.75
1	1	55	GLU	N-CA-C	-5.80	101.10	110.32
1	d	521	ALA	N-CA-C	5.79	117.67	111.36
1	M	143	TYR	N-CA-C	5.79	119.16	111.75
1	I	231	GLN	N-CA-C	-5.73	105.04	111.28
2	H	31	VAL	N-CA-C	5.72	116.66	108.93
2	G	101	LEU	CA-C-N	5.71	125.69	120.03
2	G	101	LEU	C-N-CA	5.71	125.69	120.03
2	h	331	VAL	N-CA-C	5.71	116.64	108.93
1	M	213	LEU	N-CA-C	-5.70	99.09	108.49
1	Y	225	ILE	N-CA-C	-5.69	99.55	107.80
2	C	31	VAL	N-CA-C	5.67	116.59	108.93
2	L	31	VAL	N-CA-C	5.66	116.57	108.93
2	g	353	VAL	CB-CA-C	-5.65	104.48	111.94
1	W	221	ALA	N-CA-C	5.65	117.52	111.36
2	j	518	ILE	CB-CA-C	-5.62	103.45	112.16
2	e	413	ASP	CA-C-N	5.61	125.22	119.56
2	e	413	ASP	C-N-CA	5.61	125.22	119.56
1	K	228	SER	N-CA-C	-5.57	105.20	111.28
2	N	31	VAL	N-CA-C	5.57	116.45	108.93
2	E	31	VAL	N-CA-C	5.57	116.45	108.93
2	P	113	ASP	CA-C-N	5.56	125.18	119.56
2	P	113	ASP	C-N-CA	5.56	125.18	119.56
1	a	513	LEU	N-CA-C	-5.56	98.69	108.20
1	k	432	GLU	N-CA-C	5.56	118.06	110.55
2	R	101	LEU	CA-C-N	5.56	125.76	120.31
2	R	101	LEU	C-N-CA	5.56	125.76	120.31
1	A	11	GLN	N-CA-C	-5.55	105.63	112.90
1	I	60	VAL	N-CA-C	5.55	116.11	108.12
1	A	161	GLU	CA-C-N	5.54	125.06	119.19
1	A	161	GLU	C-N-CA	5.54	125.06	119.19
1	B	58	ASP	N-CA-C	5.54	116.99	111.07
2	X	31	VAL	N-CA-C	5.54	116.40	108.93
1	3	396	GLY	N-CA-C	-5.53	106.09	112.50
2	C	113	ASP	CA-C-N	5.53	125.14	119.56
2	C	113	ASP	C-N-CA	5.53	125.14	119.56
2	e	401	LEU	CA-C-N	5.53	125.73	120.31
2	e	401	LEU	C-N-CA	5.53	125.73	120.31
2	N	113	ASP	CA-C-N	5.52	125.14	119.56
2	N	113	ASP	C-N-CA	5.52	125.14	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	101	LEU	CA-C-N	5.51	125.71	120.31
2	Z	101	LEU	C-N-CA	5.51	125.71	120.31
2	Z	31	VAL	N-CA-C	5.51	116.36	108.93
1	M	130	TYR	N-CA-C	5.50	116.96	111.07
1	S	96	GLY	N-CA-C	-5.50	106.13	112.50
1	A	102	VAL	CB-CA-C	-5.48	104.74	112.14
2	L	113	ASP	CA-C-N	5.46	125.08	119.56
2	L	113	ASP	C-N-CA	5.46	125.08	119.56
2	P	219	GLU	N-CA-C	5.45	117.92	111.33
2	V	31	VAL	N-CA-C	5.42	116.25	108.93
1	Y	228	SER	N-CA-C	-5.41	105.38	111.28
1	3	526	THR	N-CA-C	5.41	117.41	109.24
2	v	331	VAL	N-CA-C	5.41	116.23	108.93
2	T	31	VAL	N-CA-C	5.41	116.23	108.93
1	W	96	GLY	N-CA-C	-5.40	106.24	112.50
2	4	413	ASP	CA-C-N	5.38	124.99	119.56
2	4	413	ASP	C-N-CA	5.38	124.99	119.56
2	Z	113	ASP	CA-C-N	5.37	124.99	119.56
2	Z	113	ASP	C-N-CA	5.37	124.99	119.56
2	X	208	SER	N-CA-C	5.37	117.13	111.28
1	k	430	TYR	N-CA-C	5.35	116.80	111.07
1	a	396	GLY	N-CA-C	-5.35	106.30	112.50
1	Q	227	GLY	N-CA-C	5.34	120.95	111.02
2	C	101	LEU	CA-C-N	5.34	125.54	120.31
2	C	101	LEU	C-N-CA	5.34	125.54	120.31
1	A	132	GLU	N-CA-C	5.34	117.75	110.55
1	f	396	GLY	N-CA-C	-5.33	106.32	112.50
1	o	476	SER	N-CA-C	-5.32	103.51	110.53
1	B	60	VAL	N-CA-C	5.31	115.55	108.11
2	x	319	ARG	N-CA-C	5.30	118.38	109.95
2	X	113	ASP	CA-C-N	5.29	124.90	119.56
2	X	113	ASP	C-N-CA	5.29	124.90	119.56
1	o	360	VAL	N-CA-C	5.28	115.51	108.11
2	G	92	ALA	N-CA-C	-5.27	106.82	113.20
1	Q	96	GLY	N-CA-C	-5.26	106.39	112.50
2	t	413	ASP	CA-C-N	5.26	124.88	119.56
2	t	413	ASP	C-N-CA	5.26	124.88	119.56
1	O	84	THR	N-CA-C	5.26	116.70	111.07
2	C	103	LEU	N-CA-C	-5.25	99.73	108.34
2	P	103	LEU	N-CA-C	-5.24	99.90	108.76
2	J	31	VAL	N-CA-C	5.24	116.00	108.93
2	P	172	TYR	N-CA-C	-5.23	105.49	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	54	SER	N-CA-C	5.22	116.78	108.79
2	2	12	VAL	CB-CA-C	-5.22	102.62	110.55
1	1	213	LEU	N-CA-C	-5.21	98.35	107.73
2	P	53	VAL	CB-CA-C	-5.21	105.20	112.02
1	k	529	ALA	N-CA-C	-5.21	105.72	111.71
2	t	319	ARG	N-CA-C	5.20	118.22	110.52
1	b	513	LEU	N-CA-C	-5.20	98.09	107.75
1	K	183	ILE	CB-CA-C	-5.19	105.24	112.04
1	d	513	LEU	N-CA-C	-5.19	98.10	107.75
1	I	213	LEU	N-CA-C	-5.18	100.08	108.52
1	K	116	LYS	CA-C-N	5.15	125.08	119.78
1	K	116	LYS	C-N-CA	5.15	125.08	119.78
1	o	396	GLY	N-CA-C	-5.14	106.53	112.50
2	h	413	ASP	CA-C-N	5.14	124.75	119.56
2	h	413	ASP	C-N-CA	5.14	124.75	119.56
1	q	416	LYS	CA-C-N	5.14	125.04	119.85
1	q	416	LYS	C-N-CA	5.14	125.04	119.85
1	D	149	ASP	N-CA-C	5.12	118.38	107.67
2	n	353	VAL	CB-CA-C	-5.12	105.18	111.94
2	N	12	VAL	CB-CA-C	-5.11	102.78	110.55
1	b	396	GLY	N-CA-C	-5.11	106.58	112.50
1	w	513	LEU	N-CA-C	-5.10	99.48	108.20
1	U	227	GLY	N-CA-C	5.10	120.50	111.02
2	X	172	TYR	N-CA-C	-5.10	105.81	111.36
1	A	218	PRO	N-CA-C	5.09	120.76	113.47
1	F	29	SER	N-CA-C	5.09	118.02	110.48
1	A	56	LEU	N-CA-C	-5.09	107.73	114.04
1	S	116	LYS	CA-C-N	5.08	124.84	119.76
1	S	116	LYS	C-N-CA	5.08	124.84	119.76
2	l	516	ALA	N-CA-C	-5.08	105.63	111.07
1	D	102	VAL	CB-CA-C	-5.07	105.22	112.22
2	H	172	TYR	N-CA-C	-5.07	105.84	111.36
1	S	68	PHE	N-CA-C	5.06	116.49	110.97
2	X	83	LEU	N-CA-C	-5.03	105.69	111.07
1	M	49	SER	N-CA-C	5.02	116.75	111.28
1	W	47	SER	N-CA-C	5.01	117.30	110.24
1	b	432	GLU	N-CA-C	5.01	117.26	110.35
1	q	513	LEU	N-CA-C	-5.01	100.57	108.73
2	x	322	GLN	N-CA-C	-5.01	99.13	107.99
1	D	56	LEU	N-CA-C	-5.00	107.13	113.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1633	0	1633	70	0
1	3	1625	0	1622	68	0
1	A	1633	0	1633	106	0
1	B	1633	0	1633	87	0
1	D	1625	0	1622	145	0
1	F	1490	0	1483	84	0
1	I	1640	0	1642	90	0
1	K	1633	0	1633	80	0
1	M	1589	0	1587	86	0
1	O	1633	0	1633	56	0
1	Q	1633	0	1633	97	0
1	S	1633	0	1633	103	0
1	U	1633	0	1633	58	0
1	W	1487	0	1477	70	0
1	Y	1625	0	1622	109	0
1	a	1633	0	1633	70	0
1	b	1633	0	1633	72	0
1	d	1633	0	1633	84	0
1	f	1633	0	1633	65	0
1	i	1633	0	1633	72	0
1	k	1633	0	1633	80	0
1	m	1612	0	1606	48	0
1	o	1633	0	1633	78	0
1	q	1633	0	1633	91	0
1	s	1633	0	1633	82	0
1	u	1633	0	1633	68	0
1	w	1633	0	1633	110	0
1	y	1633	0	1633	124	0
2	2	1606	0	1593	48	0
2	4	1606	0	1593	43	0
2	C	1606	0	1593	48	0
2	E	1606	0	1593	71	0
2	G	1606	0	1593	49	0
2	H	1606	0	1593	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1606	0	1593	49	0
2	L	1606	0	1593	57	0
2	N	1606	0	1593	49	0
2	P	1606	0	1593	40	0
2	R	1606	0	1593	72	0
2	T	1606	0	1593	47	0
2	V	1610	0	1596	65	0
2	X	1606	0	1593	58	0
2	Z	1606	0	1593	60	0
2	c	1596	0	1583	56	0
2	e	1606	0	1593	36	0
2	g	1606	0	1593	50	0
2	h	1588	0	1572	36	0
2	j	1606	0	1593	58	0
2	l	1606	0	1593	45	0
2	n	1606	0	1593	35	0
2	p	1606	0	1593	37	0
2	r	1606	0	1593	49	0
2	t	1606	0	1593	57	0
2	v	1615	0	1601	51	0
2	x	1606	0	1593	43	0
2	z	1606	0	1593	61	0
3	1	3	0	0	1	0
3	2	1	0	0	0	0
3	3	5	0	0	2	0
3	4	7	0	0	1	0
3	A	2	0	0	2	0
3	B	2	0	0	1	0
3	E	4	0	0	2	0
3	F	3	0	0	2	0
3	G	2	0	0	1	0
3	H	1	0	0	1	0
3	I	4	0	0	3	0
3	J	2	0	0	0	0
3	K	3	0	0	4	0
3	L	1	0	0	0	0
3	M	1	0	0	1	0
3	N	6	0	0	4	0
3	O	3	0	0	1	0
3	P	4	0	0	0	0
3	R	3	0	0	2	0
3	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1	0	0	1	0
3	U	1	0	0	0	0
3	V	6	0	0	0	0
3	X	4	0	0	0	0
3	a	5	0	0	2	0
3	b	3	0	0	0	0
3	c	6	0	0	0	0
3	d	2	0	0	0	0
3	e	5	0	0	3	0
3	f	1	0	0	0	0
3	g	3	0	0	0	0
3	h	3	0	0	3	0
3	i	1	0	0	0	0
3	j	3	0	0	0	0
3	k	2	0	0	1	0
3	l	3	0	0	1	0
3	n	2	0	0	1	0
3	o	1	0	0	0	0
3	p	2	0	0	0	0
3	q	1	0	0	1	0
3	r	2	0	0	0	0
3	s	2	0	0	0	0
3	t	2	0	0	0	0
3	u	2	0	0	3	0
3	v	4	0	0	0	0
3	w	4	0	0	2	0
3	x	1	0	0	0	0
3	y	2	0	0	0	0
3	z	4	0	0	1	0
All	All	90443	0	89905	3512	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 19.

All (3512) 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:D:13:MET:N	1:D:13:MET:HE3	1.40	1.36
1:D:35:TYR:CE2	1:D:40:LEU:HB2	1.65	1.32
1:a:313:MET:HA	1:a:313:MET:CE	1.63	1.26
1:M:35:TYR:CE1	1:M:37:GLY:HA3	1.68	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:230:LEU:HD23	1:S:230:LEU:C	1.51	1.25
1:B:19:LEU:HD23	1:B:19:LEU:C	1.61	1.23
1:w:315:GLU:CG	1:y:310:GLU:HG3	1.66	1.23
1:s:517:ARG:NH2	1:s:523:ARG:HG3	1.53	1.22
1:1:229:ALA:O	1:1:233:LEU:HD13	1.41	1.18
1:Y:14:ARG:HH22	2:c:309:PRO:HB3	1.04	1.18
1:Y:35:TYR:HE1	1:Y:37:GLY:CA	1.57	1.18
2:E:165:ARG:HG3	2:E:213:LEU:HD22	1.20	1.18
1:S:217:ARG:NH2	1:S:223:ARG:HG3	1.58	1.17
1:U:10:GLU:HA	1:1:15:GLU:OE2	1.44	1.16
1:M:35:TYR:CE1	1:M:37:GLY:CA	2.30	1.15
1:Y:35:TYR:CE1	1:Y:37:GLY:CA	2.30	1.15
1:Y:35:TYR:CE1	1:Y:37:GLY:HA3	1.81	1.15
2:v:509:ARG:O	2:v:513:LEU:HD13	1.44	1.14
1:S:35:TYR:CE1	1:S:37:GLY:HA3	1.83	1.14
1:q:335:TYR:HE1	1:q:337:GLY:HA3	1.08	1.14
1:F:159:THR:HG21	2:r:459:ASP:HB2	1.27	1.14
1:f:529:ALA:O	1:f:533:LEU:HD13	1.46	1.13
1:q:335:TYR:CE1	1:q:337:GLY:CA	2.30	1.13
1:K:178:THR:HB	1:K:233:LEU:HD22	1.24	1.13
1:s:315:GLU:OE2	1:3:310:GLU:HG2	1.47	1.12
1:I:11:GLN:HG2	1:I:14:ARG:NH2	1.63	1.12
1:w:478:THR:HB	1:w:533:LEU:HD21	1.20	1.12
1:q:335:TYR:CE1	1:q:337:GLY:HA3	1.83	1.12
1:s:335:TYR:CE1	1:s:337:GLY:HA3	1.84	1.12
1:1:231:GLN:HA	1:1:234:LEU:CD1	1.78	1.11
1:y:478:THR:HA	1:y:533:LEU:HD11	1.30	1.11
1:s:526:THR:CG2	1:s:527:GLY:H	1.63	1.10
1:a:313:MET:CA	1:a:313:MET:HE3	1.80	1.10
1:y:478:THR:CA	1:y:533:LEU:HD11	1.82	1.09
2:t:318:ARG:HD2	2:t:491:PHE:O	1.52	1.09
1:F:159:THR:CG2	2:r:459:ASP:HB2	1.82	1.09
1:s:335:TYR:HE1	1:s:337:GLY:HA3	0.97	1.09
1:s:526:THR:HG22	1:s:527:GLY:N	1.63	1.08
1:S:231:GLN:HE21	1:S:234:LEU:HD12	1.13	1.08
1:B:19:LEU:HD23	1:B:19:LEU:O	1.51	1.08
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.35	1.08
2:G:187:VAL:HA	2:V:222:SER:HB3	1.13	1.08
1:D:10:GLU:OE2	1:Q:19:LEU:HB2	1.51	1.08
1:o:476:SER:HB3	1:o:479:ASP:OD1	1.54	1.08
1:w:315:GLU:HG2	1:y:310:GLU:HG3	1.08	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:227:GLY:CA	1:S:230:LEU:HB3	1.84	1.07
1:w:315:GLU:CD	1:y:310:GLU:CG	2.27	1.07
1:3:335:TYR:HE1	1:3:337:GLY:HA3	1.15	1.07
1:S:35:TYR:CE1	1:S:37:GLY:CA	2.37	1.07
1:a:313:MET:HA	1:a:313:MET:HE3	1.29	1.07
1:w:452:HIS:HB3	1:w:471:TYR:CE2	1.90	1.07
1:w:415:ALA:HB3	1:y:412:THR:HG23	1.33	1.06
1:3:335:TYR:CE1	1:3:337:GLY:HA3	1.89	1.06
1:d:348:ARG:NH1	1:k:435:ARG:HH11	1.52	1.06
1:S:173:GLU:HG3	1:S:174:ASN:OD1	1.54	1.06
1:S:231:GLN:NE2	1:S:234:LEU:HD12	1.70	1.05
1:Y:35:TYR:HE1	1:Y:37:GLY:HA3	0.90	1.05
1:B:11:GLN:O	1:B:14:ARG:HB2	1.55	1.05
1:d:437:GLU:HG2	1:q:348:ARG:HH22	1.20	1.05
1:Q:35:TYR:CE1	1:Q:38:GLY:N	2.25	1.04
1:w:452:HIS:HB3	1:w:471:TYR:HE2	1.15	1.04
2:L:14:MET:HE3	2:L:105:ALA:HB2	1.39	1.04
1:D:12:ALA:C	1:D:13:MET:HE3	1.83	1.04
1:y:478:THR:HB	1:y:533:LEU:CD2	1.86	1.04
1:s:526:THR:HG22	1:s:527:GLY:H	0.88	1.03
1:y:428:ALA:HB2	1:y:434:LYS:HB3	1.41	1.02
1:B:19:LEU:C	1:B:19:LEU:CD2	2.30	1.02
1:q:335:TYR:HE1	1:q:337:GLY:CA	1.69	1.02
1:y:339:VAL:O	1:y:512:VAL:HG23	1.58	1.02
1:D:90:ASP:OD1	1:D:93:ASP:HB2	1.59	1.02
1:s:335:TYR:CE1	1:s:337:GLY:CA	2.43	1.02
1:1:20:ALA:O	1:1:24:ILE:HG13	1.58	1.02
1:D:35:TYR:CE2	1:D:40:LEU:CB	2.43	1.01
1:Y:173:GLU:HG3	1:Y:174:ASN:ND2	1.75	1.01
1:w:315:GLU:CD	1:y:310:GLU:HG3	1.84	1.01
1:K:230:LEU:O	1:K:234:LEU:HB2	1.60	1.01
1:S:35:TYR:HE1	1:S:37:GLY:HA3	1.12	1.00
1:k:335:TYR:CE1	1:k:337:GLY:HA3	1.96	1.00
2:T:37:THR:HG21	2:T:43:THR:HG23	1.44	1.00
1:S:48:ARG:NH2	1:1:137:GLU:HG2	1.75	1.00
1:w:479:ASP:O	1:w:483:ILE:HG13	1.61	1.00
1:y:341:PHE:HB3	1:y:353:ILE:HD13	1.39	1.00
2:x:515:ARG:O	2:x:519:GLU:HG3	1.59	1.00
1:w:335:TYR:CE1	1:w:337:GLY:HA3	1.96	1.00
1:q:335:TYR:CE1	1:q:337:GLY:N	2.30	0.99
2:E:165:ARG:CG	2:E:213:LEU:HD22	1.90	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:348:ARG:HH12	1:k:435:ARG:NH1	1.60	0.99
1:s:335:TYR:HE1	1:s:337:GLY:CA	1.75	0.99
1:D:35:TYR:HE2	1:D:40:LEU:CB	1.74	0.99
1:U:112:THR:HG23	1:1:115:ALA:HB3	1.40	0.99
1:A:217:ARG:NH1	1:A:223:ARG:HB2	1.75	0.99
1:S:230:LEU:C	1:S:230:LEU:CD2	2.30	0.98
1:Y:14:ARG:NH2	2:c:309:PRO:HB3	1.77	0.98
1:w:478:THR:CB	1:w:533:LEU:HD21	1.92	0.98
2:E:144:LEU:HB2	3:E:242:HOH:O	1.61	0.98
1:y:341:PHE:HB3	1:y:353:ILE:CD1	1.93	0.98
1:w:340:LEU:HD12	1:w:512:VAL:HG12	1.40	0.98
2:G:187:VAL:CA	2:V:222:SER:HB3	1.93	0.98
1:w:335:TYR:CE1	1:w:337:GLY:N	2.30	0.98
1:W:115:ALA:HB3	1:Y:112:THR:HG23	1.45	0.98
1:D:12:ALA:HB3	1:D:13:MET:HE1	1.44	0.97
1:i:525:ILE:HG22	1:i:530:LEU:HB2	1.45	0.97
1:o:313:MET:HA	1:o:313:MET:CE	1.94	0.97
2:t:461:ASP:CG	2:t:509:ARG:HH21	1.71	0.97
1:I:11:GLN:CD	1:I:14:ARG:HH21	1.72	0.97
2:e:461:ASP:CG	2:e:509:ARG:HH21	1.72	0.97
1:M:152:HIS:HB3	1:M:171:TYR:CE2	1.99	0.97
1:q:526:THR:O	1:q:530:LEU:HB2	1.65	0.97
1:A:59:ARG:HD2	1:A:129:HIS:HA	1.46	0.97
1:S:227:GLY:HA2	1:S:230:LEU:HB3	1.45	0.97
1:f:348:ARG:HH22	1:w:437:GLU:CG	1.77	0.97
1:m:335:TYR:CE1	1:m:337:GLY:HA3	2.00	0.96
1:y:533:LEU:O	1:y:533:LEU:HD13	1.63	0.96
1:1:231:GLN:CA	1:1:234:LEU:HD12	1.92	0.96
1:W:228:SER:O	1:W:231:GLN:HG2	1.65	0.96
1:F:97:ARG:HD2	1:M:49:SER:HB2	1.47	0.96
1:I:115:ALA:HB3	1:S:112:THR:HG23	1.44	0.96
1:w:335:TYR:CE1	1:w:337:GLY:CA	2.48	0.95
1:1:231:GLN:HA	1:1:234:LEU:HD12	0.99	0.95
2:Z:40:TYR:CE1	2:Z:109:ILE:HD13	2.00	0.95
1:Y:35:TYR:HD1	1:Y:37:GLY:H	1.13	0.95
1:S:230:LEU:HD23	1:S:230:LEU:O	1.67	0.95
1:3:335:TYR:CE1	1:3:337:GLY:CA	2.48	0.95
1:a:313:MET:HA	1:a:313:MET:HE2	1.47	0.95
1:M:35:TYR:HE1	1:M:37:GLY:HA3	1.09	0.94
1:S:35:TYR:CE1	1:S:37:GLY:N	2.36	0.94
1:q:333:LEU:HD21	1:q:340:LEU:HB3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:225:ILE:HG22	1:S:230:LEU:HB2	1.47	0.94
2:t:314:MET:HE3	2:t:405:ALA:HB2	1.49	0.94
2:R:37:THR:HG21	2:R:59:TYR:HD2	1.28	0.94
1:o:437:GLU:HG2	1:u:348:ARG:HH21	1.27	0.94
1:A:217:ARG:HH11	1:A:223:ARG:HB2	1.26	0.93
1:D:13:MET:N	1:D:13:MET:CE	2.30	0.93
1:S:35:TYR:CD1	1:S:37:GLY:N	2.37	0.93
1:q:451:PRO:HD2	3:q:38:HOH:O	1.68	0.93
1:A:135:ARG:CB	1:A:135:ARG:HH11	1.82	0.93
1:s:335:TYR:HD1	1:s:337:GLY:H	1.13	0.93
2:t:318:ARG:NH1	2:t:493:THR:CG2	2.31	0.93
1:y:341:PHE:CB	1:y:353:ILE:HD13	1.99	0.92
2:e:444:LEU:HB2	3:e:8:HOH:O	1.67	0.92
1:Y:35:TYR:CD1	1:Y:37:GLY:N	2.38	0.92
1:Y:35:TYR:CE1	1:Y:38:GLY:N	2.38	0.92
1:f:415:ALA:HB3	1:w:412:THR:HG23	1.48	0.92
1:M:112:THR:HG22	1:M:113:GLU:HG3	1.50	0.92
1:D:35:TYR:HE2	1:D:40:LEU:N	1.67	0.92
1:K:35:TYR:CE1	1:K:37:GLY:HA3	2.05	0.92
2:r:513:LEU:O	2:r:517:ILE:HD13	1.68	0.92
1:w:311:GLN:HA	1:w:314:ARG:HD2	1.51	0.92
1:w:315:GLU:OE2	1:y:310:GLU:HB2	1.67	0.92
1:W:179:ASP:O	1:W:183:ILE:HG13	1.68	0.91
1:I:35:TYR:CE1	1:I:37:GLY:HA3	2.06	0.91
1:a:313:MET:HE2	1:a:316:ARG:HD3	1.53	0.91
1:u:412:THR:HG23	1:3:415:ALA:HB3	1.52	0.91
1:q:335:TYR:CD1	1:q:337:GLY:N	2.38	0.91
1:d:335:TYR:CE1	1:d:337:GLY:HA3	2.06	0.91
1:I:11:GLN:CG	1:I:14:ARG:NH2	2.34	0.91
1:D:181:LEU:HD23	1:D:233:LEU:CD2	2.01	0.91
1:f:348:ARG:HH22	1:w:437:GLU:HG2	1.36	0.91
1:A:97:ARG:HD2	1:A:97:ARG:O	1.71	0.90
1:O:210:VAL:HB	1:O:230:LEU:HD21	1.52	0.90
1:o:412:THR:HG22	1:o:413:GLU:HG3	1.53	0.90
1:D:20:ALA:O	1:D:24:ILE:HG13	1.71	0.90
1:D:112:THR:HG23	1:Q:115:ALA:HB3	1.53	0.90
1:K:51:GLN:HB3	1:K:209:GLU:OE1	1.71	0.90
2:E:165:ARG:HG3	2:E:213:LEU:CD2	2.00	0.90
1:1:112:THR:HG22	1:1:113:GLU:HG3	1.53	0.90
1:M:15:GLU:HB2	2:j:519:GLU:HB3	1.52	0.90
1:D:115:ALA:HB3	1:K:112:THR:HG23	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:412:THR:HG22	1:u:413:GLU:HG3	1.52	0.90
1:A:135:ARG:NH1	1:A:135:ARG:HB3	1.87	0.89
1:Q:112:THR:HG22	1:Q:113:GLU:HG3	1.54	0.89
1:Y:14:ARG:HH22	2:c:309:PRO:CB	1.85	0.89
1:i:415:ALA:HB3	1:s:412:THR:HG23	1.54	0.89
1:M:35:TYR:CD1	1:M:37:GLY:N	2.41	0.89
2:Z:107:TYR:HB2	2:Z:197:ILE:HG22	1.52	0.89
1:M:129:HIS:HB2	1:M:132:GLU:OE2	1.73	0.89
1:q:333:LEU:HD23	1:q:333:LEU:O	1.72	0.89
2:T:37:THR:CG2	2:T:43:THR:HG23	2.03	0.89
2:t:318:ARG:NH1	2:t:493:THR:HG23	1.85	0.89
1:D:219:ARG:NH2	1:D:220:ARG:HD3	1.87	0.89
1:s:527:GLY:O	1:s:531:GLN:HG3	1.71	0.89
1:U:112:THR:HG22	1:U:113:GLU:HG3	1.54	0.89
1:f:311:GLN:HG2	1:f:314:ARG:NH2	1.88	0.89
1:i:311:GLN:HE21	1:i:314:ARG:HH21	1.13	0.89
1:m:412:THR:HG22	1:m:413:GLU:HG3	1.54	0.89
1:b:530:LEU:CD2	1:b:534:LEU:HD21	2.04	0.89
1:i:311:GLN:NE2	1:i:314:ARG:HH21	1.69	0.88
1:I:230:LEU:O	1:I:234:LEU:HG	1.73	0.88
1:b:527:GLY:O	1:b:531:GLN:HG3	1.73	0.88
1:3:412:THR:HG22	1:3:413:GLU:HG3	1.55	0.88
2:E:134:GLU:HB2	3:E:241:HOH:O	1.72	0.88
1:y:412:THR:HG22	1:y:413:GLU:HG3	1.55	0.88
1:b:415:ALA:HB3	1:i:412:THR:HG23	1.56	0.88
1:S:69:ASN:HB2	1:l:105:GLN:HG2	1.55	0.88
1:u:355:GLU:HB2	1:u:522:PHE:CG	2.08	0.88
2:V:217:ILE:HG23	2:V:221:ARG:NH1	1.87	0.88
1:W:178:THR:HG23	1:W:179:ASP:OD1	1.74	0.88
1:s:517:ARG:HH22	1:s:523:ARG:HG3	1.35	0.88
1:y:313:MET:CE	1:y:313:MET:HA	2.04	0.88
1:i:335:TYR:CE1	1:i:337:GLY:HA3	2.08	0.87
1:d:412:THR:HG22	1:d:413:GLU:HG3	1.55	0.87
1:b:310:GLU:HG3	1:b:311:GLN:N	1.88	0.87
1:f:311:GLN:HE21	1:f:314:ARG:HH21	1.17	0.87
1:K:35:TYR:HE1	1:K:37:GLY:HA3	1.37	0.87
1:Q:182:ARG:NH1	1:Q:234:LEU:HD22	1.88	0.87
1:y:313:MET:HA	1:y:313:MET:HE3	1.57	0.87
1:y:478:THR:HB	1:y:533:LEU:HD21	1.56	0.87
1:y:478:THR:CB	1:y:533:LEU:HD11	2.03	0.87
2:t:318:ARG:HH11	2:t:493:THR:HG23	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:TYR:HE2	1:D:40:LEU:CA	1.88	0.87
1:M:176:SER:HB3	1:M:179:ASP:OD1	1.74	0.87
1:a:525:ILE:HG22	1:a:530:LEU:HB2	1.57	0.87
1:d:437:GLU:HG2	1:q:348:ARG:NH2	1.88	0.87
1:F:81:PHE:HB2	3:F:249:HOH:O	1.73	0.87
1:I:11:GLN:NE2	1:I:14:ARG:HE	1.73	0.86
1:O:112:THR:HG22	1:O:113:GLU:HG3	1.54	0.86
1:m:335:TYR:HE1	1:m:337:GLY:HA3	1.38	0.86
1:q:412:THR:HG22	1:q:413:GLU:HG3	1.56	0.86
1:s:412:THR:HG22	1:s:413:GLU:HG3	1.56	0.86
1:Y:55:GLU:HB2	1:Y:222:PHE:CG	2.10	0.86
2:V:217:ILE:O	2:V:221:ARG:HB2	1.75	0.86
1:w:412:THR:HG22	1:w:413:GLU:HG3	1.56	0.86
1:S:230:LEU:HD23	1:S:231:GLN:N	1.90	0.86
2:N:198:ASP:OD1	2:N:200:ASP:HB2	1.74	0.86
2:t:318:ARG:HD3	2:t:490:ILE:HG22	1.56	0.86
1:S:231:GLN:NE2	1:S:234:LEU:CD1	2.39	0.86
1:A:127:VAL:HG21	1:A:213:LEU:HB3	1.56	0.86
1:D:181:LEU:CD2	1:D:233:LEU:CD2	2.54	0.86
1:S:35:TYR:HE1	1:S:37:GLY:CA	1.79	0.85
2:E:107:TYR:HB2	2:E:197:ILE:HG22	1.56	0.85
2:R:164:LEU:HD13	2:R:213:LEU:CD1	2.06	0.85
1:d:335:TYR:CE1	1:d:337:GLY:N	2.44	0.85
1:i:412:THR:HG22	1:i:413:GLU:HG3	1.58	0.85
1:q:335:TYR:CD2	1:q:338:GLY:O	2.30	0.85
2:Z:40:TYR:CD1	2:Z:109:ILE:HD13	2.12	0.85
1:w:340:LEU:CD1	1:w:512:VAL:HG12	2.05	0.85
1:U:35:TYR:CD2	1:U:38:GLY:O	2.30	0.85
1:Y:178:THR:CB	1:Y:233:LEU:HG	2.07	0.85
1:a:482:ARG:HH12	1:a:534:LEU:C	1.84	0.85
1:K:35:TYR:CD2	1:K:38:GLY:O	2.30	0.85
1:u:481:LEU:HD22	1:u:533:LEU:HD23	1.56	0.85
1:a:313:MET:CE	1:a:316:ARG:HD3	2.07	0.85
1:i:335:TYR:CD2	1:i:338:GLY:O	2.30	0.85
1:y:478:THR:OG1	1:y:533:LEU:CD1	2.25	0.85
2:V:209:ARG:O	2:V:212:GLU:HG2	1.75	0.85
1:S:112:THR:HG22	1:S:113:GLU:HG3	1.55	0.84
2:4:301:OZT:H17	2:4:333:LYS:NZ	1.92	0.84
1:K:112:THR:HG22	1:K:113:GLU:HG3	1.57	0.84
1:M:127:VAL:CG1	1:M:215:ALA:HB2	2.06	0.84
1:Q:35:TYR:HD1	1:Q:37:GLY:N	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:112:THR:HG22	1:Y:113:GLU:HG3	1.57	0.84
1:A:35:TYR:CD2	1:A:38:GLY:O	2.30	0.84
1:I:231:GLN:O	1:I:235:VAL:HG22	1.77	0.84
1:b:530:LEU:HD22	1:b:534:LEU:HD21	1.57	0.84
1:o:517:ARG:NH2	1:o:523:ARG:HG3	1.92	0.84
2:G:187:VAL:HA	2:V:222:SER:CB	2.05	0.84
1:W:112:THR:HG22	1:W:113:GLU:HG3	1.57	0.84
1:D:35:TYR:CE2	1:D:38:GLY:O	2.30	0.84
1:F:159:THR:HG22	2:r:459:ASP:OD2	1.78	0.84
1:q:529:ALA:O	1:q:533:LEU:HD23	1.78	0.84
1:3:311:GLN:HG2	1:3:311:GLN:O	1.75	0.84
1:D:15:GLU:OE1	1:K:10:GLU:HG2	1.77	0.84
1:I:35:TYR:CD2	1:I:38:GLY:O	2.30	0.84
1:w:315:GLU:CD	1:y:310:GLU:HG2	2.03	0.84
1:Q:35:TYR:CE1	1:Q:37:GLY:CA	2.61	0.84
1:y:314:ARG:O	1:y:318:GLU:HG2	1.78	0.84
1:y:478:THR:CB	1:y:533:LEU:CD1	2.56	0.84
1:y:478:THR:OG1	1:y:533:LEU:HD13	1.78	0.84
1:Q:35:TYR:HE1	1:Q:37:GLY:HA3	1.41	0.83
2:r:513:LEU:O	2:r:517:ILE:CD1	2.24	0.83
1:D:40:LEU:CD1	1:D:212:VAL:HG12	2.09	0.83
1:Q:35:TYR:HD1	1:Q:37:GLY:H	1.24	0.83
1:w:335:TYR:CD2	1:w:338:GLY:O	2.30	0.83
1:M:35:TYR:CE1	1:M:37:GLY:N	2.45	0.83
1:D:35:TYR:CZ	1:D:38:GLY:O	2.31	0.83
1:I:11:GLN:NE2	1:I:14:ARG:HH21	1.75	0.83
1:O:182:ARG:HH12	1:O:234:LEU:HA	1.42	0.83
1:k:335:TYR:CE1	1:k:337:GLY:CA	2.62	0.83
1:s:335:TYR:CD1	1:s:337:GLY:N	2.46	0.83
2:V:172:TYR:CE1	2:V:218:ILE:CD1	2.62	0.83
1:y:478:THR:HB	1:y:533:LEU:HD22	1.60	0.83
1:S:35:TYR:HD1	1:S:37:GLY:H	1.27	0.83
1:1:22:LYS:O	1:1:26:ARG:HG3	1.80	0.82
1:D:35:TYR:CE2	1:D:40:LEU:N	2.46	0.82
1:F:33:LEU:HD21	1:F:40:LEU:HD23	1.58	0.82
1:Y:178:THR:HG23	1:Y:179:ASP:OD1	1.78	0.82
1:A:135:ARG:HH11	1:A:135:ARG:HB2	1.45	0.82
1:d:335:TYR:CE1	1:d:337:GLY:CA	2.62	0.82
1:M:18:GLU:HG3	2:j:522:SER:C	2.04	0.82
1:D:181:LEU:CD2	1:D:233:LEU:HD22	2.10	0.82
1:U:11:GLN:HE21	1:U:11:GLN:HA	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:315:GLU:CG	1:y:310:GLU:CG	2.54	0.82
2:V:212:GLU:HG3	2:V:213:LEU:N	1.95	0.82
1:Q:35:TYR:CE1	1:Q:37:GLY:HA3	2.15	0.82
2:H:107:TYR:HB2	2:H:197:ILE:HG22	1.62	0.82
2:v:517:ILE:O	2:v:521:ARG:HG3	1.79	0.82
1:s:481:LEU:HD23	1:s:533:LEU:HB3	1.62	0.81
1:a:412:THR:HG22	1:a:413:GLU:HG3	1.62	0.81
1:d:529:ALA:O	1:d:533:LEU:HD13	1.79	0.81
1:B:98:GLN:O	1:B:102:VAL:HG23	1.81	0.81
1:Q:35:TYR:CE1	1:Q:37:GLY:C	2.58	0.81
2:J:37:THR:HG21	2:J:43:THR:HG23	1.62	0.81
1:a:313:MET:HE3	1:a:313:MET:N	1.93	0.81
1:f:412:THR:HG22	1:f:413:GLU:HG3	1.60	0.81
1:S:227:GLY:C	1:S:230:LEU:HB3	2.06	0.81
2:J:192:PRO:O	2:J:210:ILE:HD13	1.80	0.81
1:I:112:THR:HG22	1:I:113:GLU:HG3	1.62	0.81
2:e:465:ARG:HG3	2:e:513:LEU:HD22	1.63	0.81
1:A:36:ALA:HA	1:A:174:ASN:HD22	1.45	0.81
1:Y:35:TYR:CE1	1:Y:37:GLY:C	2.59	0.81
2:h:498:ASP:OD1	2:h:500:ASP:HB2	1.81	0.81
1:A:135:ARG:CB	1:A:135:ARG:NH1	2.43	0.81
1:Q:35:TYR:HE1	1:Q:37:GLY:CA	1.93	0.81
1:q:333:LEU:CD2	1:q:340:LEU:HB3	2.11	0.80
2:g:487:VAL:HG13	2:v:521:ARG:CB	2.11	0.80
2:t:318:ARG:CD	2:t:491:PHE:O	2.28	0.80
1:M:218:PRO:HD2	3:M:249:HOH:O	1.80	0.80
1:D:98:GLN:O	1:D:102:VAL:HG23	1.82	0.80
1:I:11:GLN:NE2	1:I:14:ARG:NH2	2.30	0.80
1:k:435:ARG:HH22	1:k:451:PRO:HB3	1.45	0.80
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.63	0.80
1:d:529:ALA:O	1:d:533:LEU:CD1	2.30	0.80
1:k:412:THR:HG22	1:k:413:GLU:HG3	1.63	0.80
1:w:340:LEU:HD12	1:w:512:VAL:CG1	2.11	0.80
1:K:182:ARG:HG2	3:K:250:HOH:O	1.81	0.80
1:a:526:THR:O	1:a:530:LEU:CB	2.30	0.80
1:w:315:GLU:OE2	1:y:310:GLU:CB	2.30	0.80
1:S:173:GLU:CG	1:S:174:ASN:OD1	2.30	0.80
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.64	0.80
1:f:311:GLN:NE2	1:f:314:ARG:HH21	1.78	0.80
1:y:478:THR:HA	1:y:533:LEU:CD1	2.12	0.80
2:r:464:LEU:O	2:r:464:LEU:CD2	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:319:ARG:HG3	2:t:320:SER:N	1.94	0.80
1:M:176:SER:CB	1:M:179:ASP:OD1	2.30	0.79
1:w:452:HIS:CB	1:w:471:TYR:HE2	1.94	0.79
1:y:533:LEU:O	1:y:533:LEU:CD1	2.30	0.79
2:J:37:THR:CG2	2:J:43:THR:HG23	2.11	0.79
1:o:476:SER:CB	1:o:479:ASP:OD1	2.30	0.79
1:q:359:ARG:HD2	1:q:429:HIS:HA	1.63	0.79
2:z:337:THR:CG2	2:z:343:THR:HG23	2.13	0.79
2:z:472:TYR:CD2	2:z:521:ARG:NH1	2.50	0.79
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.63	0.79
1:I:11:GLN:NE2	1:I:14:ARG:NE	2.30	0.79
1:F:115:ALA:HB3	1:W:112:THR:HG23	1.63	0.79
2:t:461:ASP:CG	2:t:509:ARG:NH2	2.40	0.79
1:o:437:GLU:HG2	1:u:348:ARG:NH2	1.98	0.79
2:z:472:TYR:CE2	2:z:521:ARG:NH1	2.51	0.79
1:Q:140:ARG:NH2	1:Q:155:VAL:H	1.81	0.79
2:V:209:ARG:O	2:V:212:GLU:CG	2.31	0.79
1:A:41:PHE:HB3	1:A:53:ILE:HD13	1.65	0.79
1:y:533:LEU:CD1	1:y:533:LEU:C	2.56	0.79
1:A:182:ARG:HH12	1:A:234:LEU:C	1.90	0.79
2:2:1:OZT:H17	2:2:33:LYS:NZ	1.98	0.78
2:E:214:ALA:O	2:E:218:ILE:HG13	1.82	0.78
2:z:472:TYR:HE2	2:z:521:ARG:HH11	1.30	0.78
2:4:301:OZT:H17	2:4:333:LYS:HZ3	1.46	0.78
1:I:11:GLN:HG2	1:I:14:ARG:HH22	1.44	0.78
1:w:315:GLU:HG2	1:y:310:GLU:CG	2.03	0.78
1:3:335:TYR:CD1	1:3:337:GLY:N	2.52	0.78
1:I:31:VAL:HG12	1:I:33:LEU:CD2	2.14	0.78
1:b:412:THR:HG22	1:b:413:GLU:HG3	1.62	0.78
2:H:165:ARG:HG3	2:H:213:LEU:HD22	1.64	0.78
2:E:215:ARG:O	2:E:219:GLU:HG3	1.82	0.78
2:R:164:LEU:HD13	2:R:213:LEU:HD11	1.63	0.78
2:V:214:ALA:O	2:V:218:ILE:HG12	1.83	0.78
1:o:313:MET:HA	1:o:313:MET:HE3	1.64	0.78
1:K:35:TYR:CE1	1:K:37:GLY:CA	2.67	0.78
1:3:517:ARG:HD3	1:3:520:ARG:O	1.83	0.78
1:k:335:TYR:HE1	1:k:337:GLY:HA3	1.43	0.78
1:k:517:ARG:NH2	1:k:523:ARG:HG3	1.99	0.78
2:H:107:TYR:CE2	2:H:199:ALA:HA	2.19	0.78
2:z:513:LEU:O	2:z:517:ILE:HG13	1.81	0.78
1:Q:35:TYR:CD2	1:Q:38:GLY:O	2.36	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:527:GLY:O	1:s:531:GLN:CG	2.32	0.78
1:d:348:ARG:NH1	1:k:435:ARG:NH1	2.23	0.78
2:P:37:THR:HG21	2:P:43:THR:HG23	1.64	0.78
1:F:182:ARG:HD2	3:F:250:HOH:O	1.83	0.77
1:1:229:ALA:O	1:1:233:LEU:CD1	2.30	0.77
1:o:313:MET:HA	1:o:313:MET:HE2	1.65	0.77
1:d:310:GLU:HG2	1:q:315:GLU:OE2	1.83	0.77
2:v:509:ARG:O	2:v:513:LEU:CD1	2.31	0.77
1:D:35:TYR:CD2	1:D:38:GLY:O	2.37	0.77
1:1:41:PHE:HB3	1:1:53:ILE:HD13	1.67	0.77
1:f:529:ALA:O	1:f:533:LEU:CD1	2.30	0.77
1:s:369:ASN:HB2	1:3:405:GLN:HG2	1.64	0.77
1:y:356:LEU:HB2	1:y:360:VAL:HG23	1.64	0.77
2:t:301:OZT:HA	2:t:317:ASP:OD2	1.84	0.77
1:D:13:MET:HE3	1:D:13:MET:CA	2.14	0.77
1:w:311:GLN:HG3	1:w:314:ARG:HD3	1.66	0.77
1:f:341:PHE:HB3	1:f:353:ILE:HD13	1.65	0.77
1:o:313:MET:HE3	1:o:313:MET:CA	2.14	0.77
1:I:31:VAL:HG12	1:I:33:LEU:HD23	1.66	0.77
1:F:113:GLU:O	1:F:113:GLU:HG2	1.85	0.77
1:i:311:GLN:HE21	1:i:314:ARG:NH2	1.81	0.77
2:h:307:LYS:HD3	3:h:42:HOH:O	1.85	0.77
1:Y:227:GLY:HA2	1:Y:230:LEU:HD12	1.66	0.77
1:d:335:TYR:CD1	1:d:337:GLY:N	2.52	0.77
1:s:341:PHE:HB3	1:s:353:ILE:HD13	1.66	0.77
1:A:57:TYR:HB3	1:A:60:VAL:HG12	1.67	0.76
2:P:37:THR:CG2	2:P:43:THR:HG23	2.15	0.76
1:D:11:GLN:HA	1:D:11:GLN:OE1	1.83	0.76
1:Q:217:ARG:NH2	1:Q:223:ARG:HG3	2.00	0.76
1:k:435:ARG:HH22	1:k:451:PRO:CB	1.98	0.76
1:y:339:VAL:O	1:y:512:VAL:CG2	2.32	0.76
1:F:58:ASP:HB3	1:F:219:ARG:O	1.86	0.76
1:Q:162:PRO:HG3	1:i:474:ASN:O	1.85	0.76
1:S:217:ARG:HH22	1:S:223:ARG:HG3	1.49	0.76
1:m:335:TYR:CE1	1:m:337:GLY:CA	2.66	0.76
2:R:37:THR:CG2	2:R:59:TYR:HD2	1.99	0.76
1:w:311:GLN:CA	1:w:314:ARG:HD2	2.16	0.76
2:Z:107:TYR:HB2	2:Z:197:ILE:CG2	2.16	0.76
1:S:48:ARG:HH21	1:1:137:GLU:HG2	1.45	0.76
3:u:20:HOH:O	2:4:410:HIS:CD2	2.38	0.76
1:D:12:ALA:HB3	1:D:13:MET:CE	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:37:THR:HG21	2:R:59:TYR:CD2	2.17	0.76
1:D:113:GLU:O	1:D:113:GLU:HG2	1.85	0.75
1:W:230:LEU:HD13	1:W:230:LEU:C	2.11	0.75
1:Q:35:TYR:CD1	1:Q:37:GLY:N	2.55	0.75
2:R:209:ARG:O	2:R:213:LEU:HG	1.86	0.75
2:c:337:THR:CG2	2:c:343:THR:HG23	2.16	0.75
1:Y:36:ALA:HB2	1:Y:174:ASN:HA	1.67	0.75
1:D:18:GLU:OE1	1:D:18:GLU:HA	1.86	0.75
1:S:10:GLU:O	1:S:14:ARG:HD2	1.86	0.75
1:Y:176:SER:OG	1:Y:179:ASP:CG	2.30	0.75
2:C:38:ASP:C	2:C:38:ASP:OD1	2.30	0.75
2:g:337:THR:CG2	2:g:343:THR:HG23	2.16	0.75
1:A:155:VAL:HG12	1:A:160:THR:HG22	1.68	0.75
1:I:35:TYR:CE1	1:I:37:GLY:CA	2.70	0.75
1:i:344:GLU:HG3	1:i:344:GLU:O	1.87	0.75
1:q:341:PHE:HB3	1:q:353:ILE:HD13	1.69	0.75
1:3:335:TYR:HD1	1:3:337:GLY:H	1.33	0.75
2:T:38:ASP:C	2:T:38:ASP:OD1	2.30	0.75
2:T:192:PRO:O	2:T:210:ILE:HD13	1.87	0.75
2:Z:38:ASP:C	2:Z:38:ASP:OD1	2.30	0.75
1:I:11:GLN:CD	1:I:14:ARG:NH2	2.45	0.75
1:Q:140:ARG:HE	1:Q:154:VAL:HG13	1.50	0.75
2:n:338:ASP:C	2:n:338:ASP:OD1	2.30	0.75
1:B:11:GLN:O	1:B:14:ARG:CB	2.35	0.75
1:i:331:VAL:HG12	1:i:333:LEU:CD2	2.16	0.75
1:w:328:LYS:HB3	1:w:344:GLU:HG3	1.67	0.75
2:E:165:ARG:CB	2:E:213:LEU:HD22	2.17	0.75
1:b:341:PHE:HB3	1:b:353:ILE:HD13	1.69	0.74
2:t:318:ARG:HH12	2:t:493:THR:CG2	1.97	0.74
2:R:38:ASP:C	2:R:38:ASP:OD1	2.30	0.74
2:h:435:GLY:HA2	3:h:42:HOH:O	1.87	0.74
1:D:97:ARG:HD2	1:D:97:ARG:C	2.12	0.74
1:D:153:PHE:CD1	1:D:167:LEU:HD13	2.22	0.74
1:f:348:ARG:NH2	1:w:437:GLU:CG	2.50	0.74
1:w:335:TYR:CZ	1:w:337:GLY:HA3	2.22	0.74
1:F:159:THR:CG2	2:r:459:ASP:CB	2.65	0.74
1:I:11:GLN:HE21	1:I:14:ARG:NE	1.84	0.74
2:L:14:MET:HE3	2:L:105:ALA:CB	2.16	0.74
1:k:310:GLU:HG2	1:k:314:ARG:HD2	1.70	0.74
1:u:481:LEU:HD22	1:u:533:LEU:CD2	2.16	0.74
1:w:335:TYR:CD1	1:w:337:GLY:N	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ASP:C	2:H:38:ASP:OD1	2.30	0.74
3:I:251:HOH:O	2:C:110:HIS:HD2	1.71	0.74
2:T:130:ASN:HB2	3:T:241:HOH:O	1.87	0.74
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.70	0.74
1:K:47:SER:HB2	1:M:149:ASP:OD2	1.88	0.74
2:Z:37:THR:CG2	2:Z:43:THR:HG23	2.17	0.74
2:g:318:ARG:HD3	2:g:493:THR:HG23	1.70	0.74
2:E:107:TYR:HB2	2:E:197:ILE:CG2	2.17	0.74
2:r:464:LEU:O	2:r:464:LEU:HD23	1.87	0.74
1:D:219:ARG:HH22	2:E:64:GLU:CD	1.95	0.74
1:B:155:VAL:HG12	1:B:160:THR:HG22	1.70	0.73
1:w:473:GLU:O	1:w:474:ASN:HB2	1.88	0.73
1:K:178:THR:HB	1:K:233:LEU:CD2	2.12	0.73
2:2:19:ARG:HG3	2:2:20:SER:N	2.04	0.73
2:e:318:ARG:HD3	2:e:493:THR:HG23	1.70	0.73
1:F:35:TYR:OH	1:F:212:VAL:HB	1.88	0.73
1:I:11:GLN:HE21	1:I:14:ARG:CZ	2.01	0.73
2:L:38:ASP:C	2:L:38:ASP:OD1	2.30	0.73
2:N:38:ASP:C	2:N:38:ASP:OD1	2.30	0.73
2:c:337:THR:HG21	2:c:343:THR:HG23	1.70	0.73
1:Q:35:TYR:CE2	1:Q:38:GLY:O	2.41	0.73
1:u:340:LEU:HD13	1:u:512:VAL:HG12	1.69	0.73
2:G:38:ASP:C	2:G:38:ASP:OD1	2.30	0.73
1:I:11:GLN:CG	1:I:14:ARG:HH21	2.00	0.73
1:S:28:LYS:HB3	1:S:44:GLU:HG3	1.70	0.73
1:q:335:TYR:HD1	1:q:337:GLY:H	1.35	0.73
2:E:19:ARG:HG3	2:E:20:SER:N	2.04	0.73
1:D:35:TYR:OH	1:D:212:VAL:HB	1.88	0.73
1:y:335:TYR:OH	1:y:512:VAL:HG21	1.88	0.73
2:L:37:THR:CG2	2:L:43:THR:HG23	2.18	0.73
2:r:318:ARG:HD3	2:r:493:THR:HG23	1.71	0.73
1:d:328:LYS:HB3	1:d:344:GLU:HG3	1.69	0.73
2:2:115:GLN:OE1	2:2:115:GLN:HA	1.89	0.73
1:I:181:LEU:HD23	1:I:233:LEU:HB3	1.70	0.73
1:s:481:LEU:CD2	1:s:533:LEU:HD13	2.19	0.73
1:O:28:LYS:HB3	1:O:44:GLU:HG3	1.70	0.73
1:s:481:LEU:HD22	1:s:533:LEU:HD13	1.71	0.73
1:3:328:LYS:HB3	1:3:344:GLU:HG3	1.70	0.73
2:V:18:ARG:HD3	2:V:193:THR:HG23	1.71	0.73
2:j:491:PHE:CE2	2:j:514:ALA:HB3	2.24	0.73
2:r:407:TYR:HB2	2:r:497:ILE:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:O	1:A:113:GLU:HG2	1.88	0.73
1:O:10:GLU:O	1:O:14:ARG:HG3	1.89	0.73
1:k:517:ARG:HH21	1:k:523:ARG:HG3	1.53	0.73
1:s:328:LYS:HB3	1:s:344:GLU:HG3	1.71	0.73
2:C:37:THR:HG21	2:C:43:THR:HG23	1.69	0.73
2:L:165:ARG:HA	2:L:213:LEU:HD13	1.71	0.73
1:D:35:TYR:CE1	1:D:38:GLY:O	2.41	0.72
1:I:227:GLY:HA2	1:I:230:LEU:HB2	1.70	0.72
1:W:28:LYS:HB3	1:W:44:GLU:HG3	1.71	0.72
2:J:18:ARG:HD3	2:J:193:THR:HG23	1.71	0.72
1:M:127:VAL:HG11	1:M:215:ALA:HB2	1.70	0.72
1:O:217:ARG:NH2	1:O:223:ARG:HG3	2.04	0.72
2:2:1:OZT:H17	2:2:33:LYS:HZ3	1.52	0.72
1:D:40:LEU:HD13	1:D:212:VAL:HG12	1.69	0.72
1:i:331:VAL:CG1	1:i:333:LEU:HD22	2.19	0.72
2:g:301:OZT:C7	2:g:333:LYS:NZ	2.53	0.72
2:P:38:ASP:C	2:P:38:ASP:OD1	2.30	0.72
2:2:38:ASP:C	2:2:38:ASP:OD1	2.30	0.72
2:g:338:ASP:OD1	2:g:338:ASP:C	2.30	0.72
2:x:338:ASP:C	2:x:338:ASP:OD1	2.30	0.72
2:z:338:ASP:C	2:z:338:ASP:OD1	2.30	0.72
1:d:412:THR:HG23	1:q:415:ALA:HB3	1.71	0.72
1:o:328:LYS:HB3	1:o:344:GLU:HG3	1.70	0.72
1:3:341:PHE:HB3	1:3:353:ILE:HD13	1.70	0.72
1:B:205:VAL:CG2	1:B:206:ALA:H	2.02	0.72
2:c:319:ARG:HG3	2:c:320:SER:N	2.03	0.72
1:U:28:LYS:HB3	1:U:44:GLU:HG3	1.72	0.72
1:u:341:PHE:HB3	1:u:353:ILE:HD13	1.70	0.72
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.72	0.72
1:S:217:ARG:HH21	1:S:223:ARG:HG3	1.50	0.72
1:a:341:PHE:HB3	1:a:353:ILE:HD13	1.71	0.72
1:b:441:ILE:HD12	1:b:441:ILE:N	2.05	0.72
1:y:478:THR:CB	1:y:533:LEU:HD21	2.20	0.72
1:3:530:LEU:HD23	1:3:530:LEU:O	1.90	0.72
2:C:18:ARG:HD3	2:C:193:THR:HG23	1.71	0.72
2:T:37:THR:HG21	2:T:43:THR:CG2	2.19	0.72
1:F:155:VAL:HG12	1:F:160:THR:HG22	1.70	0.72
1:i:530:LEU:O	1:i:530:LEU:HD22	1.90	0.72
1:k:481:LEU:HD23	1:k:533:LEU:HB3	1.71	0.72
1:w:478:THR:CB	1:w:533:LEU:CD2	2.67	0.72
2:R:18:ARG:HD3	2:R:193:THR:HG23	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:331:VAL:HG12	1:i:333:LEU:HD22	1.72	0.71
1:S:231:GLN:HA	1:S:234:LEU:HD12	1.72	0.71
1:Y:41:PHE:HB3	1:Y:53:ILE:HD13	1.72	0.71
1:o:412:THR:HG23	1:u:415:ALA:HB3	1.71	0.71
1:w:340:LEU:CD1	1:w:512:VAL:CG1	2.68	0.71
1:w:478:THR:HB	1:w:533:LEU:CD2	2.11	0.71
1:y:313:MET:HE2	1:y:316:ARG:HD3	1.70	0.71
1:f:530:LEU:O	1:f:534:LEU:HG	1.90	0.71
1:o:313:MET:CE	1:o:313:MET:CA	2.68	0.71
2:L:107:TYR:HB2	2:L:197:ILE:HG22	1.70	0.71
2:Z:165:ARG:HG3	2:Z:213:LEU:HD22	1.71	0.71
1:A:123:CYS:HA	1:A:139:TYR:O	1.91	0.71
1:F:205:VAL:CG2	1:F:206:ALA:H	2.03	0.71
1:W:152:HIS:HB3	1:W:171:TYR:CE2	2.25	0.71
1:Y:177:LEU:HD12	1:Y:177:LEU:O	1.90	0.71
1:i:341:PHE:HB3	1:i:353:ILE:HD13	1.71	0.71
1:D:12:ALA:CB	1:D:13:MET:HE1	2.18	0.71
1:B:38:GLY:HA3	1:B:213:LEU:O	1.90	0.71
1:D:115:ALA:CB	1:K:112:THR:HG23	2.19	0.71
1:M:28:LYS:HB3	1:M:44:GLU:HG3	1.72	0.71
1:O:230:LEU:O	1:O:234:LEU:HD22	1.89	0.71
1:U:173:GLU:O	1:U:174:ASN:HB2	1.89	0.71
1:b:310:GLU:CG	1:b:311:GLN:N	2.53	0.71
1:A:36:ALA:HA	1:A:174:ASN:ND2	2.05	0.71
1:B:35:TYR:CE1	1:B:37:GLY:HA3	2.26	0.71
1:Y:35:TYR:CE1	1:Y:37:GLY:N	2.57	0.71
1:Y:35:TYR:HD1	1:Y:37:GLY:N	1.82	0.71
1:3:478:THR:OG1	1:3:533:LEU:CD1	2.39	0.71
1:f:328:LYS:HB3	1:f:344:GLU:HG3	1.72	0.71
1:1:28:LYS:HB3	1:1:44:GLU:HG3	1.72	0.71
1:b:328:LYS:HB3	1:b:344:GLU:HG3	1.73	0.71
1:u:481:LEU:O	1:u:485:VAL:HG23	1.89	0.71
1:y:328:LYS:HB3	1:y:344:GLU:HG3	1.72	0.71
1:D:219:ARG:NH2	2:E:64:GLU:OE1	2.24	0.71
1:Q:144:ASP:OD1	1:Q:146:SER:CB	2.39	0.71
1:k:328:LYS:HB3	1:k:344:GLU:HG3	1.71	0.71
1:o:356:LEU:HB2	1:o:360:VAL:HG22	1.72	0.71
2:t:338:ASP:C	2:t:338:ASP:OD1	2.30	0.71
1:D:155:VAL:HG12	1:D:160:THR:HG22	1.73	0.70
1:a:412:THR:HG23	1:o:415:ALA:HB3	1.73	0.70
1:a:517:ARG:NH2	1:a:523:ARG:HG3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:509:GLU:OE1	1:d:524:ARG:NH2	2.24	0.70
1:y:335:TYR:HE1	1:y:337:GLY:HA3	1.56	0.70
1:y:355:GLU:HB2	1:y:522:PHE:CG	2.26	0.70
2:J:38:ASP:OD2	2:J:38:ASP:C	2.34	0.70
2:g:337:THR:HG21	2:g:343:THR:HG23	1.74	0.70
1:F:36:ALA:HA	1:F:174:ASN:HD22	1.56	0.70
1:d:348:ARG:HH12	1:k:435:ARG:HH11	0.77	0.70
1:D:232:ALA:O	1:D:233:LEU:C	2.34	0.70
1:b:530:LEU:O	1:b:534:LEU:HG	1.90	0.70
1:w:310:GLU:HG3	1:w:312:ALA:H	1.55	0.70
2:j:319:ARG:HG3	2:j:320:SER:N	2.06	0.70
1:I:48:ARG:HH21	1:S:137:GLU:CG	2.03	0.70
1:S:227:GLY:O	1:S:231:GLN:N	2.23	0.70
1:A:205:VAL:CG2	1:A:206:ALA:H	2.04	0.70
1:F:178:THR:HB	1:F:233:LEU:HD23	1.73	0.70
1:I:130:TYR:CD1	1:I:216:ASN:O	2.44	0.70
1:s:517:ARG:HH21	1:s:523:ARG:HG3	1.54	0.70
2:H:37:THR:HG21	2:H:59:TYR:HD2	1.55	0.70
1:Q:28:LYS:HB3	1:Q:44:GLU:HG3	1.72	0.70
1:W:230:LEU:HD13	1:W:230:LEU:O	1.92	0.70
1:i:311:GLN:NE2	1:i:314:ARG:NH2	2.38	0.70
1:w:311:GLN:CB	1:w:314:ARG:HD2	2.22	0.70
2:G:19:ARG:HG3	2:G:20:SER:N	2.06	0.70
2:R:107:TYR:HB2	2:R:197:ILE:HG22	1.73	0.70
1:M:58:ASP:OD1	1:M:219:ARG:NH1	2.24	0.70
1:o:316:ARG:NH2	1:o:417:PRO:HD3	2.07	0.70
1:o:525:ILE:HG22	1:o:530:LEU:HB2	1.72	0.70
2:R:212:GLU:CD	2:R:215:ARG:HH21	2.00	0.70
1:D:90:ASP:OD1	1:D:93:ASP:CB	2.39	0.70
1:I:15:GLU:OE2	1:S:10:GLU:CD	2.34	0.70
1:K:230:LEU:HG	1:K:234:LEU:HD12	1.73	0.70
1:q:442:THR:HB	1:q:444:ASP:OD1	1.92	0.70
2:2:198:ASP:OD1	2:2:200:ASP:HB2	1.92	0.70
1:D:181:LEU:HD22	1:D:233:LEU:HD22	1.74	0.69
1:Y:14:ARG:NH2	2:c:309:PRO:CB	2.49	0.69
1:q:359:ARG:NH2	1:q:428:ALA:O	2.23	0.69
2:g:487:VAL:HG13	2:v:521:ARG:HB3	1.74	0.69
1:I:31:VAL:CG1	1:I:33:LEU:CD2	2.69	0.69
1:Y:181:LEU:O	1:Y:185:VAL:HG23	1.92	0.69
1:a:315:GLU:CD	1:b:310:GLU:HB3	2.16	0.69
1:q:328:LYS:HB3	1:q:344:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:478:THR:CA	1:y:533:LEU:HD21	2.22	0.69
2:G:37:THR:HG21	2:G:43:THR:HG23	1.74	0.69
2:g:487:VAL:HG13	2:v:521:ARG:HB2	1.73	0.69
1:D:10:GLU:OE2	1:Q:19:LEU:CB	2.35	0.69
1:D:57:TYR:OH	1:D:91:ARG:NH1	2.25	0.69
1:I:165:ASN:HB2	3:I:252:HOH:O	1.91	0.69
1:d:319:LEU:HD21	1:d:416:LYS:HG3	1.71	0.69
2:L:1:OZT:H17	2:L:17:ASP:OD1	1.91	0.69
2:Z:37:THR:HG21	2:Z:59:TYR:HD2	1.56	0.69
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.72	0.69
1:B:229:ALA:O	1:B:232:ALA:HB3	1.93	0.69
1:D:205:VAL:CG2	1:D:206:ALA:H	2.05	0.69
1:Y:28:LYS:HB3	1:Y:44:GLU:HG3	1.73	0.69
1:o:354:SER:CB	1:o:375:ARG:HD2	2.23	0.69
1:D:35:TYR:CE2	1:D:39:VAL:C	2.70	0.69
2:H:186:LEU:HD11	2:H:218:ILE:HD12	1.72	0.69
1:B:217:ARG:HB3	1:B:217:ARG:HH11	1.57	0.69
2:R:129:TRP:HD1	3:R:243:HOH:O	1.74	0.69
2:j:318:ARG:HD3	2:j:493:THR:HG23	1.74	0.69
1:F:217:ARG:HB3	1:F:217:ARG:HH11	1.58	0.69
1:M:41:PHE:HB3	1:M:53:ILE:HD13	1.75	0.69
1:Q:144:ASP:CG	1:Q:146:SER:HG	2.00	0.69
1:S:176:SER:HB2	1:S:179:ASP:CG	2.18	0.69
1:U:41:PHE:HB3	1:U:53:ILE:HD13	1.73	0.69
1:o:335:TYR:CE1	1:o:337:GLY:CA	2.75	0.69
1:w:341:PHE:HB3	1:w:353:ILE:HD13	1.75	0.69
1:y:335:TYR:CE1	1:y:337:GLY:HA3	2.28	0.69
1:y:533:LEU:HD13	1:y:533:LEU:C	2.15	0.69
2:G:18:ARG:HD3	2:G:193:THR:HG23	1.73	0.69
2:C:37:THR:CG2	2:C:43:THR:HG23	2.22	0.69
2:L:19:ARG:HG3	2:L:20:SER:N	2.06	0.69
2:z:514:ALA:O	2:z:518:ILE:HG13	1.93	0.69
1:Q:10:GLU:CB	1:Y:15:GLU:OE2	2.40	0.69
1:m:328:LYS:HB3	1:m:344:GLU:HG3	1.75	0.69
1:B:114:GLN:HG2	1:B:115:ALA:H	1.56	0.68
1:I:165:ASN:CB	3:I:252:HOH:O	2.39	0.68
1:Y:35:TYR:CD2	1:Y:38:GLY:O	2.46	0.68
1:k:428:ALA:HB2	1:k:434:LYS:HB3	1.74	0.68
2:4:301:OZT:C7	2:4:333:LYS:NZ	2.56	0.68
1:M:35:TYR:HD1	1:M:37:GLY:H	1.33	0.68
2:R:14:MET:HE2	2:R:103:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.75	0.68
1:1:181:LEU:HD23	1:1:233:LEU:HB3	1.74	0.68
1:w:311:GLN:HA	1:w:314:ARG:CD	2.22	0.68
1:D:205:VAL:N	1:D:208:LEU:HG	2.08	0.68
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.75	0.68
1:Y:178:THR:CG2	1:Y:179:ASP:OD1	2.42	0.68
1:1:225:ILE:HG21	1:1:233:LEU:HD22	1.74	0.68
2:N:19:ARG:HG3	2:N:20:SER:N	2.08	0.68
2:l:319:ARG:HG3	2:l:320:SER:N	2.09	0.68
1:Q:140:ARG:HH21	1:Q:155:VAL:H	1.40	0.68
1:W:127:VAL:HB	1:W:213:LEU:HD23	1.76	0.68
1:A:127:VAL:HG13	1:A:215:ALA:HB2	1.75	0.68
1:F:152:HIS:HB3	1:F:171:TYR:CE2	2.29	0.68
1:d:526:THR:HG22	1:d:527:GLY:N	2.08	0.68
2:z:337:THR:HG21	2:z:343:THR:HG23	1.73	0.68
1:A:97:ARG:HD2	1:A:97:ARG:C	2.18	0.68
1:D:40:LEU:HD12	1:D:212:VAL:HG12	1.75	0.68
1:1:230:LEU:O	1:1:234:LEU:HG	1.94	0.68
2:4:319:ARG:HG3	2:4:320:SER:N	2.08	0.68
1:W:178:THR:O	1:W:182:ARG:HG3	1.94	0.68
1:k:335:TYR:CD1	1:k:337:GLY:N	2.62	0.68
1:o:341:PHE:HB3	1:o:353:ILE:HD13	1.76	0.68
1:s:481:LEU:HD22	1:s:533:LEU:CD1	2.24	0.68
1:U:10:GLU:HG3	1:U:12:ALA:HB3	1.76	0.68
1:W:178:THR:CG2	1:W:179:ASP:OD1	2.41	0.68
1:a:526:THR:CG2	1:a:527:GLY:N	2.57	0.68
1:u:355:GLU:HB2	1:u:522:PHE:CB	2.24	0.68
1:Q:10:GLU:HB3	1:Y:15:GLU:OE2	1.93	0.67
1:W:176:SER:OG	1:W:179:ASP:CG	2.37	0.67
1:u:356:LEU:HB2	1:u:360:VAL:HG22	1.74	0.67
1:Y:178:THR:OG1	1:Y:233:LEU:HG	1.94	0.67
1:D:35:TYR:CG	1:D:38:GLY:O	2.47	0.67
1:M:129:HIS:HB2	1:M:132:GLU:CD	2.19	0.67
1:W:225:ILE:HG22	1:W:230:LEU:HB2	1.75	0.67
1:o:335:TYR:CD1	1:o:337:GLY:N	2.61	0.67
1:A:152:HIS:HB3	1:A:171:TYR:CE2	2.29	0.67
1:k:450:GLU:HB3	3:k:11:HOH:O	1.93	0.67
1:m:335:TYR:HD1	1:m:337:GLY:H	1.43	0.67
1:m:531:GLN:C	1:m:531:GLN:OE1	2.38	0.67
1:S:227:GLY:O	1:S:230:LEU:HB3	1.95	0.67
1:U:137:GLU:HG2	1:1:48:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:415:ALA:HB3	1:w:412:THR:CG2	2.23	0.67
1:s:335:TYR:HD1	1:s:337:GLY:N	1.85	0.67
1:D:81:PHE:CE2	1:D:85:ARG:HG3	2.30	0.67
1:U:217:ARG:NH2	1:U:223:ARG:HG3	2.10	0.67
1:d:341:PHE:HB3	1:d:353:ILE:HD13	1.75	0.67
1:o:437:GLU:CG	1:u:348:ARG:HH21	2.03	0.67
1:y:313:MET:HE3	1:y:313:MET:CA	2.24	0.67
1:y:335:TYR:HD1	1:y:337:GLY:H	1.40	0.67
2:C:19:ARG:HG3	2:C:20:SER:N	2.08	0.67
2:E:1:OZT:O	2:E:140:GLY:HA3	1.94	0.67
2:c:306:LEU:HD12	2:c:306:LEU:C	2.20	0.67
2:n:318:ARG:HD3	2:n:493:THR:HG23	1.76	0.67
2:v:319:ARG:HG3	2:v:320:SER:N	2.09	0.67
1:M:152:HIS:HB3	1:M:171:TYR:CZ	2.29	0.67
2:T:19:ARG:HG3	2:T:20:SER:N	2.10	0.67
2:c:301:OZT:H17	2:c:317:ASP:OD1	1.95	0.67
2:j:314:MET:HE2	2:j:403:LEU:HD13	1.77	0.67
1:A:229:ALA:O	1:A:233:LEU:HD13	1.95	0.67
1:K:11:GLN:OE1	2:j:509:ARG:HG3	1.94	0.67
1:O:233:LEU:C	1:O:234:LEU:HD13	2.19	0.67
1:Q:230:LEU:HD23	1:Q:230:LEU:C	2.20	0.67
1:i:335:TYR:CE1	1:i:337:GLY:CA	2.75	0.67
2:E:18:ARG:HD3	2:E:193:THR:HG23	1.75	0.67
2:V:209:ARG:O	2:V:213:LEU:HG	1.95	0.67
2:X:37:THR:HG21	2:X:59:TYR:HD2	1.60	0.67
2:r:464:LEU:CD2	2:r:464:LEU:C	2.68	0.67
1:F:54:SER:CB	1:F:75:ARG:HD2	2.25	0.67
1:3:355:GLU:HB2	1:3:522:PHE:CG	2.29	0.67
1:B:165:ASN:HB3	3:B:249:HOH:O	1.95	0.67
2:R:37:THR:CG2	2:R:43:THR:HG23	2.25	0.67
2:V:14:MET:HE2	2:V:103:LEU:HD13	1.78	0.67
1:A:57:TYR:HB3	1:A:60:VAL:CG1	2.24	0.66
1:o:476:SER:HB3	1:o:479:ASP:CG	2.18	0.66
1:w:415:ALA:CB	1:y:412:THR:HG23	2.19	0.66
2:Z:18:ARG:HD3	2:Z:193:THR:HG23	1.75	0.66
2:l:465:ARG:HG3	2:l:513:LEU:HD22	1.76	0.66
1:B:79:ILE:HD13	2:C:68:LYS:HB3	1.75	0.66
1:y:310:GLU:HA	1:y:310:GLU:OE1	1.93	0.66
2:r:464:LEU:O	2:r:464:LEU:HD22	1.96	0.66
1:o:335:TYR:HD1	1:o:337:GLY:H	1.38	0.66
1:A:127:VAL:CG2	1:A:213:LEU:HB3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:TYR:CD1	1:D:38:GLY:O	2.48	0.66
1:F:115:ALA:CB	1:W:112:THR:HG23	2.25	0.66
1:K:35:TYR:HD1	1:K:37:GLY:H	1.44	0.66
1:Q:182:ARG:HH11	1:Q:234:LEU:HD22	1.58	0.66
1:m:335:TYR:CD1	1:m:337:GLY:N	2.63	0.66
1:w:315:GLU:OE2	1:y:310:GLU:CG	2.42	0.66
1:B:113:GLU:HG2	1:B:113:GLU:O	1.95	0.66
1:u:328:LYS:HB3	1:u:344:GLU:HG3	1.77	0.66
2:g:338:ASP:OD1	2:g:340:TYR:N	2.28	0.66
1:a:328:LYS:HB3	1:a:344:GLU:HG3	1.76	0.66
2:R:19:ARG:HG3	2:R:20:SER:N	2.09	0.66
2:V:172:TYR:HE1	2:V:218:ILE:HD12	1.61	0.66
1:S:227:GLY:HA2	1:S:230:LEU:HD13	1.76	0.66
1:i:527:GLY:O	1:i:531:GLN:HB2	1.96	0.66
1:u:340:LEU:HD13	1:u:512:VAL:CG1	2.26	0.66
2:T:38:ASP:OD1	2:T:40:TYR:N	2.28	0.66
2:n:319:ARG:HG3	2:n:320:SER:N	2.10	0.66
2:z:319:ARG:HG3	2:z:320:SER:N	2.09	0.66
1:F:56:LEU:HB2	1:F:60:VAL:HG22	1.78	0.66
1:I:16:ARG:NH2	1:I:111:PHE:O	2.29	0.66
1:d:415:ALA:HB3	1:k:412:THR:HG23	1.78	0.66
2:E:90:ASN:HA	2:E:93:ALA:HB3	1.78	0.66
2:L:37:THR:HG21	2:L:43:THR:HG23	1.78	0.66
1:B:81:PHE:HE2	1:B:98:GLN:HE21	1.43	0.66
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.78	0.66
1:3:479:ASP:O	1:3:483:ILE:HG13	1.96	0.66
2:L:38:ASP:OD1	2:L:40:TYR:N	2.28	0.66
1:U:53:ILE:O	1:U:224:ARG:NH2	2.26	0.66
1:f:517:ARG:NH2	1:f:523:ARG:HG3	2.10	0.66
2:X:18:ARG:HD3	2:X:193:THR:HG23	1.76	0.66
2:x:337:THR:HG21	2:x:343:THR:HG23	1.77	0.66
1:S:214:ASP:OD2	1:S:216:ASN:N	2.30	0.65
1:f:324:ILE:HD11	1:f:420:VAL:O	1.96	0.65
1:i:517:ARG:NH2	1:i:523:ARG:HG3	2.10	0.65
1:D:116:LYS:HB2	1:K:13:MET:HE1	1.78	0.65
1:F:114:GLN:HG2	1:F:115:ALA:H	1.60	0.65
1:b:517:ARG:NH2	1:b:523:ARG:HG3	2.11	0.65
2:N:165:ARG:HD3	3:N:245:HOH:O	1.96	0.65
2:n:465:ARG:HA	2:n:513:LEU:HD13	1.79	0.65
1:Q:182:ARG:NH1	1:Q:234:LEU:CD2	2.58	0.65
1:B:115:ALA:HB3	1:I:112:THR:HG23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:GLN:NE2	1:I:14:ARG:CZ	2.59	0.65
1:K:35:TYR:CD1	1:K:37:GLY:N	2.64	0.65
1:Q:144:ASP:OD1	1:Q:146:SER:HB2	1.94	0.65
1:o:355:GLU:HB2	1:o:522:PHE:CG	2.31	0.65
2:G:37:THR:CG2	2:G:43:THR:HG23	2.26	0.65
2:J:165:ARG:HA	2:J:213:LEU:HD13	1.79	0.65
2:N:38:ASP:OD1	2:N:40:TYR:N	2.30	0.65
2:R:169:GLU:CB	2:R:217:ILE:HD13	2.25	0.65
2:2:18:ARG:HD3	2:2:193:THR:HG23	1.79	0.65
1:A:114:GLN:HG2	1:A:115:ALA:H	1.62	0.65
1:M:14:ARG:HD3	2:j:520:SER:HA	1.78	0.65
2:Z:38:ASP:OD1	2:Z:40:TYR:N	2.30	0.65
2:2:38:ASP:OD1	2:2:40:TYR:N	2.30	0.65
2:j:491:PHE:CE2	2:j:514:ALA:CB	2.80	0.65
1:W:83:ASP:OD2	2:X:65:HIS:HD2	1.79	0.65
1:s:514:ASP:OD2	1:s:516:ASN:N	2.30	0.65
2:H:38:ASP:OD1	2:H:40:TYR:N	2.30	0.65
2:P:38:ASP:OD1	2:P:40:TYR:N	2.30	0.65
2:x:338:ASP:OD1	2:x:340:TYR:N	2.30	0.65
2:J:38:ASP:OD2	2:J:40:TYR:N	2.30	0.65
2:R:212:GLU:OE1	2:R:215:ARG:NH2	2.30	0.65
2:X:38:ASP:OD1	2:X:41:THR:N	2.30	0.65
1:B:51:GLN:HA	1:B:209:GLU:OE2	1.96	0.65
1:Q:182:ARG:HH12	1:Q:234:LEU:CA	2.09	0.65
1:S:10:GLU:HG2	1:S:13:MET:HB2	1.79	0.65
1:W:214:ASP:OD1	1:W:216:ASN:N	2.30	0.65
1:d:335:TYR:CD2	1:d:338:GLY:O	2.50	0.65
1:f:310:GLU:OE1	1:f:311:GLN:N	2.30	0.65
2:E:198:ASP:OD1	2:E:200:ASP:N	2.30	0.65
2:J:19:ARG:HG3	2:J:20:SER:N	2.11	0.65
2:P:164:LEU:HD13	2:P:213:LEU:CD1	2.27	0.65
2:c:464:LEU:HD13	2:c:513:LEU:CD1	2.26	0.65
2:g:319:ARG:HG3	2:g:320:SER:N	2.11	0.65
1:B:10:GLU:C	1:B:12:ALA:N	2.52	0.65
1:K:51:GLN:N	1:K:51:GLN:OE1	2.30	0.65
1:S:10:GLU:HG3	1:S:11:GLN:N	2.10	0.65
1:y:341:PHE:HB3	1:y:353:ILE:HD11	1.79	0.65
2:C:38:ASP:OD1	2:C:40:TYR:N	2.30	0.65
1:D:181:LEU:HD22	1:D:233:LEU:CD2	2.26	0.64
1:O:225:ILE:HG23	1:O:229:ALA:HB1	1.79	0.64
1:Q:35:TYR:HE1	1:Q:37:GLY:C	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:517:ARG:NH1	1:d:520:ARG:O	2.30	0.64
1:y:473:GLU:O	1:y:474:ASN:ND2	2.30	0.64
2:L:8:TYR:CZ	2:L:11:GLY:HA3	2.32	0.64
2:R:212:GLU:N	2:R:212:GLU:OE2	2.30	0.64
1:1:217:ARG:NH2	1:1:223:ARG:HG3	2.13	0.64
1:d:310:GLU:OE1	1:d:312:ALA:N	2.30	0.64
2:P:19:ARG:HG3	2:P:20:SER:N	2.12	0.64
2:R:38:ASP:OD1	2:R:40:TYR:N	2.30	0.64
2:n:338:ASP:OD1	2:n:340:TYR:N	2.30	0.64
1:D:32:ALA:HB3	1:D:154:VAL:HB	1.79	0.64
1:D:214:ASP:OD1	1:D:216:ASN:N	2.30	0.64
1:k:519:ARG:HH22	2:l:364:GLU:CD	2.05	0.64
1:u:344:GLU:HG3	1:u:344:GLU:O	1.96	0.64
1:u:479:ASP:O	1:u:483:ILE:HG13	1.97	0.64
2:V:19:ARG:HG3	2:V:20:SER:N	2.11	0.64
2:Z:19:ARG:HG3	2:Z:20:SER:N	2.12	0.64
2:Z:107:TYR:CE2	2:Z:199:ALA:HA	2.32	0.64
2:h:318:ARG:HD3	2:h:493:THR:HG23	1.79	0.64
2:t:338:ASP:OD1	2:t:340:TYR:N	2.30	0.64
1:K:45:ASN:ND2	1:K:50:LEU:O	2.30	0.64
1:W:40:LEU:CD1	1:W:212:VAL:HG12	2.26	0.64
1:o:335:TYR:CE1	1:o:337:GLY:HA3	2.32	0.64
2:g:301:OZT:H27	2:g:333:LYS:NZ	2.13	0.64
1:K:83:ASP:OD2	2:L:65:HIS:HD2	1.81	0.64
1:o:335:TYR:HE1	1:o:337:GLY:HA3	1.61	0.64
2:G:38:ASP:OD1	2:G:40:TYR:N	2.30	0.64
2:x:337:THR:CG2	2:x:343:THR:HG23	2.27	0.64
1:O:163:ILE:HG23	1:O:187:ALA:O	1.97	0.64
1:S:178:THR:HA	1:S:233:LEU:HD22	1.80	0.64
1:a:526:THR:O	1:a:530:LEU:N	2.30	0.64
1:d:331:VAL:HG12	1:d:333:LEU:CD2	2.28	0.64
1:m:517:ARG:NH2	1:m:523:ARG:CD	2.61	0.64
2:L:12:VAL:HG22	2:L:197:ILE:HB	1.80	0.64
1:B:16:ARG:HH21	1:B:111:PHE:C	2.05	0.64
1:K:182:ARG:CG	3:K:250:HOH:O	2.40	0.64
1:U:58:ASP:OD1	1:U:219:ARG:NH1	2.31	0.64
1:o:463:ILE:HG23	1:o:487:ALA:O	1.98	0.64
1:y:478:THR:OG1	1:y:533:LEU:HD11	1.95	0.64
2:L:38:ASP:OD1	2:L:39:ASP:N	2.31	0.64
2:e:319:ARG:HG3	2:e:320:SER:N	2.13	0.64
2:g:301:OZT:H17	2:g:333:LYS:NZ	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:318:ARG:HD3	2:z:493:THR:HG23	1.80	0.64
1:F:205:VAL:N	1:F:208:LEU:HG	2.13	0.64
2:z:338:ASP:OD1	2:z:340:TYR:N	2.30	0.64
1:A:127:VAL:CG1	1:A:215:ALA:HB2	2.28	0.63
1:Q:31:VAL:HG12	1:Q:33:LEU:HD23	1.80	0.63
1:S:227:GLY:HA2	1:S:230:LEU:CB	2.23	0.63
1:y:313:MET:CE	1:y:316:ARG:HD3	2.27	0.63
2:H:19:ARG:HG3	2:H:20:SER:N	2.12	0.63
1:A:217:ARG:HH11	1:A:223:ARG:CB	2.07	0.63
1:I:13:MET:HE2	1:I:16:ARG:HD3	1.80	0.63
1:U:35:TYR:CE1	1:U:37:GLY:HA3	2.32	0.63
1:Y:14:ARG:HH12	2:c:415:GLN:HB3	1.63	0.63
1:3:335:TYR:CE1	1:3:337:GLY:N	2.66	0.63
2:P:18:ARG:HD3	2:P:193:THR:HG23	1.80	0.63
1:a:526:THR:O	1:a:530:LEU:HB3	1.98	0.63
1:y:478:THR:CB	1:y:533:LEU:CD2	2.69	0.63
1:s:514:ASP:OD1	1:s:516:ASN:HB2	1.98	0.63
1:w:481:LEU:O	1:w:485:VAL:HG23	1.97	0.63
2:E:165:ARG:CG	2:E:213:LEU:CD2	2.69	0.63
2:L:18:ARG:HD3	2:L:193:THR:HG23	1.81	0.63
2:r:314:MET:HE2	2:r:403:LEU:HD13	1.80	0.63
2:r:319:ARG:HG3	2:r:320:SER:N	2.11	0.63
1:S:214:ASP:OD2	1:S:214:ASP:C	2.40	0.63
1:U:10:GLU:CA	1:1:15:GLU:OE2	2.35	0.63
1:u:412:THR:HG22	1:u:413:GLU:CG	2.28	0.63
2:R:169:GLU:HB2	2:R:217:ILE:CD1	2.29	0.63
2:n:338:ASP:OD1	2:n:341:THR:N	2.32	0.63
1:I:11:GLN:HE21	1:I:11:GLN:HA	1.63	0.63
1:A:51:GLN:HA	1:A:209:GLU:OE2	1.97	0.63
1:I:128:ALA:CB	1:I:134:LYS:HB3	2.21	0.63
1:K:59:ARG:NH2	1:K:215:ALA:HA	2.13	0.63
1:w:463:ILE:HD13	1:w:488:LEU:HD23	1.80	0.63
2:N:161:ASP:OD2	2:N:209:ARG:NH1	2.32	0.63
1:k:481:LEU:HD21	1:k:534:LEU:HD11	1.80	0.63
2:H:18:ARG:HD3	2:H:193:THR:HG23	1.80	0.63
1:A:217:ARG:NH1	1:A:223:ARG:CB	2.56	0.63
1:I:35:TYR:CD1	1:I:37:GLY:N	2.67	0.63
1:b:473:GLU:O	1:b:474:ASN:HB2	1.97	0.63
1:w:383:ASP:OD2	2:x:365:HIS:HD2	1.81	0.63
1:y:478:THR:CA	1:y:533:LEU:CD1	2.70	0.63
1:I:35:TYR:CE1	1:I:37:GLY:N	2.66	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:526:THR:O	1:a:530:LEU:HB2	1.97	0.62
1:m:341:PHE:HB3	1:m:353:ILE:HD13	1.80	0.62
1:q:441:ILE:HD12	1:q:441:ILE:N	2.14	0.62
1:A:57:TYR:CB	1:A:60:VAL:CG1	2.77	0.62
1:1:181:LEU:CD2	1:1:233:LEU:HB3	2.29	0.62
1:d:310:GLU:OE1	1:d:311:GLN:N	2.31	0.62
1:m:517:ARG:NH2	1:m:523:ARG:HD3	2.14	0.62
1:q:435:ARG:NH2	1:q:473:GLU:OE2	2.32	0.62
1:u:333:LEU:N	1:u:333:LEU:HD23	2.14	0.62
2:V:217:ILE:CG2	2:V:221:ARG:NH1	2.59	0.62
2:l:318:ARG:HD3	2:l:493:THR:HG23	1.79	0.62
2:v:338:ASP:OD2	2:v:338:ASP:C	2.42	0.62
1:D:112:THR:HG22	1:D:113:GLU:N	2.15	0.62
1:D:114:GLN:HG2	1:D:115:ALA:H	1.63	0.62
1:1:83:ASP:OD2	2:2:65:HIS:HD2	1.82	0.62
1:b:310:GLU:HG3	1:b:311:GLN:H	1.62	0.62
2:C:161:ASP:CG	2:C:209:ARG:HH21	2.08	0.62
2:V:212:GLU:HG3	2:V:213:LEU:H	1.62	0.62
2:g:301:OZT:C7	2:g:333:LYS:HZ1	2.11	0.62
2:v:511:ALA:O	2:v:515:ARG:HG3	2.00	0.62
1:O:159:THR:HB	3:O:251:HOH:O	1.98	0.62
1:Q:53:ILE:O	1:Q:224:ARG:NH2	2.32	0.62
2:C:1:OZT:H17	2:C:17:ASP:OD1	1.99	0.62
2:L:14:MET:CE	2:L:105:ALA:HB2	2.25	0.62
1:S:149:ASP:CG	1:S:149:ASP:O	2.42	0.62
1:Y:55:GLU:HG3	1:Y:222:PHE:HB2	1.82	0.62
1:1:18:GLU:OE1	1:1:21:ARG:NH2	2.30	0.62
1:s:335:TYR:CE1	1:s:338:GLY:N	2.67	0.62
1:3:526:THR:HG22	1:3:527:GLY:N	2.13	0.62
1:A:35:TYR:CE1	1:A:37:GLY:HA3	2.34	0.62
1:I:128:ALA:HB2	1:I:134:LYS:CB	2.21	0.62
1:3:383:ASP:OD2	2:4:365:HIS:HD2	1.83	0.62
2:H:107:TYR:HB2	2:H:197:ILE:CG2	2.27	0.62
1:S:35:TYR:CD2	1:S:38:GLY:O	2.52	0.62
1:Y:179:ASP:OD1	1:Y:179:ASP:N	2.31	0.62
2:N:18:ARG:HD3	2:N:193:THR:HG23	1.81	0.62
2:V:172:TYR:CE1	2:V:218:ILE:HD12	2.33	0.62
2:x:319:ARG:HG3	2:x:320:SER:N	2.15	0.62
1:K:51:GLN:CB	1:K:209:GLU:OE1	2.46	0.62
1:S:83:ASP:OD2	2:T:65:HIS:HD2	1.83	0.62
1:i:310:GLU:O	1:i:314:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:333:LEU:HD23	1:u:333:LEU:H	1.64	0.62
1:M:35:TYR:HE1	1:M:37:GLY:CA	1.87	0.62
1:W:48:ARG:NH2	1:Y:135:ARG:O	2.33	0.62
1:Y:179:ASP:O	1:Y:183:ILE:HG13	1.99	0.62
1:b:310:GLU:OE1	1:b:311:GLN:HA	2.00	0.62
2:Z:37:THR:HG23	2:Z:43:THR:HG23	1.82	0.62
1:A:36:ALA:CA	1:A:174:ASN:HD22	2.11	0.62
1:i:442:THR:OG1	1:i:446:SER:HB2	2.00	0.62
1:m:517:ARG:HH21	1:m:523:ARG:CD	2.13	0.62
2:V:130:ASN:HD22	2:V:131:ILE:N	1.97	0.62
1:I:130:TYR:HD1	1:I:216:ASN:O	1.83	0.61
1:Y:178:THR:HB	1:Y:233:LEU:CG	2.30	0.61
1:l:173:GLU:O	1:l:174:ASN:HB2	1.98	0.61
1:k:341:PHE:HB3	1:k:353:ILE:HD13	1.82	0.61
2:h:319:ARG:HG3	2:h:320:SER:N	2.15	0.61
2:c:337:THR:HG21	2:c:359:TYR:HD2	1.65	0.61
2:z:337:THR:HG21	2:z:359:TYR:HD2	1.64	0.61
2:4:486:LEU:HG	3:4:23:HOH:O	2.00	0.61
1:B:114:GLN:HG2	1:B:115:ALA:N	2.15	0.61
1:a:315:GLU:OE2	1:b:310:GLU:HB3	2.00	0.61
1:d:310:GLU:OE1	1:d:310:GLU:C	2.43	0.61
1:i:313:MET:HE2	1:i:316:ARG:HD3	1.82	0.61
2:J:161:ASP:CG	2:J:209:ARG:HH21	2.08	0.61
1:a:478:THR:HB	1:a:533:LEU:HD21	1.82	0.61
1:s:449:ASP:CG	1:s:449:ASP:O	2.42	0.61
1:y:428:ALA:CB	1:y:434:LYS:HB3	2.25	0.61
2:R:37:THR:HG23	2:R:43:THR:HG23	1.82	0.61
2:X:37:THR:CG2	2:X:43:THR:HG23	2.31	0.61
1:D:28:LYS:HB3	1:D:44:GLU:HG3	1.81	0.61
1:Q:31:VAL:HG12	1:Q:33:LEU:CD2	2.31	0.61
1:Y:173:GLU:CG	1:Y:174:ASN:ND2	2.60	0.61
1:Y:186:ALA:HA	1:Y:189:ARG:HG3	1.81	0.61
1:Y:217:ARG:HH21	1:Y:223:ARG:HG3	1.64	0.61
1:i:389:TYR:HD1	2:c:374:LEU:HD21	1.66	0.61
1:q:335:TYR:CE1	1:q:338:GLY:N	2.68	0.61
1:y:525:ILE:HG22	1:y:530:LEU:HB2	1.82	0.61
2:H:1:OZT:H17	2:H:33:LYS:NZ	2.15	0.61
2:z:472:TYR:HD2	2:z:521:ARG:NH1	1.98	0.61
1:S:177:LEU:HD12	1:S:177:LEU:O	2.00	0.61
1:S:230:LEU:CD2	1:S:231:GLN:N	2.57	0.61
1:i:443:TYR:CD2	1:i:444:ASP:N	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:442:THR:CB	1:q:444:ASP:OD1	2.48	0.61
1:q:526:THR:O	1:q:530:LEU:N	2.30	0.61
2:R:164:LEU:CD1	2:R:213:LEU:HD11	2.30	0.61
2:X:107:TYR:HB2	2:X:197:ILE:HG22	1.82	0.61
1:S:214:ASP:OD2	1:S:215:ALA:N	2.33	0.61
1:s:331:VAL:HG12	1:s:333:LEU:CD2	2.29	0.61
1:y:359:ARG:NH2	1:y:428:ALA:O	2.30	0.61
1:M:112:THR:HG22	1:M:113:GLU:CG	2.27	0.61
1:Y:217:ARG:NH1	1:Y:220:ARG:O	2.34	0.61
1:f:473:GLU:O	1:f:474:ASN:HB2	1.99	0.61
2:E:1:OZT:H17	2:E:17:ASP:OD1	2.00	0.61
1:A:219:ARG:NH2	2:H:64:GLU:OE1	2.33	0.61
1:Q:35:TYR:CD1	1:Q:38:GLY:N	2.50	0.61
1:k:481:LEU:HD22	1:k:533:LEU:HD23	1.83	0.61
1:o:412:THR:HG22	1:o:413:GLU:CG	2.29	0.61
1:y:430:TYR:C	1:y:430:TYR:CD2	2.77	0.61
1:D:56:LEU:HB2	1:D:60:VAL:HG22	1.82	0.61
2:N:14:MET:HE2	2:N:103:LEU:HD13	1.83	0.61
2:T:130:ASN:HD22	2:T:131:ILE:N	1.99	0.61
2:Z:37:THR:HG21	2:Z:43:THR:HG23	1.81	0.61
2:Z:40:TYR:CE1	2:Z:109:ILE:CD1	2.81	0.61
1:Q:173:GLU:O	1:Q:174:ASN:HB2	2.01	0.61
1:l:35:TYR:CE1	1:l:37:GLY:HA3	2.36	0.61
1:q:340:LEU:CD1	1:q:512:VAL:HG12	2.31	0.61
2:V:217:ILE:HG23	2:V:221:ARG:HH11	1.61	0.61
1:D:219:ARG:HH22	1:D:220:ARG:HD3	1.62	0.60
1:I:173:GLU:O	1:I:174:ASN:HB2	2.01	0.60
1:i:333:LEU:N	1:i:333:LEU:HD23	2.16	0.60
1:B:112:THR:HG22	1:B:113:GLU:N	2.16	0.60
1:K:112:THR:HG22	1:K:113:GLU:CG	2.30	0.60
1:Y:178:THR:HB	1:Y:233:LEU:HD11	1.83	0.60
1:d:357:TYR:O	1:d:358:ASP:C	2.42	0.60
1:k:519:ARG:NH2	2:l:364:GLU:OE1	2.34	0.60
1:o:318:GLU:O	1:o:319:LEU:C	2.41	0.60
1:Q:182:ARG:HH12	1:Q:234:LEU:HA	1.64	0.60
1:W:40:LEU:HD13	1:W:212:VAL:HG12	1.82	0.60
1:l:112:THR:HG22	1:l:113:GLU:CG	2.30	0.60
1:f:348:ARG:HH22	1:w:437:GLU:HG3	1.63	0.60
2:H:14:MET:HE2	2:H:103:LEU:HD13	1.83	0.60
2:2:1:OZT:C7	2:2:33:LYS:NZ	2.64	0.60
2:t:314:MET:HE2	2:t:403:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:511:ALA:O	2:x:515:ARG:HG3	2.01	0.60
1:F:229:ALA:O	1:F:233:LEU:HD12	2.01	0.60
1:W:181:LEU:O	1:W:185:VAL:HG23	2.01	0.60
2:E:165:ARG:HB2	2:E:213:LEU:CD2	2.31	0.60
2:R:218:ILE:O	2:R:218:ILE:HG22	2.01	0.60
2:c:318:ARG:HD3	2:c:493:THR:HG23	1.82	0.60
2:c:469:GLU:HA	2:c:517:ILE:HD13	1.83	0.60
1:A:56:LEU:CD1	1:A:62:PHE:HB2	2.31	0.60
1:F:97:ARG:NE	1:M:49:SER:O	2.34	0.60
1:B:54:SER:CB	1:B:75:ARG:HD2	2.32	0.60
1:k:335:TYR:CE1	1:k:337:GLY:N	2.69	0.60
1:s:412:THR:HG22	1:s:413:GLU:CG	2.31	0.60
2:P:164:LEU:HD13	2:P:213:LEU:HD12	1.83	0.60
2:t:318:ARG:HH12	2:t:493:THR:HG21	1.66	0.60
1:B:205:VAL:N	1:B:208:LEU:HG	2.16	0.60
1:F:48:ARG:HH22	1:W:135:ARG:HH11	1.47	0.60
1:Q:35:TYR:CD1	1:Q:37:GLY:CA	2.85	0.60
1:f:335:TYR:CE1	1:f:337:GLY:HA3	2.37	0.60
1:y:368:PHE:HA	1:y:371:PHE:CE2	2.37	0.60
1:y:383:ASP:OD2	2:z:365:HIS:HD2	1.84	0.60
2:V:215:ARG:O	2:V:219:GLU:HG3	2.01	0.60
2:l:494:ALA:HB3	2:l:510:ILE:HD11	1.83	0.60
1:B:176:SER:HB3	1:B:179:ASP:OD2	2.02	0.60
1:D:35:TYR:CE2	1:D:40:LEU:CA	2.78	0.60
1:l:56:LEU:HD13	1:l:99:LEU:HD13	1.84	0.60
1:q:359:ARG:CD	1:q:429:HIS:HA	2.32	0.60
1:u:463:ILE:HG23	1:u:487:ALA:HB1	1.82	0.60
2:R:107:TYR:HB2	2:R:197:ILE:CG2	2.30	0.60
2:t:461:ASP:OD1	2:t:509:ARG:NH2	2.31	0.60
2:z:337:THR:HG23	2:z:343:THR:HG23	1.83	0.60
1:A:205:VAL:N	1:A:208:LEU:HG	2.16	0.60
1:W:163:ILE:HG23	1:W:187:ALA:HB1	1.83	0.60
1:Y:178:THR:HB	1:Y:233:LEU:CD1	2.32	0.60
1:f:526:THR:HG22	1:f:527:GLY:N	2.15	0.60
2:H:1:OZT:C7	2:H:33:LYS:NZ	2.65	0.60
1:a:521:ALA:N	3:a:50:HOH:O	2.35	0.60
1:k:383:ASP:OD2	2:l:365:HIS:HD2	1.84	0.60
1:m:310:GLU:HG2	1:m:312:ALA:H	1.67	0.60
2:h:407:TYR:HB2	2:h:497:ILE:HG22	1.83	0.60
1:B:62:PHE:C	1:B:62:PHE:CD1	2.80	0.59
1:K:178:THR:CB	1:K:233:LEU:HD22	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:14:ARG:NH2	2:c:309:PRO:CG	2.65	0.59
1:u:392:ARG:NH2	3:u:20:HOH:O	2.35	0.59
1:w:348:ARG:HH22	1:y:434:LYS:HG2	1.67	0.59
2:p:314:MET:HE2	2:p:403:LEU:HD13	1.82	0.59
1:D:62:PHE:C	1:D:62:PHE:CD1	2.79	0.59
1:K:210:VAL:HG21	1:K:230:LEU:HD11	1.83	0.59
1:U:35:TYR:HB2	1:U:175:ALA:O	2.01	0.59
1:u:412:THR:CG2	1:3:415:ALA:HB3	2.29	0.59
1:u:463:ILE:CG2	1:u:487:ALA:HB1	2.32	0.59
2:H:38:ASP:OD1	2:H:41:THR:N	2.35	0.59
2:h:465:ARG:HG3	2:h:513:LEU:HD22	1.84	0.59
1:M:92:ARG:HH12	1:M:132:GLU:CD	2.10	0.59
1:Q:163:ILE:HG23	1:Q:187:ALA:O	2.02	0.59
1:U:226:THR:HG22	1:U:227:GLY:N	2.17	0.59
1:3:463:ILE:HG23	1:3:487:ALA:O	2.02	0.59
2:V:37:THR:HG21	2:V:59:TYR:HD2	1.66	0.59
2:t:407:TYR:HB2	2:t:497:ILE:HG22	1.83	0.59
1:s:481:LEU:CD2	1:s:533:LEU:CD1	2.80	0.59
1:w:355:GLU:HB2	1:w:522:PHE:CG	2.37	0.59
2:E:37:THR:HG21	2:E:43:THR:HG23	1.84	0.59
2:c:337:THR:HG21	2:c:343:THR:CG2	2.33	0.59
1:A:54:SER:CB	1:A:75:ARG:HD2	2.32	0.59
1:A:59:ARG:NH2	1:A:217:ARG:O	2.34	0.59
1:s:335:TYR:CE1	1:s:337:GLY:C	2.80	0.59
2:J:37:THR:HG21	2:J:43:THR:CG2	2.31	0.59
2:x:314:MET:HE2	2:x:403:LEU:HD13	1.83	0.59
1:A:112:THR:HG22	1:A:113:GLU:N	2.17	0.59
1:D:54:SER:CB	1:D:75:ARG:HD2	2.33	0.59
1:I:59:ARG:NH2	1:I:128:ALA:O	2.30	0.59
1:U:178:THR:O	1:U:182:ARG:HG3	2.03	0.59
1:W:214:ASP:OD1	1:W:214:ASP:C	2.45	0.59
1:i:473:GLU:O	1:i:474:ASN:HB2	2.02	0.59
1:y:412:THR:HG22	1:y:413:GLU:CG	2.32	0.59
2:X:37:THR:HG21	2:X:43:THR:HG23	1.85	0.59
2:X:40:TYR:CE1	2:X:109:ILE:HD13	2.38	0.59
1:D:227:GLY:O	1:D:230:LEU:HB3	2.01	0.59
1:S:181:LEU:HD23	1:S:233:LEU:HB3	1.83	0.59
1:y:481:LEU:HD21	1:y:530:LEU:CD2	2.32	0.59
1:3:412:THR:HG22	1:3:413:GLU:CG	2.30	0.59
2:N:165:ARG:HA	2:N:213:LEU:HD13	1.83	0.59
1:B:59:ARG:NH2	1:B:128:ALA:O	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:231:GLN:HA	1:S:234:LEU:CD1	2.32	0.59
1:1:35:TYR:HE1	1:1:37:GLY:HA3	1.68	0.59
1:a:510:VAL:HG12	1:a:525:ILE:HD12	1.84	0.59
1:k:315:GLU:OE2	1:m:310:GLU:HG3	2.02	0.59
1:m:412:THR:HG22	1:m:413:GLU:CG	2.30	0.59
2:R:192:PRO:O	2:R:210:ILE:HD13	2.02	0.59
1:Y:14:ARG:HH21	2:c:309:PRO:HG3	1.68	0.59
1:Y:112:THR:HG22	1:Y:113:GLU:CG	2.32	0.59
1:i:526:THR:HG22	1:i:527:GLY:N	2.16	0.59
1:y:481:LEU:HD21	1:y:530:LEU:HD21	1.84	0.59
2:V:37:THR:CG2	2:V:43:THR:HG23	2.33	0.59
1:A:28:LYS:HB3	1:A:44:GLU:HG3	1.85	0.59
1:A:62:PHE:CD1	1:A:62:PHE:C	2.81	0.59
1:B:161:GLU:HB2	1:B:162:PRO:HD3	1.85	0.59
1:B:205:VAL:HG22	1:B:206:ALA:H	1.67	0.59
1:M:152:HIS:CB	1:M:171:TYR:CE2	2.82	0.59
1:O:173:GLU:O	1:O:174:ASN:HB2	2.03	0.59
1:Y:217:ARG:NH2	1:Y:223:ARG:HG3	2.17	0.59
1:1:163:ILE:HG23	1:1:187:ALA:O	2.02	0.59
1:d:412:THR:HG22	1:d:413:GLU:CG	2.31	0.59
2:j:491:PHE:HE2	2:j:514:ALA:HB3	1.67	0.59
1:D:181:LEU:HD23	1:D:233:LEU:HD23	1.83	0.58
1:M:179:ASP:O	1:M:183:ILE:HG13	2.03	0.58
1:f:313:MET:HA	1:f:313:MET:HE3	1.83	0.58
1:o:473:GLU:HG3	1:o:474:ASN:OD1	2.03	0.58
1:s:368:PHE:HA	1:s:371:PHE:CE2	2.38	0.58
2:L:12:VAL:CG1	2:L:118:GLY:CA	2.80	0.58
2:P:14:MET:HE2	2:P:103:LEU:HD13	1.84	0.58
2:V:37:THR:HG21	2:V:43:THR:HG23	1.85	0.58
1:B:152:HIS:HB3	1:B:171:TYR:CE2	2.37	0.58
1:F:165:ASN:HD22	2:r:500:ASP:CG	2.11	0.58
1:Y:14:ARG:NH2	2:c:309:PRO:HG3	2.18	0.58
1:a:315:GLU:CG	1:b:310:GLU:HB3	2.33	0.58
1:s:473:GLU:O	1:s:474:ASN:HB2	2.02	0.58
1:3:328:LYS:HG2	3:3:129:HOH:O	2.03	0.58
2:C:38:ASP:OD1	2:C:39:ASP:N	2.36	0.58
2:V:156:GLN:OE1	2:V:165:ARG:NH2	2.36	0.58
1:3:441:ILE:HD12	1:3:441:ILE:N	2.18	0.58
2:v:430:ASN:HD22	2:v:431:ILE:N	2.01	0.58
1:F:112:THR:HG22	1:F:113:GLU:N	2.18	0.58
1:i:412:THR:HG22	1:i:413:GLU:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:212:GLU:CD	2:R:215:ARG:NH2	2.61	0.58
2:j:430:ASN:HD22	2:j:431:ILE:N	2.00	0.58
2:v:318:ARG:HD3	2:v:493:THR:HG23	1.85	0.58
1:F:36:ALA:HA	1:F:174:ASN:ND2	2.18	0.58
1:I:35:TYR:CZ	1:I:37:GLY:HA3	2.38	0.58
2:E:165:ARG:CB	2:E:213:LEU:CD2	2.82	0.58
2:L:37:THR:HG21	2:L:59:TYR:HD2	1.67	0.58
1:A:97:ARG:HG3	1:O:49:SER:HB2	1.85	0.58
1:I:83:ASP:OD2	2:J:65:HIS:HD2	1.86	0.58
1:W:217:ARG:NH1	1:W:220:ARG:O	2.37	0.58
1:d:340:LEU:HD13	1:d:512:VAL:HG12	1.86	0.58
1:q:526:THR:O	1:q:530:LEU:CB	2.46	0.58
2:E:165:ARG:HB2	2:E:213:LEU:HD21	1.85	0.58
1:B:16:ARG:NH2	1:B:111:PHE:O	2.36	0.58
1:B:205:VAL:CG2	1:B:206:ALA:N	2.67	0.58
1:F:205:VAL:CG2	1:F:206:ALA:N	2.66	0.58
1:d:348:ARG:HE	1:k:437:GLU:HG2	1.68	0.58
1:o:509:GLU:OE1	1:o:524:ARG:NH2	2.36	0.58
2:X:196:ILE:HG13	2:X:205:VAL:CG2	2.33	0.58
1:D:36:ALA:HA	1:D:174:ASN:ND2	2.19	0.58
1:W:112:THR:HG22	1:W:113:GLU:CG	2.31	0.58
1:d:473:GLU:O	1:d:474:ASN:HB2	2.03	0.58
1:u:345:ASN:ND2	1:u:350:LEU:O	2.34	0.58
2:N:37:THR:HG21	2:N:43:THR:HG23	1.86	0.58
1:b:349:SER:HB2	1:i:397:ARG:HG3	1.86	0.58
1:f:313:MET:HA	1:f:313:MET:CE	2.33	0.58
1:s:481:LEU:CD2	1:s:533:LEU:HB3	2.33	0.58
1:w:412:THR:HG22	1:w:413:GLU:CG	2.31	0.58
2:L:12:VAL:HG12	2:L:118:GLY:HA3	1.85	0.58
2:j:491:PHE:HE2	2:j:514:ALA:CB	2.17	0.58
1:M:225:ILE:HG22	1:M:230:LEU:HB2	1.86	0.58
1:f:341:PHE:CB	1:f:353:ILE:HD13	2.34	0.58
1:s:526:THR:O	1:s:530:LEU:HB2	2.04	0.58
1:I:130:TYR:CE1	1:I:216:ASN:O	2.57	0.57
1:U:112:THR:HG22	1:U:113:GLU:CG	2.29	0.57
1:y:339:VAL:C	1:y:512:VAL:HG23	2.27	0.57
1:y:362:PHE:CD1	1:y:362:PHE:C	2.82	0.57
2:J:165:ARG:HG3	2:J:213:LEU:HD22	1.86	0.57
2:g:314:MET:HE2	2:g:403:LEU:HD13	1.84	0.57
1:D:16:ARG:HB3	1:D:117:PRO:HG3	1.84	0.57
1:D:59:ARG:NH2	1:D:215:ALA:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:GLN:HG2	1:D:115:ALA:N	2.19	0.57
1:O:112:THR:HG22	1:O:113:GLU:CG	2.32	0.57
1:Q:35:TYR:CG	1:Q:38:GLY:O	2.57	0.57
1:i:485:VAL:HG21	1:i:534:LEU:HD11	1.85	0.57
1:q:353:ILE:HG21	1:q:511:ALA:HB3	1.87	0.57
1:s:517:ARG:NH2	1:s:523:ARG:CG	2.48	0.57
1:y:357:TYR:CB	1:y:360:VAL:HG22	2.34	0.57
2:X:6:LEU:C	2:X:6:LEU:HD12	2.29	0.57
2:j:464:LEU:HD13	2:j:513:LEU:CD1	2.34	0.57
2:t:318:ARG:HD3	2:t:490:ILE:CG2	2.33	0.57
1:D:40:LEU:CD1	1:D:212:VAL:CG1	2.83	0.57
1:U:225:ILE:HG22	1:U:230:LEU:HB2	1.85	0.57
1:W:53:ILE:HG21	1:W:211:ALA:HB3	1.85	0.57
1:q:473:GLU:O	1:q:474:ASN:HB2	2.04	0.57
1:3:476:SER:HB3	1:3:479:ASP:CG	2.29	0.57
1:3:476:SER:HB3	1:3:479:ASP:OD1	2.04	0.57
2:4:314:MET:HE2	2:4:403:LEU:HD13	1.85	0.57
1:U:56:LEU:HD11	1:U:62:PHE:HB2	1.86	0.57
2:G:161:ASP:CG	2:G:209:ARG:HH21	2.12	0.57
2:J:14:MET:HE2	2:J:103:LEU:HD13	1.86	0.57
2:2:14:MET:HE2	2:2:103:LEU:HD13	1.85	0.57
1:U:163:ILE:HG23	1:U:187:ALA:O	2.04	0.57
1:d:340:LEU:CD1	1:d:512:VAL:HG12	2.33	0.57
1:f:311:GLN:HG2	1:f:314:ARG:HH22	1.65	0.57
2:G:14:MET:HE2	2:G:103:LEU:HD13	1.85	0.57
2:G:37:THR:HG21	2:G:59:TYR:HD2	1.69	0.57
2:X:165:ARG:HG3	2:X:213:LEU:HD22	1.87	0.57
2:g:301:OZT:H27	2:g:333:LYS:HE2	1.86	0.57
1:D:56:LEU:HD13	1:D:99:LEU:HD13	1.87	0.57
1:K:173:GLU:O	1:K:174:ASN:HB2	2.04	0.57
1:Q:137:GLU:HG2	1:Y:48:ARG:HH21	1.69	0.57
1:Y:178:THR:HB	1:Y:233:LEU:HG	1.85	0.57
1:i:444:ASP:CG	1:i:446:SER:HG	2.12	0.57
1:m:530:LEU:O	1:m:530:LEU:HD23	2.04	0.57
2:L:12:VAL:CG1	2:L:118:GLY:HA2	2.35	0.57
2:P:83:LEU:HD13	2:P:123:PHE:CE1	2.40	0.57
1:A:205:VAL:HG22	1:A:206:ALA:H	1.68	0.57
1:Y:141:ILE:HD12	1:Y:141:ILE:N	2.20	0.57
1:q:412:THR:HG22	1:q:413:GLU:CG	2.33	0.57
1:y:435:ARG:NH2	1:y:473:GLU:OE2	2.36	0.57
2:E:198:ASP:OD1	2:E:200:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:210:VAL:CB	1:O:230:LEU:HD21	2.32	0.57
1:Y:173:GLU:O	1:Y:174:ASN:HB2	2.04	0.57
1:Y:178:THR:CB	1:Y:233:LEU:CG	2.82	0.57
1:Y:229:ALA:O	1:Y:233:LEU:N	2.38	0.57
1:a:310:GLU:OE2	1:o:315:GLU:OE2	2.22	0.57
1:m:473:GLU:O	1:m:474:ASN:HB2	2.04	0.57
1:q:442:THR:HG1	1:q:446:SER:HB2	1.68	0.57
2:X:19:ARG:HG3	2:X:20:SER:N	2.18	0.57
2:c:465:ARG:HG3	2:c:513:LEU:HD22	1.87	0.57
2:r:513:LEU:O	2:r:517:ILE:HD12	2.04	0.57
1:A:112:THR:HG23	1:O:115:ALA:HB3	1.87	0.57
1:B:19:LEU:CD2	1:B:20:ALA:N	2.67	0.57
1:B:48:ARG:HH22	1:I:135:ARG:HH11	1.51	0.57
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.40	0.57
1:a:478:THR:HB	1:a:533:LEU:CD2	2.34	0.57
1:k:356:LEU:HD13	1:k:399:LEU:HD13	1.87	0.57
1:m:531:GLN:C	1:m:531:GLN:CD	2.72	0.57
2:H:37:THR:CG2	2:H:43:THR:HG23	2.34	0.57
2:T:18:ARG:HD3	2:T:193:THR:HG23	1.87	0.57
2:j:515:ARG:O	2:j:519:GLU:HG3	2.04	0.57
1:D:12:ALA:CB	1:D:13:MET:CE	2.81	0.57
1:a:526:THR:HG22	1:a:527:GLY:N	2.19	0.57
1:q:340:LEU:HD13	1:q:512:VAL:CG1	2.35	0.57
2:J:130:ASN:HD22	2:J:131:ILE:N	2.03	0.57
2:g:337:THR:HG21	2:g:359:TYR:HD2	1.68	0.57
2:x:337:THR:HG21	2:x:359:TYR:HD2	1.70	0.57
1:d:443:TYR:CD2	1:d:444:ASP:N	2.73	0.56
3:u:20:HOH:O	2:4:410:HIS:HD2	1.83	0.56
1:3:481:LEU:HD23	1:3:533:LEU:HB3	1.85	0.56
1:D:233:LEU:HG	1:D:233:LEU:O	2.05	0.56
1:U:181:LEU:HD23	1:U:233:LEU:HB3	1.87	0.56
1:W:152:HIS:HB3	1:W:171:TYR:HE2	1.67	0.56
1:o:354:SER:HB2	1:o:375:ARG:HD2	1.87	0.56
1:w:335:TYR:HE1	1:w:337:GLY:HA3	1.63	0.56
1:3:478:THR:OG1	1:3:533:LEU:HD12	2.05	0.56
2:C:164:LEU:HD13	2:C:213:LEU:CD1	2.35	0.56
2:R:13:VAL:HG21	2:R:164:LEU:HD23	1.87	0.56
2:t:429:TRP:O	2:4:350:ALA:HB2	2.05	0.56
1:A:59:ARG:NH1	1:A:128:ALA:O	2.34	0.56
1:D:40:LEU:HD13	1:D:212:VAL:CG1	2.35	0.56
1:F:90:ASP:HB2	1:F:93:ASP:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:GLN:HG2	1:F:115:ALA:N	2.20	0.56
1:S:49:SER:HB2	1:1:97:ARG:HG3	1.87	0.56
1:W:173:GLU:HG3	1:W:174:ASN:OD1	2.05	0.56
1:W:173:GLU:O	1:W:174:ASN:HB2	2.04	0.56
1:Y:55:GLU:HB2	1:Y:222:PHE:CB	2.35	0.56
1:1:12:ALA:O	1:1:16:ARG:HG3	2.05	0.56
1:f:463:ILE:HG23	1:f:487:ALA:O	2.05	0.56
1:k:338:GLY:HA3	1:k:513:LEU:O	2.05	0.56
1:q:529:ALA:O	1:q:533:LEU:CD2	2.52	0.56
1:y:357:TYR:N	1:y:360:VAL:HG23	2.20	0.56
2:L:107:TYR:HB2	2:L:197:ILE:CG2	2.35	0.56
2:R:169:GLU:HA	2:R:217:ILE:HD13	1.87	0.56
2:t:430:ASN:HD22	2:t:431:ILE:N	2.03	0.56
2:x:514:ALA:O	2:x:518:ILE:HG13	2.05	0.56
1:Q:112:THR:HG22	1:Q:113:GLU:CG	2.32	0.56
1:u:340:LEU:CD1	1:u:512:VAL:HG12	2.35	0.56
1:B:227:GLY:O	1:B:228:SER:C	2.46	0.56
1:I:112:THR:HG22	1:I:113:GLU:CG	2.33	0.56
1:i:441:ILE:HD12	1:i:441:ILE:N	2.21	0.56
1:q:340:LEU:HD13	1:q:512:VAL:HG12	1.87	0.56
1:y:335:TYR:CE1	1:y:337:GLY:CA	2.88	0.56
1:y:430:TYR:CD1	1:y:518:PRO:HA	2.41	0.56
2:r:407:TYR:HB2	2:r:497:ILE:CG2	2.36	0.56
1:Q:182:ARG:NH1	1:Q:234:LEU:HA	2.20	0.56
1:Q:230:LEU:HA	1:Q:233:LEU:HD12	1.87	0.56
1:o:355:GLU:HG2	1:o:355:GLU:O	2.05	0.56
2:J:214:ALA:O	2:J:218:ILE:HG13	2.05	0.56
2:L:14:MET:HE2	2:L:103:LEU:HD13	1.87	0.56
1:F:51:GLN:HA	1:F:209:GLU:OE2	2.05	0.56
1:k:350:LEU:HD11	1:m:447:ILE:HG12	1.86	0.56
2:c:518:ILE:HG22	2:c:519:GLU:N	2.20	0.56
2:n:331:VAL:HG11	2:n:333:LYS:HE3	1.87	0.56
1:A:40:LEU:HD13	1:A:212:VAL:HG12	1.87	0.56
1:M:217:ARG:NH2	1:M:223:ARG:HG3	2.21	0.56
1:W:163:ILE:CG2	1:W:187:ALA:HB1	2.35	0.56
1:W:230:LEU:C	1:W:230:LEU:CD1	2.79	0.56
1:q:383:ASP:OD2	2:r:365:HIS:HD2	1.89	0.56
2:E:6:LEU:C	2:E:6:LEU:HD12	2.30	0.56
2:Z:37:THR:HG21	2:Z:59:TYR:CD2	2.39	0.56
2:e:314:MET:HE2	2:e:403:LEU:HD13	1.87	0.56
2:e:461:ASP:CG	2:e:509:ARG:NH2	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:301:OZT:H27	2:g:333:LYS:CE	2.36	0.56
2:v:314:MET:HE2	2:v:403:LEU:HD13	1.88	0.56
1:A:214:ASP:OD2	1:A:223:ARG:NH2	2.39	0.56
1:D:36:ALA:HA	1:D:174:ASN:HD22	1.70	0.56
1:D:36:ALA:CA	1:D:174:ASN:HD22	2.19	0.56
1:f:313:MET:HE3	1:f:313:MET:CA	2.36	0.56
2:v:340:TYR:CE1	2:v:409:ILE:HD13	2.41	0.56
1:D:56:LEU:CD1	1:D:62:PHE:HB2	2.36	0.55
1:M:83:ASP:OD2	2:N:65:HIS:HD2	1.88	0.55
1:O:18:GLU:HG3	1:O:22:LYS:HE3	1.87	0.55
1:b:356:LEU:HD13	1:b:399:LEU:HD13	1.88	0.55
1:b:442:THR:OG1	1:b:446:SER:HB2	2.05	0.55
1:k:519:ARG:NH2	2:l:364:GLU:CD	2.64	0.55
2:H:107:TYR:CE2	2:H:199:ALA:CA	2.89	0.55
2:v:513:LEU:HD12	2:v:513:LEU:N	2.21	0.55
1:A:98:GLN:O	1:A:102:VAL:HG23	2.06	0.55
1:A:127:VAL:HG21	1:A:213:LEU:CB	2.34	0.55
1:A:205:VAL:CG2	1:A:206:ALA:N	2.66	0.55
1:D:152:HIS:HB3	1:D:171:TYR:CE2	2.41	0.55
1:l:35:TYR:CD2	1:l:38:GLY:O	2.59	0.55
1:a:313:MET:HE1	1:a:316:ARG:HD3	1.88	0.55
1:b:526:THR:O	1:b:530:LEU:HB2	2.07	0.55
1:A:114:GLN:HG2	1:A:115:ALA:N	2.21	0.55
1:d:335:TYR:CZ	1:d:337:GLY:HA3	2.42	0.55
1:u:526:THR:HG22	1:u:527:GLY:N	2.21	0.55
2:H:76:PHE:CE2	2:H:80:ILE:HD11	2.42	0.55
1:d:331:VAL:HG12	1:d:333:LEU:HD23	1.89	0.55
2:J:38:ASP:OD2	2:J:41:THR:N	2.38	0.55
2:j:301:OZT:O	2:j:440:GLY:HA3	2.06	0.55
1:i:328:LYS:HB3	1:i:344:GLU:HG3	1.88	0.55
1:q:442:THR:OG1	1:q:446:SER:HB2	2.06	0.55
1:w:368:PHE:HA	1:w:371:PHE:CE2	2.41	0.55
2:X:1:OZT:C7	2:X:33:LYS:NZ	2.69	0.55
2:v:391:LEU:C	2:v:393:ALA:H	2.14	0.55
2:4:318:ARG:HD3	2:4:493:THR:HG23	1.89	0.55
1:A:161:GLU:HB2	1:A:162:PRO:HD3	1.89	0.55
1:D:35:TYR:OH	1:D:212:VAL:CB	2.55	0.55
1:D:152:HIS:HB3	1:D:171:TYR:CZ	2.42	0.55
1:F:35:TYR:CE2	1:F:40:LEU:HB2	2.42	0.55
1:F:98:GLN:O	1:F:102:VAL:HG23	2.06	0.55
1:F:176:SER:HB3	1:F:179:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:368:PHE:HA	1:i:371:PHE:CE2	2.42	0.55
1:k:435:ARG:NH2	1:k:451:PRO:CB	2.68	0.55
1:q:405:GLN:HG2	1:y:369:ASN:HB2	1.88	0.55
2:H:37:THR:HG21	2:H:43:THR:HG23	1.89	0.55
2:H:186:LEU:HD11	2:H:218:ILE:CD1	2.36	0.55
2:G:130:ASN:HD22	2:G:131:ILE:N	2.05	0.55
2:N:45:ILE:CD1	3:N:243:HOH:O	2.55	0.55
2:N:130:ASN:HD22	2:N:131:ILE:N	2.05	0.55
2:c:358:LEU:HD12	2:c:358:LEU:O	2.07	0.55
2:l:514:ALA:O	2:l:518:ILE:HG13	2.07	0.55
1:S:112:THR:HG22	1:S:113:GLU:CG	2.34	0.55
1:k:519:ARG:NH2	2:l:364:GLU:OE2	2.30	0.55
1:k:527:GLY:C	1:k:529:ALA:N	2.60	0.55
1:m:368:PHE:HA	1:m:371:PHE:CE2	2.42	0.55
1:o:479:ASP:OD1	1:o:479:ASP:N	2.30	0.55
2:X:1:OZT:H27	2:X:33:LYS:NZ	2.21	0.55
2:h:430:ASN:HD22	2:h:431:ILE:N	2.04	0.55
2:n:335:TYR:CZ	2:n:353:VAL:HG13	2.42	0.55
2:n:430:ASN:HD22	2:n:431:ILE:N	2.04	0.55
2:p:465:ARG:HA	2:p:513:LEU:HD13	1.88	0.55
1:B:83:ASP:OD2	2:C:65:HIS:HD2	1.89	0.55
1:B:182:ARG:HG2	1:B:182:ARG:HH11	1.71	0.55
1:d:517:ARG:NH2	1:d:523:ARG:HG3	2.22	0.55
1:i:527:GLY:O	1:i:531:GLN:N	2.30	0.55
1:s:312:ALA:O	1:s:316:ARG:HG3	2.07	0.55
2:R:130:ASN:HD22	2:R:131:ILE:N	2.05	0.55
1:k:331:VAL:HG12	1:k:333:LEU:HD23	1.88	0.55
2:G:185:ASP:OD1	2:G:188:ARG:HB2	2.07	0.55
1:B:35:TYR:CE1	1:B:37:GLY:CA	2.90	0.55
1:F:159:THR:CG2	2:r:459:ASP:OD2	2.53	0.55
1:W:41:PHE:CB	1:W:53:ILE:HD13	2.36	0.55
1:l:41:PHE:CB	1:l:53:ILE:HD13	2.36	0.55
2:n:306:LEU:C	2:n:306:LEU:HD12	2.32	0.55
1:B:69:ASN:HB2	1:I:105:GLN:HG2	1.89	0.54
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.42	0.54
1:b:362:PHE:CD1	1:b:362:PHE:C	2.85	0.54
1:k:481:LEU:HD21	1:k:534:LEU:CD1	2.37	0.54
1:u:481:LEU:CD2	1:u:533:LEU:HG	2.37	0.54
2:J:169:GLU:HA	2:J:217:ILE:HD13	1.89	0.54
1:d:437:GLU:CG	1:q:348:ARG:NH2	2.67	0.54
1:u:368:PHE:HA	1:u:371:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:172:TYR:CE1	2:V:218:ILE:HD11	2.42	0.54
2:X:215:ARG:O	2:X:219:GLU:HG3	2.06	0.54
2:Z:37:THR:CG2	2:Z:59:TYR:HD2	2.19	0.54
2:j:495:VAL:HG22	2:j:504:ASP:OD1	2.07	0.54
2:j:507:GLU:O	2:j:507:GLU:HG2	2.07	0.54
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.90	0.54
1:d:354:SER:CB	1:d:375:ARG:HD2	2.37	0.54
1:s:335:TYR:CE1	1:s:337:GLY:N	2.73	0.54
1:s:349:SER:HB2	1:3:397:ARG:HG3	1.88	0.54
1:u:481:LEU:HD22	1:u:533:LEU:CG	2.37	0.54
2:V:209:ARG:O	2:V:212:GLU:HG3	2.06	0.54
1:A:59:ARG:CD	1:A:129:HIS:HA	2.30	0.54
1:D:205:VAL:CG2	1:D:206:ALA:N	2.69	0.54
1:K:79:ILE:HD12	2:L:69:LEU:HD23	1.89	0.54
1:Y:178:THR:HG23	1:Y:179:ASP:N	2.23	0.54
1:d:362:PHE:CD1	1:d:362:PHE:C	2.84	0.54
1:k:412:THR:HG22	1:k:413:GLU:CG	2.37	0.54
2:H:132:GLU:HG3	2:H:137:GLN:HB2	1.90	0.54
2:j:513:LEU:O	2:j:514:ALA:C	2.51	0.54
1:F:62:PHE:CD1	1:F:62:PHE:C	2.85	0.54
1:a:341:PHE:CB	1:a:353:ILE:HD13	2.38	0.54
2:H:1:OZT:H27	2:H:33:LYS:HE2	1.89	0.54
2:C:198:ASP:OD1	2:C:200:ASP:N	2.30	0.54
2:L:37:THR:HG23	2:L:43:THR:HG23	1.88	0.54
1:W:54:SER:CB	1:W:75:ARG:HD2	2.38	0.54
1:o:368:PHE:HA	1:o:371:PHE:CE2	2.42	0.54
1:y:335:TYR:CD1	1:y:337:GLY:N	2.75	0.54
2:l:383:LEU:HD13	2:l:423:PHE:CE1	2.43	0.54
2:p:465:ARG:HG3	2:p:513:LEU:HD22	1.88	0.54
2:4:514:ALA:O	2:4:518:ILE:HG13	2.08	0.54
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.43	0.54
1:W:47:SER:HB2	1:Y:149:ASP:OD1	2.08	0.54
1:s:315:GLU:OE2	1:3:310:GLU:CG	2.40	0.54
1:w:474:ASN:N	1:w:474:ASN:HD22	2.06	0.54
2:g:337:THR:HG23	2:g:343:THR:HG23	1.88	0.54
1:F:205:VAL:HG23	1:F:206:ALA:H	1.72	0.54
1:I:138:LEU:HD12	1:I:138:LEU:N	2.23	0.54
1:M:54:SER:CB	1:M:75:ARG:HD2	2.38	0.54
1:k:335:TYR:HD1	1:k:337:GLY:H	1.53	0.54
1:3:530:LEU:C	1:3:530:LEU:CD2	2.81	0.54
2:V:209:ARG:C	2:V:212:GLU:HG2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:314:MET:HE1	2:x:403:LEU:O	2.08	0.54
2:x:318:ARG:HD3	2:x:493:THR:HG23	1.90	0.54
2:4:301:OZT:C7	2:4:333:LYS:HZ1	2.19	0.54
1:I:11:GLN:HE21	1:I:14:ARG:NH2	2.02	0.54
1:M:127:VAL:HG23	1:M:213:LEU:HD23	1.90	0.54
1:d:463:ILE:HG23	1:d:487:ALA:O	2.08	0.54
1:f:379:ILE:HG23	2:g:368:LYS:HE3	1.89	0.54
1:k:368:PHE:HA	1:k:371:PHE:CE2	2.43	0.54
1:k:526:THR:HG22	1:k:526:THR:O	2.08	0.54
1:q:335:TYR:CE1	1:q:337:GLY:C	2.86	0.54
1:q:341:PHE:CB	1:q:353:ILE:HD13	2.37	0.54
1:w:463:ILE:HG23	1:w:487:ALA:C	2.32	0.54
2:n:314:MET:HE1	2:n:403:LEU:O	2.08	0.54
2:v:513:LEU:CD1	2:v:513:LEU:N	2.71	0.54
2:z:407:TYR:HB2	2:z:497:ILE:HG22	1.89	0.54
1:F:182:ARG:HH12	1:F:234:LEU:C	2.16	0.54
1:o:340:LEU:HD13	1:o:512:VAL:HG12	1.90	0.54
1:s:341:PHE:CB	1:s:353:ILE:HD13	2.35	0.54
2:J:83:LEU:HD13	2:J:123:PHE:CE1	2.43	0.54
2:P:37:THR:HG21	2:P:59:TYR:HD2	1.73	0.54
2:X:14:MET:HE2	2:X:103:LEU:HD13	1.90	0.54
2:n:314:MET:HE2	2:n:403:LEU:HD13	1.90	0.54
1:D:33:LEU:N	1:D:33:LEU:HD23	2.23	0.53
1:K:176:SER:O	1:K:177:LEU:C	2.51	0.53
1:S:41:PHE:CB	1:S:53:ILE:HD13	2.38	0.53
1:q:333:LEU:HD23	1:q:333:LEU:C	2.28	0.53
2:X:1:OZT:H27	2:X:33:LYS:HZ1	1.74	0.53
2:Z:130:ASN:HD22	2:Z:131:ILE:N	2.06	0.53
2:2:1:OZT:H27	2:2:33:LYS:HE2	1.89	0.53
2:c:464:LEU:HD13	2:c:513:LEU:HD11	1.89	0.53
2:g:301:OZT:H17	2:g:333:LYS:HZ3	1.73	0.53
1:F:79:ILE:HD13	2:G:68:LYS:HB3	1.90	0.53
1:K:115:ALA:HB3	1:M:112:THR:HG23	1.91	0.53
1:o:339:VAL:HG12	1:o:340:LEU:N	2.23	0.53
1:o:517:ARG:HH22	1:o:523:ARG:HG3	1.72	0.53
1:y:357:TYR:HB3	1:y:360:VAL:HG22	1.90	0.53
1:y:463:ILE:HG23	1:y:487:ALA:O	2.07	0.53
2:C:83:LEU:HD13	2:C:123:PHE:CZ	2.43	0.53
2:Z:83:LEU:HD13	2:Z:123:PHE:CE1	2.42	0.53
2:l:465:ARG:HA	2:l:513:LEU:HD13	1.89	0.53
2:n:407:TYR:HB2	2:n:497:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:163:ILE:HG23	1:M:187:ALA:O	2.09	0.53
1:O:225:ILE:HG23	1:O:229:ALA:CB	2.37	0.53
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.43	0.53
1:Y:18:GLU:OE2	2:c:414:PRO:HD2	2.08	0.53
1:q:335:TYR:CG	1:q:338:GLY:O	2.62	0.53
1:s:349:SER:HB2	1:3:397:ARG:CG	2.38	0.53
2:J:145:PHE:CE1	2:Z:144:LEU:HD13	2.43	0.53
1:D:11:GLN:OE1	1:D:11:GLN:CA	2.52	0.53
1:D:127:VAL:HG21	1:D:213:LEU:HB3	1.90	0.53
1:1:128:ALA:HB2	1:1:134:LYS:HB3	1.88	0.53
1:o:479:ASP:O	1:o:483:ILE:HG13	2.08	0.53
1:q:368:PHE:HA	1:q:371:PHE:CE2	2.44	0.53
1:3:333:LEU:N	1:3:333:LEU:HD23	2.24	0.53
2:C:14:MET:HE2	2:C:103:LEU:HD13	1.89	0.53
2:X:31:VAL:HG11	2:X:33:LYS:HE3	1.91	0.53
2:2:35:TYR:CZ	2:2:53:VAL:HG13	2.44	0.53
2:c:383:LEU:HD13	2:c:423:PHE:CE1	2.44	0.53
2:z:314:MET:HE2	2:z:403:LEU:HD13	1.90	0.53
1:1:10:GLU:O	1:1:14:ARG:HG3	2.08	0.53
1:f:412:THR:HG22	1:f:413:GLU:CG	2.35	0.53
2:X:164:LEU:HD13	2:X:213:LEU:CD1	2.39	0.53
2:j:331:VAL:HG11	2:j:333:LYS:HE3	1.90	0.53
1:S:57:TYR:OH	1:S:86:GLY:HA3	2.08	0.53
1:W:68:PHE:HA	1:W:71:PHE:CE2	2.43	0.53
1:d:526:THR:HG22	1:d:527:GLY:H	1.72	0.53
1:s:441:ILE:N	1:s:441:ILE:HD12	2.23	0.53
1:s:481:LEU:HD23	1:s:533:LEU:HD13	1.91	0.53
2:r:348:THR:OG1	2:r:351:VAL:HG23	2.08	0.53
2:v:338:ASP:OD2	2:v:340:TYR:N	2.42	0.53
2:z:444:LEU:HB2	3:z:115:HOH:O	2.08	0.53
1:s:397:ARG:C	1:s:397:ARG:HD2	2.34	0.53
2:C:83:LEU:HD13	2:C:123:PHE:CE1	2.43	0.53
2:N:45:ILE:HD12	2:N:45:ILE:N	2.24	0.53
2:t:331:VAL:CG1	2:t:333:LYS:HE3	2.39	0.53
1:S:48:ARG:HH21	1:1:137:GLU:CG	2.18	0.53
1:1:54:SER:CB	1:1:75:ARG:HD2	2.39	0.53
1:d:318:GLU:OE1	1:d:318:GLU:HA	2.07	0.53
1:d:452:HIS:HB3	1:d:471:TYR:CE2	2.44	0.53
1:q:517:ARG:NH2	1:q:523:ARG:HG3	2.23	0.53
1:w:478:THR:OG1	1:w:533:LEU:CD2	2.56	0.53
2:E:130:ASN:HD22	2:E:131:ILE:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:430:ASN:HD22	2:l:431:ILE:N	2.07	0.53
2:p:318:ARG:HD3	2:p:493:THR:HG23	1.89	0.53
2:z:384:ALA:O	2:z:388:ARG:HG3	2.07	0.53
1:D:60:VAL:HG21	1:D:99:LEU:HD12	1.91	0.53
1:M:152:HIS:CD2	1:M:171:TYR:HE2	2.26	0.53
1:Q:161:GLU:HB3	1:i:474:ASN:HB3	1.90	0.53
1:Y:83:ASP:OD2	2:Z:65:HIS:HD2	1.92	0.53
1:a:315:GLU:HG2	1:b:310:GLU:HB3	1.90	0.53
1:d:341:PHE:CB	1:d:353:ILE:HD13	2.39	0.53
1:d:355:GLU:OE2	1:d:520:ARG:HD2	2.09	0.53
1:k:527:GLY:C	1:k:529:ALA:H	2.17	0.53
2:R:169:GLU:HB2	2:R:217:ILE:HD13	1.90	0.53
2:t:314:MET:CE	2:t:405:ALA:HB2	2.32	0.53
1:S:176:SER:HB2	1:S:179:ASP:OD2	2.08	0.53
1:w:481:LEU:HD23	1:w:533:LEU:HD13	1.90	0.53
1:y:428:ALA:HB2	1:y:434:LYS:CB	2.28	0.53
1:y:473:GLU:O	1:y:474:ASN:CB	2.55	0.53
2:J:168:VAL:HG12	2:J:217:ILE:HD12	1.90	0.53
2:P:37:THR:HG21	2:P:43:THR:CG2	2.35	0.53
2:2:130:ASN:HD22	2:2:131:ILE:N	2.07	0.53
2:4:383:LEU:HD13	2:4:423:PHE:CZ	2.44	0.53
1:Q:217:ARG:HH21	1:Q:223:ARG:HG3	1.73	0.52
1:W:141:ILE:HD12	1:W:141:ILE:N	2.24	0.52
1:W:184:ALA:O	1:W:188:LEU:HG	2.09	0.52
1:f:354:SER:CB	1:f:375:ARG:HD2	2.39	0.52
1:k:355:GLU:OE2	1:k:520:ARG:HD2	2.08	0.52
1:k:528:SER:O	1:k:531:GLN:CB	2.57	0.52
1:y:316:ARG:NH2	1:y:417:PRO:HD3	2.24	0.52
2:C:132:GLU:HG3	2:C:137:GLN:HB2	1.91	0.52
2:J:213:LEU:O	2:J:217:ILE:HG13	2.10	0.52
2:L:31:VAL:HG11	2:L:33:LYS:HE3	1.91	0.52
2:c:337:THR:HG23	2:c:343:THR:HG23	1.88	0.52
2:j:517:ILE:O	2:j:521:ARG:HG3	2.09	0.52
1:A:130:TYR:CE1	1:A:216:ASN:O	2.61	0.52
1:A:176:SER:OG	1:A:178:THR:HG22	2.09	0.52
1:U:56:LEU:CD1	1:U:62:PHE:HB2	2.40	0.52
1:U:226:THR:CG2	1:U:227:GLY:N	2.72	0.52
1:1:152:HIS:HB3	1:1:171:TYR:CE2	2.44	0.52
1:b:527:GLY:O	1:b:531:GLN:CG	2.53	0.52
2:P:1:OZT:H17	2:P:33:LYS:NZ	2.23	0.52
2:P:132:GLU:HG3	2:P:137:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:169:GLU:HB2	2:R:217:ILE:HD11	1.90	0.52
2:j:407:TYR:HB2	2:j:497:ILE:HG22	1.91	0.52
2:r:457:VAL:HG22	2:r:463:GLY:HA2	1.91	0.52
1:D:35:TYR:OH	1:D:212:VAL:CG1	2.57	0.52
1:D:161:GLU:HB2	1:D:162:PRO:HD3	1.91	0.52
1:D:223:ARG:HG2	1:D:224:ARG:N	2.24	0.52
1:F:205:VAL:HG23	1:F:206:ALA:N	2.24	0.52
1:F:205:VAL:HG22	1:F:206:ALA:H	1.73	0.52
1:U:128:ALA:HB2	1:U:134:LYS:HB3	1.91	0.52
1:Y:177:LEU:HG	1:Y:233:LEU:CD2	2.39	0.52
1:f:415:ALA:CB	1:w:412:THR:HG23	2.30	0.52
1:o:335:TYR:CE1	1:o:337:GLY:N	2.78	0.52
1:o:339:VAL:CG1	1:o:340:LEU:N	2.72	0.52
1:y:452:HIS:HB3	1:y:471:TYR:CE2	2.44	0.52
2:c:314:MET:HE2	2:c:403:LEU:HD13	1.91	0.52
2:t:517:ILE:O	2:t:521:ARG:HG3	2.09	0.52
2:z:430:ASN:HD22	2:z:431:ILE:N	2.07	0.52
1:B:207:SER:O	1:B:208:LEU:HD23	2.09	0.52
1:D:51:GLN:HA	1:D:209:GLU:OE2	2.09	0.52
1:K:49:SER:CB	1:M:139:TYR:OH	2.56	0.52
1:M:17:SER:HA	1:M:143:TYR:HE2	1.75	0.52
1:b:314:ARG:HG3	1:b:314:ARG:HH11	1.74	0.52
1:k:333:LEU:HD21	1:k:484:ALA:HB2	1.91	0.52
2:T:164:LEU:HD13	2:T:213:LEU:CD1	2.39	0.52
2:z:337:THR:HG21	2:z:343:THR:CG2	2.40	0.52
1:D:153:PHE:CD1	1:D:167:LEU:CD1	2.93	0.52
1:I:15:GLU:OE2	1:S:10:GLU:OE2	2.27	0.52
1:K:69:ASN:HB3	1:M:104:ALA:HB1	1.91	0.52
1:S:178:THR:HB	1:S:233:LEU:CD2	2.39	0.52
1:Y:35:TYR:CZ	1:Y:38:GLY:N	2.77	0.52
1:d:356:LEU:HB2	1:d:360:VAL:HG22	1.90	0.52
1:y:478:THR:HG1	1:y:533:LEU:HD13	1.75	0.52
2:E:83:LEU:HD13	2:E:123:PHE:CE1	2.44	0.52
2:V:65:HIS:CE1	2:V:69:LEU:HD11	2.43	0.52
2:V:164:LEU:HD13	2:V:213:LEU:HD11	1.91	0.52
2:2:107:TYR:CE1	2:2:117:ALA:HB3	2.45	0.52
2:z:340:TYR:HD2	2:z:407:TYR:HB3	1.74	0.52
1:K:12:ALA:HB2	2:j:512:GLU:OE1	2.10	0.52
1:i:362:PHE:CD1	1:i:362:PHE:C	2.88	0.52
1:o:311:GLN:HA	1:o:314:ARG:HD2	1.92	0.52
2:E:1:OZT:H27	2:E:33:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:301:OZT:H27	2:g:333:LYS:HZ1	1.71	0.52
2:x:434:GLU:OE2	2:z:329:ARG:NH1	2.43	0.52
1:K:171:TYR:C	1:K:171:TYR:CD2	2.88	0.52
1:W:55:GLU:OE2	1:W:220:ARG:HD2	2.10	0.52
1:d:526:THR:CG2	1:d:527:GLY:N	2.73	0.52
1:o:482:ARG:NH2	1:o:534:LEU:C	2.68	0.52
2:H:1:OZT:H17	2:H:33:LYS:HZ3	1.74	0.52
2:R:83:LEU:HD13	2:R:123:PHE:CE1	2.45	0.52
2:R:169:GLU:CA	2:R:217:ILE:HD13	2.39	0.52
2:T:83:LEU:HD13	2:T:123:PHE:CZ	2.44	0.52
2:e:430:ASN:HD22	2:e:431:ILE:N	2.08	0.52
1:D:205:VAL:HG23	1:D:206:ALA:H	1.74	0.52
1:M:134:LYS:HG2	1:M:135:ARG:N	2.24	0.52
1:U:22:LYS:O	1:U:26:ARG:HG3	2.10	0.52
1:d:412:THR:CG2	1:q:415:ALA:HB3	2.39	0.52
1:i:335:TYR:CD1	1:i:337:GLY:N	2.76	0.52
1:q:510:VAL:HG12	1:q:525:ILE:HD12	1.91	0.52
1:s:335:TYR:CD1	1:s:337:GLY:CA	2.90	0.52
1:u:441:ILE:N	1:u:441:ILE:HD12	2.25	0.52
2:R:39:ASP:N	2:R:39:ASP:OD1	2.42	0.52
2:T:83:LEU:HD13	2:T:123:PHE:CE1	2.44	0.52
2:l:383:LEU:HD13	2:l:423:PHE:CZ	2.44	0.52
2:p:464:LEU:HD13	2:p:513:LEU:HD12	1.90	0.52
1:B:28:LYS:HB3	1:B:44:GLU:HG3	1.92	0.52
1:I:40:LEU:HD12	1:I:212:VAL:HG12	1.92	0.52
1:M:68:PHE:HA	1:M:71:PHE:CE2	2.45	0.52
1:U:112:THR:CG2	1:l:115:ALA:HB3	2.28	0.52
1:b:412:THR:HG22	1:b:413:GLU:CG	2.36	0.52
1:d:529:ALA:O	1:d:533:LEU:HD12	2.07	0.52
1:k:528:SER:O	1:k:531:GLN:HB3	2.10	0.52
1:q:333:LEU:CD2	1:q:333:LEU:N	2.73	0.52
1:s:526:THR:CG2	1:s:527:GLY:N	2.34	0.52
1:y:441:ILE:HD12	1:y:441:ILE:N	2.25	0.52
2:J:198:ASP:OD2	2:J:200:ASP:HB2	2.10	0.52
2:j:349:ALA:O	2:j:353:VAL:HG23	2.10	0.52
2:z:331:VAL:HG11	2:z:333:LYS:HE3	1.92	0.52
1:D:13:MET:CE	1:D:13:MET:CA	2.86	0.52
1:D:167:LEU:O	1:D:168:LYS:C	2.53	0.52
1:f:348:ARG:NH2	1:w:437:GLU:OE2	2.42	0.52
1:m:357:TYR:OH	1:m:386:GLY:HA3	2.10	0.52
2:H:58:LEU:HD12	2:H:58:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:129:TRP:O	2:2:50:ALA:HB2	2.10	0.52
2:Z:14:MET:HE2	2:Z:103:LEU:HD13	1.92	0.52
2:x:429:TRP:O	2:z:350:ALA:HB2	2.10	0.52
1:B:48:ARG:HH22	1:I:135:ARG:NH1	2.07	0.51
1:f:452:HIS:HB3	1:f:471:TYR:CE2	2.45	0.51
1:f:526:THR:CG2	1:f:527:GLY:N	2.73	0.51
2:E:31:VAL:HG11	2:E:33:LYS:HE3	1.91	0.51
2:R:169:GLU:CB	2:R:217:ILE:CD1	2.88	0.51
1:K:163:ILE:HG23	1:K:187:ALA:O	2.09	0.51
1:Y:68:PHE:HA	1:Y:71:PHE:CE2	2.46	0.51
2:n:513:LEU:O	2:n:514:ALA:C	2.50	0.51
2:x:486:LEU:HD11	2:x:518:ILE:HD12	1.91	0.51
1:B:167:LEU:O	1:B:168:LYS:C	2.54	0.51
1:F:56:LEU:HD13	1:F:99:LEU:HD13	1.92	0.51
1:a:441:ILE:HD12	1:a:441:ILE:N	2.25	0.51
1:s:362:PHE:C	1:s:362:PHE:CD1	2.88	0.51
1:y:356:LEU:HB2	1:y:360:VAL:CG2	2.36	0.51
2:J:83:LEU:HD13	2:J:123:PHE:CZ	2.45	0.51
2:T:31:VAL:HG11	2:T:33:LYS:HE3	1.92	0.51
2:c:306:LEU:HD12	2:c:306:LEU:O	2.09	0.51
2:l:512:GLU:HG2	2:l:513:LEU:N	2.25	0.51
1:D:97:ARG:HD2	1:D:97:ARG:O	2.10	0.51
1:D:182:ARG:HG2	1:D:182:ARG:HH11	1.76	0.51
1:I:182:ARG:HH12	1:I:234:LEU:C	2.17	0.51
1:a:330:VAL:HG22	1:a:343:ALA:HB1	1.92	0.51
1:d:368:PHE:HA	1:d:371:PHE:CE2	2.46	0.51
2:4:306:LEU:C	2:4:306:LEU:HD12	2.36	0.51
1:O:56:LEU:HD13	1:O:99:LEU:HD13	1.92	0.51
1:S:173:GLU:CD	1:S:174:ASN:OD1	2.53	0.51
1:i:526:THR:O	1:i:530:LEU:CB	2.59	0.51
2:J:13:VAL:HG21	2:J:164:LEU:HD23	1.93	0.51
2:P:38:ASP:OD1	2:P:39:ASP:N	2.42	0.51
1:D:163:ILE:HG23	1:D:187:ALA:O	2.10	0.51
1:F:57:TYR:HB3	1:F:60:VAL:HG13	1.93	0.51
1:K:41:PHE:CB	1:K:53:ILE:HD13	2.40	0.51
2:V:38:ASP:C	2:V:38:ASP:OD1	2.54	0.51
2:p:430:ASN:HD22	2:p:431:ILE:N	2.08	0.51
2:t:513:LEU:O	2:t:517:ILE:HG13	2.10	0.51
2:z:472:TYR:HD2	2:z:521:ARG:HH12	1.55	0.51
1:A:139:TYR:HH	1:O:49:SER:HG	1.58	0.51
1:D:15:GLU:OE1	1:K:10:GLU:CG	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASP:OD2	2:E:65:HIS:HD2	1.93	0.51
1:D:149:ASP:OD1	1:D:149:ASP:N	2.43	0.51
1:Y:177:LEU:HD12	1:Y:177:LEU:C	2.35	0.51
1:i:341:PHE:CB	1:i:353:ILE:HD13	2.41	0.51
1:k:473:GLU:O	1:k:474:ASN:HB2	2.09	0.51
1:s:428:ALA:HB2	1:s:434:LYS:HB3	1.93	0.51
1:u:517:ARG:HH21	1:u:523:ARG:HG3	1.75	0.51
1:w:348:ARG:NH2	1:y:435:ARG:O	2.44	0.51
2:P:45:ILE:N	2:P:45:ILE:HD12	2.25	0.51
2:X:1:OZT:C7	2:X:33:LYS:HZ1	2.24	0.51
2:e:383:LEU:HD13	2:e:423:PHE:CE1	2.46	0.51
2:g:430:ASN:HD22	2:g:431:ILE:N	2.09	0.51
1:I:13:MET:HA	1:I:13:MET:CE	2.40	0.51
1:s:354:SER:CB	1:s:375:ARG:HD2	2.41	0.51
2:C:31:VAL:HG11	2:C:33:LYS:HE3	1.92	0.51
1:I:41:PHE:CB	1:I:53:ILE:HD13	2.39	0.51
1:U:62:PHE:CD1	1:U:62:PHE:C	2.89	0.51
1:b:514:ASP:OD2	1:b:523:ARG:NH2	2.44	0.51
1:i:526:THR:CG2	1:i:527:GLY:N	2.73	0.51
1:w:478:THR:OG1	1:w:533:LEU:HD22	2.09	0.51
2:P:130:ASN:HD22	2:P:131:ILE:N	2.09	0.51
2:z:464:LEU:HD13	2:z:513:LEU:HD12	1.92	0.51
1:W:40:LEU:HD12	1:W:212:VAL:HG12	1.93	0.51
2:E:49:ALA:O	2:E:53:VAL:HG23	2.11	0.51
2:Z:107:TYR:CB	2:Z:197:ILE:HG22	2.35	0.51
2:r:307:LYS:HE3	2:r:418:GLY:O	2.11	0.51
1:B:90:ASP:HB2	1:B:93:ASP:H	1.74	0.50
1:D:205:VAL:HG22	1:D:206:ALA:H	1.74	0.50
1:O:41:PHE:CB	1:O:53:ILE:HD13	2.41	0.50
1:Y:173:GLU:O	1:Y:174:ASN:CB	2.60	0.50
1:a:473:GLU:O	1:a:474:ASN:HB2	2.10	0.50
1:b:368:PHE:HA	1:b:371:PHE:CE2	2.45	0.50
1:f:379:ILE:HD13	2:g:368:LYS:HB3	1.92	0.50
1:k:379:ILE:HD12	2:l:369:LEU:HD23	1.94	0.50
1:k:435:ARG:NH2	1:k:451:PRO:HB2	2.26	0.50
1:q:452:HIS:HB3	1:q:471:TYR:CE2	2.46	0.50
2:N:140:GLY:O	2:N:143:SER:HB3	2.11	0.50
2:4:335:TYR:CZ	2:4:353:VAL:HG13	2.46	0.50
1:B:11:GLN:O	1:B:14:ARG:N	2.43	0.50
1:S:231:GLN:O	1:S:234:LEU:HB2	2.11	0.50
1:f:348:ARG:NH2	1:w:437:GLU:HG2	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:368:PHE:HA	1:f:371:PHE:CE2	2.45	0.50
1:i:525:ILE:CG2	1:i:530:LEU:HB2	2.29	0.50
2:N:35:TYR:CZ	2:N:53:VAL:HG13	2.46	0.50
2:l:513:LEU:O	2:l:517:ILE:HG13	2.11	0.50
2:r:301:OZT:O	2:r:440:GLY:HA3	2.11	0.50
2:r:331:VAL:HG11	2:r:333:LYS:HE3	1.92	0.50
1:K:16:ARG:NH1	1:K:115:ALA:O	2.44	0.50
1:O:152:HIS:HB3	1:O:171:TYR:CE2	2.46	0.50
1:Q:41:PHE:CB	1:Q:53:ILE:HD13	2.38	0.50
1:b:358:ASP:OD1	1:b:519:ARG:NH1	2.44	0.50
1:o:530:LEU:O	1:o:534:LEU:HG	2.11	0.50
1:u:379:ILE:HG23	2:v:368:LYS:HE3	1.92	0.50
2:J:49:ALA:O	2:J:53:VAL:HG23	2.11	0.50
2:V:172:TYR:HE1	2:V:218:ILE:CD1	2.14	0.50
2:g:487:VAL:CG1	2:v:521:ARG:HB3	2.41	0.50
2:4:301:OZT:H27	2:4:333:LYS:HE2	1.92	0.50
1:I:178:THR:HA	1:I:233:LEU:HD13	1.94	0.50
1:K:67:LYS:NZ	1:M:144:ASP:O	2.35	0.50
1:O:182:ARG:NH1	1:O:234:LEU:HA	2.18	0.50
1:Q:144:ASP:OD2	1:Q:146:SER:OG	2.30	0.50
1:S:152:HIS:HB3	1:S:171:TYR:CE2	2.47	0.50
1:W:185:VAL:HA	1:W:188:LEU:HD12	1.93	0.50
1:l:35:TYR:CE1	1:l:37:GLY:CA	2.94	0.50
1:b:318:GLU:OE2	1:b:322:LYS:HE3	2.12	0.50
1:o:330:VAL:HG22	1:o:343:ALA:HB1	1.93	0.50
2:C:130:ASN:HD22	2:C:131:ILE:N	2.10	0.50
2:R:37:THR:HG21	2:R:43:THR:HG23	1.91	0.50
2:g:432:GLU:HG3	2:g:437:GLN:HB2	1.94	0.50
2:r:432:GLU:HG3	2:r:437:GLN:HB2	1.92	0.50
1:A:90:ASP:HB2	1:A:93:ASP:N	2.26	0.50
1:A:205:VAL:HG23	1:A:206:ALA:N	2.27	0.50
1:M:149:ASP:OD1	1:M:149:ASP:O	2.30	0.50
1:M:150:GLU:OE2	1:M:153:PHE:O	2.30	0.50
1:W:176:SER:OG	1:W:179:ASP:OD1	2.29	0.50
1:a:452:HIS:HB3	1:a:471:TYR:CE2	2.47	0.50
1:w:379:ILE:HD12	2:x:369:LEU:HD23	1.94	0.50
2:E:1:OZT:H27	2:E:33:LYS:HZ1	1.76	0.50
2:G:14:MET:CE	2:G:103:LEU:HD13	2.42	0.50
2:c:432:GLU:HG3	2:c:437:GLN:HB2	1.93	0.50
2:4:383:LEU:HD13	2:4:423:PHE:CE1	2.46	0.50
1:A:225:ILE:HG22	1:A:230:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:530:LEU:O	1:3:530:LEU:CD2	2.57	0.50
2:P:6:LEU:C	2:P:6:LEU:HD12	2.36	0.50
1:I:230:LEU:O	1:I:234:LEU:N	2.44	0.50
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.93	0.50
1:1:83:ASP:OD2	2:2:65:HIS:CD2	2.64	0.50
1:i:444:ASP:OD2	1:i:446:SER:OG	2.30	0.50
1:o:478:THR:HG23	1:o:479:ASP:N	2.26	0.50
1:s:333:LEU:N	1:s:333:LEU:HD23	2.27	0.50
1:y:311:GLN:OE1	1:y:311:GLN:O	2.30	0.50
2:H:1:OZT:O	2:H:140:GLY:HA3	2.12	0.50
2:H:144:LEU:HD13	2:E:145:PHE:CE1	2.47	0.50
2:E:14:MET:HE2	2:E:103:LEU:HD13	1.92	0.50
2:G:13:VAL:HG21	2:G:164:LEU:HD23	1.94	0.50
2:R:83:LEU:HD13	2:R:123:PHE:CZ	2.47	0.50
2:R:132:GLU:HG3	2:R:137:GLN:HB2	1.93	0.50
2:j:464:LEU:HD13	2:j:513:LEU:HD11	1.92	0.50
2:v:365:HIS:CE1	2:v:369:LEU:HD11	2.46	0.50
1:K:35:TYR:CZ	1:K:177:LEU:HD13	2.47	0.50
1:K:83:ASP:OD2	2:L:65:HIS:CD2	2.63	0.50
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.42	0.50
1:Q:144:ASP:OD1	1:Q:146:SER:OG	2.30	0.50
2:C:1:OZT:O	2:C:140:GLY:HA3	2.12	0.50
2:G:6:LEU:C	2:G:6:LEU:HD12	2.37	0.50
2:R:208:SER:O	2:R:212:GLU:OE2	2.30	0.50
2:r:430:ASN:HD22	2:r:431:ILE:N	2.09	0.50
1:B:115:ALA:HB3	1:I:112:THR:CG2	2.41	0.50
1:F:182:ARG:HG2	1:F:182:ARG:HH11	1.77	0.50
1:U:55:GLU:HB2	1:U:222:PHE:CG	2.46	0.50
1:W:48:ARG:NH2	1:Y:137:GLU:HG2	2.27	0.50
1:Y:176:SER:OG	1:Y:179:ASP:OD1	2.30	0.50
1:d:331:VAL:CG1	1:d:333:LEU:HD22	2.42	0.50
1:d:356:LEU:HG	1:d:362:PHE:HB2	1.92	0.50
1:d:383:ASP:OD2	2:e:365:HIS:HD2	1.95	0.50
1:o:356:LEU:HG	1:o:362:PHE:HB2	1.93	0.50
1:y:330:VAL:HG13	1:y:343:ALA:HB2	1.94	0.50
2:C:156:GLN:OE1	2:C:165:ARG:NH2	2.45	0.50
2:V:6:LEU:C	2:V:6:LEU:HD12	2.36	0.50
2:V:218:ILE:O	2:V:222:SER:OG	2.30	0.50
2:v:339:ASP:N	2:v:339:ASP:OD1	2.45	0.50
2:4:430:ASN:HD22	2:4:431:ILE:N	2.10	0.50
1:A:83:ASP:OD2	2:H:65:HIS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:383:ASP:OD2	2:h:365:HIS:HD2	1.95	0.49
1:d:356:LEU:HD13	1:d:399:LEU:HD13	1.94	0.49
1:u:356:LEU:HD11	1:u:362:PHE:HB2	1.94	0.49
1:u:428:ALA:HB2	1:u:434:LYS:HB3	1.93	0.49
1:w:311:GLN:HB2	1:w:314:ARG:HD2	1.92	0.49
1:y:525:ILE:CG2	1:y:530:LEU:HB2	2.41	0.49
1:y:533:LEU:C	1:y:533:LEU:HD12	2.34	0.49
2:E:49:ALA:O	2:E:53:VAL:CG2	2.59	0.49
2:J:49:ALA:O	2:J:53:VAL:CG2	2.60	0.49
2:V:209:ARG:HA	2:V:212:GLU:HG2	1.93	0.49
2:Z:164:LEU:HD13	2:Z:213:LEU:HD12	1.94	0.49
1:F:90:ASP:HB2	1:F:93:ASP:N	2.27	0.49
1:I:28:LYS:HB3	1:I:44:GLU:HG3	1.94	0.49
1:M:127:VAL:HG21	1:M:213:LEU:O	2.12	0.49
1:M:129:HIS:CB	1:M:132:GLU:OE2	2.54	0.49
1:u:362:PHE:CD1	1:u:362:PHE:C	2.90	0.49
1:w:355:GLU:HG3	1:w:522:PHE:HB2	1.94	0.49
1:w:473:GLU:O	1:w:474:ASN:CB	2.57	0.49
1:3:311:GLN:O	1:3:311:GLN:CG	2.56	0.49
2:X:1:OZT:H17	2:X:17:ASP:OD1	2.13	0.49
2:t:407:TYR:HB2	2:t:497:ILE:CG2	2.42	0.49
2:v:383:LEU:HD13	2:v:423:PHE:CE1	2.46	0.49
1:K:51:GLN:HG2	1:K:224:ARG:NH2	2.27	0.49
1:M:127:VAL:CG1	1:M:215:ALA:CB	2.87	0.49
1:Q:10:GLU:C	1:Q:12:ALA:N	2.66	0.49
1:S:149:ASP:O	1:S:149:ASP:OD1	2.30	0.49
1:q:525:ILE:CG2	1:q:530:LEU:HG	2.42	0.49
1:y:473:GLU:C	1:y:474:ASN:CG	2.80	0.49
2:G:164:LEU:HD13	2:G:213:LEU:CD1	2.42	0.49
2:G:187:VAL:N	2:V:222:SER:HB3	2.26	0.49
2:l:432:GLU:HG3	2:l:437:GLN:HB2	1.95	0.49
2:t:319:ARG:NH1	2:t:326:ILE:CD1	2.75	0.49
1:A:181:LEU:HD23	1:A:233:LEU:HB3	1.94	0.49
1:B:24:ILE:HG22	1:B:157:GLY:HA2	1.94	0.49
1:D:23:GLY:HA3	1:D:119:GLU:OE2	2.12	0.49
1:D:205:VAL:HG23	1:D:206:ALA:N	2.27	0.49
1:D:219:ARG:NH2	2:E:64:GLU:CD	2.66	0.49
1:Q:142:THR:OG1	1:Q:144:ASP:OD1	2.30	0.49
1:Y:177:LEU:HG	1:Y:233:LEU:HD21	1.93	0.49
1:a:527:GLY:O	1:a:531:GLN:N	2.38	0.49
1:d:428:ALA:HB2	1:d:434:LYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:533:LEU:HD22	1:q:533:LEU:N	2.27	0.49
1:s:449:ASP:O	1:s:449:ASP:OD1	2.30	0.49
1:w:310:GLU:CG	1:w:312:ALA:H	2.23	0.49
1:w:341:PHE:CB	1:w:353:ILE:HD13	2.41	0.49
2:P:185:ASP:OD1	2:P:188:ARG:HB2	2.11	0.49
2:g:349:ALA:O	2:g:353:VAL:CG2	2.61	0.49
2:t:338:ASP:OD1	2:t:341:THR:N	2.46	0.49
2:v:432:GLU:HG3	2:v:437:GLN:HB2	1.94	0.49
2:4:486:LEU:HD11	2:4:518:ILE:HD12	1.94	0.49
1:K:62:PHE:CD1	1:K:62:PHE:C	2.90	0.49
1:Y:178:THR:HA	1:Y:233:LEU:CD2	2.43	0.49
1:d:441:ILE:HD12	1:d:441:ILE:N	2.27	0.49
1:q:442:THR:OG1	1:q:444:ASP:OD1	2.30	0.49
1:s:330:VAL:HG22	1:s:343:ALA:HB1	1.95	0.49
2:E:132:GLU:HG3	2:E:137:GLN:HB2	1.94	0.49
2:J:198:ASP:OD1	2:J:201:GLY:O	2.30	0.49
1:A:147:ILE:HG12	1:A:148:ALA:N	2.28	0.49
1:B:178:THR:HB	1:B:233:LEU:HD23	1.94	0.49
1:O:167:LEU:O	1:O:168:LYS:C	2.55	0.49
1:a:313:MET:CE	1:a:313:MET:CA	2.42	0.49
1:i:481:LEU:HD23	1:i:533:LEU:HB3	1.95	0.49
1:o:383:ASP:OD2	2:p:365:HIS:HD2	1.96	0.49
1:q:335:TYR:CD1	1:q:335:TYR:C	2.91	0.49
1:q:354:SER:CB	1:q:375:ARG:HD2	2.42	0.49
1:s:514:ASP:OD1	1:s:516:ASN:CB	2.60	0.49
1:y:527:GLY:O	1:y:531:GLN:HB2	2.12	0.49
2:C:37:THR:HG21	2:C:43:THR:CG2	2.38	0.49
2:L:49:ALA:O	2:L:53:VAL:HG23	2.12	0.49
2:N:1:OZT:C7	2:N:33:LYS:NZ	2.76	0.49
2:P:37:THR:HG23	2:P:43:THR:HG23	1.93	0.49
2:2:83:LEU:HD13	2:2:123:PHE:CE1	2.47	0.49
2:h:314:MET:HE2	2:h:403:LEU:HD13	1.95	0.49
2:c:407:TYR:HB2	2:c:497:ILE:HG22	1.94	0.49
1:A:40:LEU:CD1	1:A:212:VAL:HG12	2.42	0.49
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.77	0.49
1:W:30:VAL:HG22	1:W:43:ALA:HB1	1.94	0.49
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.93	0.49
1:m:354:SER:CB	1:m:375:ARG:HD2	2.43	0.49
2:L:37:THR:OG1	2:L:41:THR:OG1	2.30	0.49
2:c:468:VAL:HG12	2:c:517:ILE:HD12	1.94	0.49
2:j:445:PHE:CE1	2:z:444:LEU:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:335:TYR:CZ	2:v:353:VAL:HG13	2.47	0.49
2:x:445:PHE:HZ	2:4:325:MET:HG2	1.77	0.49
1:F:217:ARG:HB3	1:F:217:ARG:NH1	2.26	0.49
1:U:41:PHE:CB	1:U:53:ILE:HD13	2.42	0.49
1:m:463:ILE:HG23	1:m:487:ALA:O	2.12	0.49
1:q:310:GLU:HG2	1:q:312:ALA:H	1.76	0.49
1:q:333:LEU:CD2	1:q:333:LEU:H	2.25	0.49
2:2:132:GLU:HG3	2:2:137:GLN:HB2	1.95	0.49
2:e:331:VAL:HG11	2:e:333:LYS:HE3	1.94	0.49
2:j:456:GLN:OE1	2:j:465:ARG:NH2	2.46	0.49
2:p:306:LEU:C	2:p:306:LEU:HD12	2.38	0.49
2:z:337:THR:OG1	2:z:341:THR:OG1	2.30	0.49
1:F:54:SER:OG	1:F:75:ARG:HD2	2.12	0.49
1:F:230:LEU:O	1:F:231:GLN:C	2.55	0.49
1:K:47:SER:CB	1:M:149:ASP:OD2	2.58	0.49
1:3:452:HIS:HB3	1:3:471:TYR:CE2	2.48	0.49
2:C:140:GLY:O	2:C:143:SER:HB3	2.12	0.49
2:G:129:TRP:O	2:X:50:ALA:HB2	2.12	0.49
2:J:37:THR:HG23	2:J:43:THR:HG23	1.91	0.49
2:V:45:ILE:HD12	2:V:45:ILE:N	2.28	0.49
1:I:11:GLN:NE2	1:I:11:GLN:HA	2.28	0.49
1:I:141:ILE:HD12	1:I:141:ILE:N	2.28	0.49
1:I:152:HIS:HB3	1:I:171:TYR:CE2	2.48	0.49
1:M:212:VAL:HG22	1:M:223:ARG:O	2.13	0.49
1:Q:35:TYR:CZ	1:Q:38:GLY:O	2.66	0.49
1:Q:162:PRO:CG	1:i:474:ASN:O	2.59	0.49
1:b:452:HIS:HB3	1:b:471:TYR:CE2	2.48	0.49
1:f:311:GLN:HE21	1:f:314:ARG:NH2	1.98	0.49
1:k:310:GLU:OE2	1:k:314:ARG:HD2	2.13	0.49
1:k:341:PHE:CB	1:k:353:ILE:HD13	2.43	0.49
1:k:481:LEU:CD2	1:k:533:LEU:HB3	2.41	0.49
1:m:526:THR:HG22	1:m:527:GLY:N	2.28	0.49
1:s:383:ASP:OD2	2:t:365:HIS:HD2	1.96	0.49
1:y:357:TYR:N	1:y:360:VAL:CG2	2.76	0.49
1:3:362:PHE:CD1	1:3:362:PHE:C	2.91	0.49
2:G:37:THR:HG21	2:G:43:THR:CG2	2.43	0.49
2:l:498:ASP:OD1	2:l:500:ASP:HB2	2.13	0.49
1:F:141:ILE:H	1:F:141:ILE:HD12	1.77	0.48
1:F:153:PHE:CD1	1:F:167:LEU:HD13	2.49	0.48
1:I:62:PHE:CD1	1:I:62:PHE:C	2.90	0.48
1:Q:107:LEU:HD12	1:Q:141:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:179:ASP:OD1	1:W:179:ASP:N	2.44	0.48
1:Y:41:PHE:CB	1:Y:53:ILE:HD13	2.42	0.48
1:a:463:ILE:HG23	1:a:487:ALA:O	2.13	0.48
1:b:467:LEU:O	1:b:468:LYS:C	2.55	0.48
1:f:362:PHE:C	1:f:362:PHE:CD1	2.91	0.48
1:m:452:HIS:HB3	1:m:471:TYR:CE2	2.47	0.48
1:o:452:HIS:HB3	1:o:471:TYR:CE2	2.48	0.48
1:o:516:ASN:OD1	1:o:516:ASN:O	2.30	0.48
1:w:311:GLN:CG	1:w:311:GLN:O	2.61	0.48
2:H:130:ASN:HD22	2:H:131:ILE:N	2.10	0.48
2:E:156:GLN:OE1	2:E:165:ARG:NH2	2.46	0.48
2:G:49:ALA:O	2:G:53:VAL:HG23	2.13	0.48
2:P:83:LEU:HD13	2:P:123:PHE:CZ	2.47	0.48
2:V:213:LEU:O	2:V:217:ILE:HG13	2.12	0.48
2:l:375:THR:O	2:l:376:PHE:C	2.54	0.48
2:n:331:VAL:CG1	2:n:333:LYS:HE3	2.43	0.48
1:B:115:ALA:CB	1:I:112:THR:HG23	2.43	0.48
1:K:167:LEU:O	1:K:168:LYS:C	2.57	0.48
1:Y:79:ILE:HD12	2:Z:69:LEU:HD23	1.94	0.48
1:b:335:TYR:CD2	1:b:338:GLY:O	2.66	0.48
1:w:311:GLN:HG3	1:w:314:ARG:CD	2.40	0.48
1:w:419:GLU:CG	3:w:94:HOH:O	2.61	0.48
2:J:1:OZT:O	2:J:140:GLY:HA3	2.13	0.48
2:L:1:OZT:H17	2:L:17:ASP:CG	2.38	0.48
2:R:198:ASP:OD2	2:R:201:GLY:O	2.31	0.48
2:c:456:GLN:OE1	2:c:465:ARG:NH2	2.47	0.48
2:x:430:ASN:HD22	2:x:431:ILE:N	2.10	0.48
2:x:432:GLU:HG3	2:x:437:GLN:HB2	1.95	0.48
2:z:440:GLY:O	2:z:443:SER:HB3	2.13	0.48
2:z:496:ILE:HG13	2:z:505:VAL:CG2	2.43	0.48
1:D:101:ASN:O	1:D:105:GLN:HG2	2.14	0.48
1:K:98:GLN:HG3	3:K:249:HOH:O	2.12	0.48
1:Q:230:LEU:O	1:Q:233:LEU:HB2	2.13	0.48
1:1:68:PHE:HA	1:1:71:PHE:CE2	2.47	0.48
1:1:156:MET:HE3	1:1:156:MET:HB2	1.72	0.48
1:f:533:LEU:HD12	1:f:533:LEU:N	2.28	0.48
1:i:335:TYR:CE1	1:i:337:GLY:N	2.80	0.48
1:i:369:ASN:HB3	1:s:404:ALA:HB1	1.94	0.48
1:w:533:LEU:C	1:w:534:LEU:HD23	2.37	0.48
1:3:530:LEU:HD23	1:3:530:LEU:C	2.37	0.48
2:N:6:LEU:C	2:N:6:LEU:HD12	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:338:ASP:OD1	2:g:339:ASP:N	2.46	0.48
2:g:349:ALA:O	2:g:353:VAL:HG23	2.14	0.48
2:j:306:LEU:C	2:j:306:LEU:HD12	2.38	0.48
1:B:205:VAL:HG23	1:B:206:ALA:N	2.29	0.48
1:I:44:GLU:HA	1:I:208:LEU:HD23	1.95	0.48
1:S:62:PHE:CD1	1:S:62:PHE:C	2.91	0.48
1:S:176:SER:O	1:S:179:ASP:HB2	2.13	0.48
1:U:181:LEU:CD2	1:U:233:LEU:HB3	2.44	0.48
1:W:62:PHE:C	1:W:62:PHE:CD1	2.91	0.48
1:Y:22:LYS:NZ	2:c:412:SER:O	2.39	0.48
1:k:310:GLU:CG	1:k:314:ARG:HD2	2.42	0.48
1:y:335:TYR:CE1	1:y:338:GLY:N	2.81	0.48
1:y:430:TYR:C	1:y:430:TYR:HD2	2.21	0.48
1:3:479:ASP:OD1	1:3:479:ASP:N	2.47	0.48
2:E:83:LEU:HD13	2:E:123:PHE:CZ	2.48	0.48
2:G:45:ILE:HD12	2:G:45:ILE:N	2.28	0.48
2:L:130:ASN:HD22	2:L:131:ILE:N	2.11	0.48
2:X:185:ASP:OD1	2:X:188:ARG:HB2	2.14	0.48
2:Z:36:ILE:HG22	2:Z:38:ASP:O	2.13	0.48
2:e:432:GLU:HG3	2:e:437:GLN:HB2	1.95	0.48
2:l:494:ALA:CB	2:l:510:ILE:HD11	2.44	0.48
2:n:337:THR:HG21	2:n:343:THR:HG23	1.96	0.48
2:p:301:OZT:O	2:p:440:GLY:HA3	2.13	0.48
2:p:432:GLU:HG3	2:p:437:GLN:HB2	1.96	0.48
2:r:464:LEU:C	2:r:464:LEU:HD22	2.35	0.48
2:t:434:GLU:OE2	2:4:329:ARG:NH1	2.46	0.48
2:z:383:LEU:HD13	2:z:423:PHE:CE1	2.48	0.48
1:D:150:GLU:OE2	1:D:153:PHE:O	2.30	0.48
1:M:92:ARG:NH1	1:M:132:GLU:OE2	2.42	0.48
1:a:348:ARG:NH2	1:b:437:GLU:HG3	2.28	0.48
1:u:379:ILE:HD13	2:v:368:LYS:HB3	1.94	0.48
2:H:8:TYR:CD1	2:H:8:TYR:C	2.91	0.48
2:L:109:ILE:H	2:L:109:ILE:HG12	1.44	0.48
2:L:211:ALA:HB1	2:L:215:ARG:HH21	1.78	0.48
2:T:101:LEU:HA	2:T:102:PRO:HD3	1.66	0.48
2:t:432:GLU:HG3	2:t:437:GLN:HB2	1.96	0.48
1:B:153:PHE:CD1	1:B:167:LEU:HD13	2.49	0.48
1:F:59:ARG:NH2	1:F:128:ALA:O	2.34	0.48
1:F:141:ILE:HD12	1:F:141:ILE:N	2.28	0.48
1:I:44:GLU:HG3	1:I:44:GLU:O	2.13	0.48
1:O:54:SER:CB	1:O:75:ARG:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:142:THR:OG1	1:Q:146:SER:HB2	2.13	0.48
1:1:226:THR:HG22	1:1:227:GLY:N	2.27	0.48
1:k:463:ILE:HG23	1:k:487:ALA:O	2.13	0.48
1:m:330:VAL:HG22	1:m:343:ALA:HB1	1.96	0.48
1:3:355:GLU:HB2	1:3:522:PHE:CB	2.43	0.48
2:H:83:LEU:HD13	2:H:123:PHE:CE1	2.48	0.48
2:C:198:ASP:OD1	2:C:199:ALA:N	2.46	0.48
2:E:198:ASP:OD1	2:E:198:ASP:C	2.56	0.48
2:L:12:VAL:CG1	2:L:118:GLY:HA3	2.43	0.48
2:R:169:GLU:CA	2:R:217:ILE:CD1	2.92	0.48
2:X:40:TYR:CD1	2:X:109:ILE:HD13	2.49	0.48
2:h:513:LEU:O	2:h:517:ILE:HG13	2.14	0.48
2:g:301:OZT:H17	2:g:317:ASP:OD1	2.14	0.48
2:j:349:ALA:O	2:j:353:VAL:CG2	2.62	0.48
2:z:432:GLU:HG3	2:z:437:GLN:HB2	1.94	0.48
1:A:54:SER:OG	1:A:75:ARG:HD2	2.13	0.48
1:B:10:GLU:C	1:B:12:ALA:H	2.15	0.48
1:B:16:ARG:NH2	1:B:111:PHE:C	2.72	0.48
1:a:310:GLU:HG3	1:a:313:MET:HB2	1.94	0.48
1:f:357:TYR:O	1:f:358:ASP:C	2.56	0.48
1:i:530:LEU:HD22	1:i:530:LEU:C	2.38	0.48
1:w:478:THR:HG23	1:w:479:ASP:N	2.28	0.48
1:y:316:ARG:CZ	1:y:417:PRO:HD3	2.44	0.48
2:H:191:PHE:HB3	2:H:192:PRO:HD2	1.95	0.48
2:L:45:ILE:HD12	2:L:45:ILE:N	2.28	0.48
2:Z:1:OZT:O	2:Z:140:GLY:HA3	2.13	0.48
2:Z:40:TYR:CE2	2:Z:201:GLY:HA2	2.48	0.48
2:g:301:OZT:H17	2:g:317:ASP:OD2	2.14	0.48
1:F:127:VAL:HG21	1:F:213:LEU:HB3	1.95	0.48
1:a:313:MET:CE	1:a:316:ARG:CD	2.87	0.48
1:a:412:THR:HG22	1:a:413:GLU:CG	2.37	0.48
2:Z:83:LEU:HD13	2:Z:123:PHE:CZ	2.49	0.48
2:t:306:LEU:C	2:t:306:LEU:HD12	2.38	0.48
1:Q:35:TYR:HE2	1:Q:40:LEU:HB2	1.79	0.48
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.95	0.48
1:W:83:ASP:OD2	2:X:65:HIS:CD2	2.62	0.48
1:W:178:THR:HG23	1:W:179:ASP:N	2.29	0.48
1:f:313:MET:HE2	1:f:316:ARG:HD3	1.95	0.48
1:o:522:PHE:CE2	1:o:524:ARG:HG2	2.49	0.48
1:q:310:GLU:HG2	1:q:311:GLN:N	2.29	0.48
1:q:443:TYR:CD2	1:q:444:ASP:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:368:PHE:HA	1:3:371:PHE:CE2	2.49	0.48
2:E:45:ILE:N	2:E:45:ILE:HD12	2.29	0.48
2:h:456:GLN:OE1	2:h:465:ARG:NH2	2.46	0.48
2:e:349:ALA:O	2:e:353:VAL:CG2	2.62	0.48
2:g:306:LEU:C	2:g:306:LEU:HD12	2.39	0.48
2:v:306:LEU:C	2:v:306:LEU:HD12	2.39	0.48
1:F:161:GLU:HB2	1:F:162:PRO:HD3	1.95	0.48
1:M:176:SER:OG	1:M:179:ASP:OD1	2.30	0.48
1:Q:62:PHE:CD1	1:Q:62:PHE:C	2.92	0.48
1:u:481:LEU:HD23	1:u:533:LEU:HG	1.95	0.48
1:y:355:GLU:HG3	1:y:522:PHE:HB2	1.96	0.48
2:J:37:THR:HG21	2:J:59:TYR:HD2	1.79	0.48
2:V:132:GLU:HG3	2:V:137:GLN:HB2	1.95	0.48
2:2:38:ASP:OD1	2:2:41:THR:N	2.46	0.48
2:2:83:LEU:HD13	2:2:123:PHE:CZ	2.48	0.48
2:j:491:PHE:CD2	2:j:514:ALA:CB	2.97	0.48
1:Y:18:GLU:HG3	2:c:413:ASP:OD2	2.14	0.47
1:y:512:VAL:HG22	1:y:513:LEU:N	2.28	0.47
2:H:31:VAL:HG11	2:H:33:LYS:HE3	1.96	0.47
2:R:86:MET:HB2	2:R:86:MET:HE3	1.76	0.47
2:V:1:OZT:H17	2:V:33:LYS:NZ	2.28	0.47
2:X:31:VAL:CG1	2:X:33:LYS:HE3	2.44	0.47
2:p:511:ALA:HB1	2:p:515:ARG:HH21	1.80	0.47
2:x:392:ALA:O	2:x:393:ALA:C	2.57	0.47
1:A:90:ASP:HB2	1:A:93:ASP:H	1.77	0.47
1:B:231:GLN:HE21	1:B:231:GLN:HB2	1.52	0.47
1:F:163:ILE:HG23	1:F:187:ALA:O	2.14	0.47
1:O:163:ILE:HG23	1:O:187:ALA:C	2.39	0.47
1:W:173:GLU:O	1:W:174:ASN:CB	2.61	0.47
1:d:310:GLU:CG	1:q:315:GLU:OE2	2.60	0.47
1:d:331:VAL:CG1	1:d:333:LEU:CD2	2.92	0.47
1:k:481:LEU:CD2	1:k:534:LEU:HD11	2.44	0.47
1:m:517:ARG:NH2	1:m:523:ARG:HG3	2.29	0.47
1:q:362:PHE:CD1	1:q:362:PHE:C	2.91	0.47
1:w:526:THR:HG22	1:w:527:GLY:N	2.29	0.47
1:y:336:ALA:H	1:y:474:ASN:HA	1.78	0.47
2:H:109:ILE:H	2:H:109:ILE:HG12	1.40	0.47
2:X:37:THR:CG2	2:X:59:TYR:HD2	2.27	0.47
2:X:196:ILE:HG13	2:X:205:VAL:HG22	1.94	0.47
2:c:345:ILE:N	2:c:345:ILE:HD12	2.29	0.47
2:4:331:VAL:HG11	2:4:333:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLY:O	1:D:89:TYR:O	2.32	0.47
1:M:176:SER:OG	1:M:178:THR:HG22	2.14	0.47
1:Y:54:SER:CB	1:Y:75:ARG:HD2	2.43	0.47
1:o:330:VAL:HG13	1:o:343:ALA:HB2	1.97	0.47
1:u:513:LEU:HD12	1:u:513:LEU:HA	1.72	0.47
2:C:144:LEU:HD13	2:R:145:PHE:CE1	2.49	0.47
2:E:86:MET:HE3	2:E:86:MET:HB2	1.72	0.47
2:L:1:OZT:H27	2:L:33:LYS:HZ1	1.79	0.47
2:R:6:LEU:C	2:R:6:LEU:HD12	2.39	0.47
2:e:513:LEU:O	2:e:516:ALA:HB3	2.15	0.47
1:B:74:LEU:HD13	1:B:122:LEU:HD21	1.96	0.47
1:F:60:VAL:HG21	1:F:99:LEU:HD12	1.96	0.47
1:S:56:LEU:HD23	1:S:56:LEU:HA	1.72	0.47
1:S:227:GLY:HA2	1:S:230:LEU:CD1	2.43	0.47
1:Y:30:VAL:HG22	1:Y:43:ALA:HB1	1.96	0.47
1:l:57:TYR:O	1:l:58:ASP:C	2.56	0.47
1:m:467:LEU:O	1:m:468:LYS:C	2.57	0.47
1:o:316:ARG:CZ	1:o:417:PRO:HD3	2.45	0.47
1:y:318:GLU:O	1:y:322:LYS:HG3	2.15	0.47
2:J:6:LEU:C	2:J:6:LEU:HD12	2.40	0.47
2:X:213:LEU:O	2:X:217:ILE:HG13	2.13	0.47
2:e:336:ILE:HD13	2:e:502:ALA:HB1	1.95	0.47
2:g:337:THR:HG21	2:g:343:THR:CG2	2.43	0.47
2:g:383:LEU:HD13	2:g:423:PHE:CE1	2.49	0.47
2:j:337:THR:HG21	2:j:343:THR:HG23	1.96	0.47
2:p:511:ALA:O	2:p:512:GLU:C	2.57	0.47
1:B:127:VAL:HG21	1:B:213:LEU:HB3	1.97	0.47
1:F:205:VAL:HG22	1:F:207:SER:OG	2.14	0.47
1:M:30:VAL:HG22	1:M:43:ALA:HB1	1.96	0.47
1:Y:55:GLU:CG	1:Y:222:PHE:HB2	2.45	0.47
1:Y:167:LEU:O	1:Y:168:LYS:C	2.57	0.47
1:Y:229:ALA:HA	1:Y:232:ALA:HB3	1.96	0.47
1:a:368:PHE:HA	1:a:371:PHE:CE2	2.50	0.47
1:q:335:TYR:CZ	1:q:338:GLY:N	2.82	0.47
1:w:311:GLN:CG	1:w:314:ARG:HD3	2.41	0.47
1:w:335:TYR:HE1	1:w:337:GLY:CA	2.19	0.47
1:w:383:ASP:OD2	2:x:365:HIS:CD2	2.65	0.47
2:C:6:LEU:C	2:C:6:LEU:HD12	2.39	0.47
2:G:144:LEU:HB2	3:G:241:HOH:O	2.15	0.47
2:J:156:GLN:OE1	2:J:165:ARG:NH2	2.47	0.47
2:L:31:VAL:HG12	2:L:33:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:107:TYR:CE2	2:N:199:ALA:HA	2.49	0.47
2:P:107:TYR:HB2	2:P:197:ILE:HG22	1.95	0.47
2:h:383:LEU:HD13	2:h:423:PHE:CE1	2.50	0.47
2:c:383:LEU:HD13	2:c:423:PHE:CZ	2.49	0.47
2:g:337:THR:OG1	2:g:341:THR:OG1	2.30	0.47
2:p:314:MET:HE1	2:p:403:LEU:O	2.15	0.47
1:B:19:LEU:HD22	1:B:20:ALA:N	2.30	0.47
1:B:178:THR:HB	1:B:233:LEU:CD2	2.44	0.47
1:U:30:VAL:HG22	1:U:43:ALA:HB1	1.96	0.47
1:1:141:ILE:HD12	1:1:141:ILE:N	2.29	0.47
1:f:312:ALA:O	1:f:316:ARG:HG3	2.15	0.47
1:m:330:VAL:HG13	1:m:343:ALA:HB2	1.97	0.47
1:u:335:TYR:CD2	1:u:338:GLY:O	2.67	0.47
1:w:452:HIS:CG	1:w:471:TYR:HE2	2.32	0.47
2:H:156:GLN:OE1	2:H:165:ARG:NH2	2.47	0.47
2:V:185:ASP:OD1	2:V:188:ARG:HB2	2.14	0.47
2:c:338:ASP:OD1	2:c:341:THR:N	2.47	0.47
2:c:491:PHE:HB3	2:c:492:PRO:HD2	1.97	0.47
2:e:349:ALA:O	2:e:353:VAL:HG23	2.15	0.47
2:z:456:GLN:OE1	2:z:465:ARG:NH2	2.47	0.47
1:A:35:TYR:CE2	1:A:38:GLY:C	2.93	0.47
1:A:40:LEU:HD13	1:A:212:VAL:CG1	2.44	0.47
1:A:68:PHE:HB2	3:A:250:HOH:O	2.15	0.47
1:B:35:TYR:CE1	1:B:37:GLY:N	2.83	0.47
1:B:61:GLY:N	1:B:213:LEU:HD21	2.30	0.47
1:B:205:VAL:HG23	1:B:206:ALA:H	1.77	0.47
1:D:57:TYR:HB3	1:D:60:VAL:HG13	1.96	0.47
1:D:71:PHE:C	1:D:71:PHE:CD1	2.92	0.47
1:F:74:LEU:HD13	1:F:122:LEU:HD21	1.95	0.47
1:I:15:GLU:OE2	1:S:10:GLU:HA	2.15	0.47
1:I:54:SER:CB	1:I:75:ARG:HD2	2.45	0.47
1:Q:182:ARG:HH12	1:Q:234:LEU:CB	2.27	0.47
1:U:152:HIS:HB3	1:U:171:TYR:CE2	2.50	0.47
1:d:423:CYS:HA	1:d:439:TYR:O	2.14	0.47
1:f:481:LEU:HD23	1:f:533:LEU:HB3	1.96	0.47
1:i:354:SER:CB	1:i:375:ARG:HD2	2.45	0.47
1:m:310:GLU:O	1:m:311:GLN:C	2.57	0.47
1:o:390:ASP:OD2	1:o:393:ASP:N	2.47	0.47
1:q:311:GLN:O	1:q:315:GLU:HB2	2.14	0.47
1:s:514:ASP:CG	1:s:516:ASN:H	2.22	0.47
2:H:1:OZT:C7	2:H:33:LYS:HZ1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:ARG:HA	2:E:213:LEU:HD13	1.96	0.47
2:J:31:VAL:HG11	2:J:33:LYS:HE3	1.96	0.47
2:J:144:LEU:HD13	2:Z:145:PHE:CE1	2.50	0.47
2:N:215:ARG:O	2:N:219:GLU:HG3	2.14	0.47
2:R:66:TYR:C	2:R:66:TYR:CD2	2.93	0.47
2:T:14:MET:HE2	2:T:103:LEU:HD13	1.97	0.47
2:T:38:ASP:OD1	2:T:39:ASP:N	2.47	0.47
2:T:86:MET:HE3	2:T:86:MET:HB2	1.68	0.47
2:g:314:MET:HE1	2:g:403:LEU:O	2.15	0.47
2:l:456:GLN:OE1	2:l:465:ARG:NH2	2.48	0.47
2:n:485:ASP:OD1	2:n:488:ARG:HB2	2.15	0.47
2:z:515:ARG:HA	2:z:518:ILE:HD12	1.96	0.47
2:4:498:ASP:OD1	2:4:501:GLY:O	2.33	0.47
1:A:179:ASP:O	1:A:183:ILE:HG13	2.15	0.47
1:B:74:LEU:HD23	1:B:74:LEU:HA	1.60	0.47
1:I:130:TYR:C	1:I:130:TYR:CD2	2.93	0.47
1:Q:230:LEU:C	1:Q:230:LEU:CD2	2.87	0.47
1:f:356:LEU:HD13	1:f:399:LEU:HD13	1.97	0.47
1:o:355:GLU:HB2	1:o:522:PHE:CB	2.45	0.47
1:q:514:ASP:CG	1:q:523:ARG:NH2	2.73	0.47
1:u:370:GLU:HB3	1:u:418:TYR:CD2	2.50	0.47
1:w:310:GLU:CD	1:w:312:ALA:HB3	2.40	0.47
2:N:132:GLU:HG3	2:N:137:GLN:HB2	1.95	0.47
2:Z:6:LEU:C	2:Z:6:LEU:HD12	2.40	0.47
2:j:485:ASP:OD1	2:j:488:ARG:HB2	2.15	0.47
2:x:331:VAL:HG11	2:x:333:LYS:HE3	1.97	0.47
2:x:338:ASP:OD1	2:x:339:ASP:N	2.47	0.47
1:D:214:ASP:OD1	1:D:214:ASP:C	2.58	0.47
1:Q:137:GLU:OE1	1:Q:139:TYR:OH	2.29	0.47
1:l:35:TYR:HD1	1:l:37:GLY:H	1.61	0.47
1:a:354:SER:CB	1:a:375:ARG:HD2	2.45	0.47
1:b:340:LEU:HD13	1:b:512:VAL:HG12	1.95	0.47
1:d:526:THR:CG2	1:d:527:GLY:H	2.28	0.47
1:q:340:LEU:CD1	1:q:512:VAL:CG1	2.93	0.47
1:u:463:ILE:HG23	1:u:487:ALA:C	2.40	0.47
1:w:415:ALA:HB3	1:y:412:THR:CG2	2.24	0.47
1:3:529:ALA:O	1:3:533:LEU:HD23	2.15	0.47
2:L:152:LYS:HG3	2:P:152:LYS:HG3	1.97	0.47
2:P:191:PHE:HB3	2:P:192:PRO:HD2	1.97	0.47
2:P:217:ILE:O	2:P:217:ILE:HG22	2.12	0.47
2:Z:132:GLU:OE1	2:Z:132:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:498:ASP:OD1	2:h:500:ASP:CB	2.58	0.47
2:p:345:ILE:HD12	2:p:345:ILE:N	2.30	0.47
2:4:349:ALA:O	2:4:353:VAL:HG23	2.15	0.47
1:D:57:TYR:HB3	1:D:60:VAL:CG1	2.45	0.47
1:I:69:ASN:HB3	1:S:104:ALA:HB1	1.96	0.47
1:K:28:LYS:HB3	1:K:44:GLU:HG3	1.97	0.47
1:U:181:LEU:HD23	1:U:233:LEU:CB	2.45	0.47
1:d:437:GLU:OE2	1:q:348:ARG:NH2	2.48	0.47
1:k:354:SER:CB	1:k:375:ARG:HD2	2.45	0.47
1:q:510:VAL:CG1	1:q:525:ILE:HD12	2.45	0.47
1:s:331:VAL:CG1	1:s:333:LEU:HD22	2.44	0.47
1:w:362:PHE:CD1	1:w:362:PHE:C	2.93	0.47
1:w:441:ILE:HD12	1:w:441:ILE:N	2.30	0.47
2:h:407:TYR:HB2	2:h:497:ILE:CG2	2.45	0.47
2:g:340:TYR:CE1	2:g:409:ILE:HD13	2.49	0.47
2:z:345:ILE:HD12	2:z:345:ILE:N	2.30	0.47
1:I:16:ARG:HH21	1:I:111:PHE:C	2.21	0.46
1:I:31:VAL:CG1	1:I:33:LEU:HD22	2.45	0.46
1:Q:140:ARG:HH21	1:Q:155:VAL:N	2.11	0.46
1:Q:152:HIS:HB3	1:Q:171:TYR:CE2	2.50	0.46
1:U:141:ILE:N	1:U:141:ILE:HD12	2.30	0.46
1:Y:14:ARG:HH21	2:c:309:PRO:CG	2.26	0.46
1:d:316:ARG:NH2	1:d:411:PHE:O	2.47	0.46
1:d:359:ARG:HA	1:d:359:ARG:HD2	1.83	0.46
1:i:452:HIS:HB3	1:i:471:TYR:CE2	2.50	0.46
1:u:467:LEU:O	1:u:468:LYS:C	2.58	0.46
1:w:331:VAL:HG12	1:w:333:LEU:CD2	2.45	0.46
2:E:65:HIS:CE1	2:E:69:LEU:HD11	2.50	0.46
2:L:1:OZT:H27	2:L:33:LYS:NZ	2.30	0.46
2:N:185:ASP:OD1	2:N:188:ARG:HB2	2.15	0.46
2:T:35:TYR:CZ	2:T:53:VAL:HG13	2.50	0.46
2:X:130:ASN:HD22	2:X:131:ILE:N	2.12	0.46
2:Z:198:ASP:OD1	2:Z:201:GLY:O	2.32	0.46
2:t:514:ALA:O	2:t:518:ILE:HG13	2.15	0.46
2:z:464:LEU:HD13	2:z:513:LEU:CD1	2.45	0.46
1:B:75:ARG:O	1:B:79:ILE:HG13	2.15	0.46
1:S:79:ILE:HD12	2:T:69:LEU:HD23	1.97	0.46
1:S:227:GLY:O	1:S:230:LEU:CB	2.62	0.46
1:b:530:LEU:CD2	1:b:534:LEU:CD2	2.88	0.46
1:y:313:MET:HA	1:y:313:MET:HE2	1.91	0.46
1:3:383:ASP:OD2	2:4:365:HIS:CD2	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LEU:HD13	2:H:123:PHE:CZ	2.50	0.46
2:C:196:ILE:HG13	2:C:205:VAL:CG2	2.45	0.46
2:J:132:GLU:HG3	2:J:137:GLN:HB2	1.98	0.46
2:R:214:ALA:O	2:R:218:ILE:HG13	2.14	0.46
2:V:31:VAL:HG11	2:V:33:LYS:HE3	1.97	0.46
2:2:198:ASP:OD1	2:2:200:ASP:CB	2.63	0.46
2:g:492:PRO:O	2:g:510:ILE:HD13	2.14	0.46
2:n:432:GLU:HG3	2:n:437:GLN:HB2	1.96	0.46
1:W:128:ALA:HB2	1:W:134:LYS:HB3	1.98	0.46
1:Y:152:HIS:HB3	1:Y:171:TYR:CE2	2.50	0.46
1:Y:176:SER:OG	1:Y:179:ASP:OD2	2.34	0.46
2:L:37:THR:HG21	2:L:43:THR:CG2	2.44	0.46
2:X:65:HIS:CE1	2:X:69:LEU:HD11	2.50	0.46
2:h:409:ILE:H	2:h:409:ILE:HG12	1.43	0.46
2:e:345:ILE:CD1	3:e:68:HOH:O	2.62	0.46
2:p:401:LEU:HA	2:p:402:PRO:HD3	1.64	0.46
2:t:319:ARG:HH11	2:t:326:ILE:HD13	1.80	0.46
1:I:11:GLN:HE22	1:I:14:ARG:HE	1.60	0.46
1:O:18:GLU:OE1	1:O:21:ARG:NH2	2.43	0.46
1:O:231:GLN:HG3	1:O:232:ALA:N	2.29	0.46
1:S:83:ASP:OD2	2:T:65:HIS:CD2	2.66	0.46
1:m:513:LEU:HD12	1:m:513:LEU:HA	1.79	0.46
1:3:481:LEU:CD2	1:3:533:LEU:HB3	2.45	0.46
2:J:109:ILE:H	2:J:109:ILE:HG12	1.46	0.46
2:Z:107:TYR:OH	2:Z:199:ALA:HB2	2.14	0.46
2:Z:132:GLU:HG3	2:Z:137:GLN:HB2	1.96	0.46
2:e:338:ASP:C	2:e:338:ASP:OD1	2.58	0.46
2:t:498:ASP:OD1	2:t:500:ASP:HB2	2.15	0.46
2:v:513:LEU:CD1	2:v:513:LEU:H	2.28	0.46
2:x:306:LEU:C	2:x:306:LEU:HD12	2.40	0.46
1:A:122:LEU:N	1:A:122:LEU:CD1	2.78	0.46
1:B:90:ASP:HB2	1:B:93:ASP:N	2.29	0.46
1:Q:79:ILE:HD13	2:R:68:LYS:HB3	1.97	0.46
1:b:341:PHE:CB	1:b:353:ILE:HD13	2.43	0.46
1:y:330:VAL:HG22	1:y:343:ALA:HB1	1.97	0.46
2:V:219:GLU:O	2:V:223:GLY:C	2.59	0.46
2:2:6:LEU:C	2:2:6:LEU:HD12	2.40	0.46
2:t:464:LEU:CD2	2:t:464:LEU:O	2.64	0.46
1:K:141:ILE:N	1:K:141:ILE:HD12	2.30	0.46
1:Q:10:GLU:CD	1:Y:15:GLU:HG2	2.40	0.46
1:d:355:GLU:HB2	1:d:522:PHE:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:508:LEU:HA	1:i:508:LEU:HD23	1.66	0.46
1:y:473:GLU:C	1:y:474:ASN:ND2	2.74	0.46
2:H:54:GLU:OE1	2:H:54:GLU:HA	2.15	0.46
2:E:59:TYR:CE2	2:E:63:LEU:HD11	2.51	0.46
2:J:45:ILE:N	2:J:45:ILE:HD12	2.30	0.46
2:L:164:LEU:HD13	2:L:213:LEU:CD1	2.45	0.46
2:N:31:VAL:HG11	2:N:33:LYS:HE3	1.96	0.46
2:P:103:LEU:HD23	2:P:103:LEU:HA	1.76	0.46
2:l:338:ASP:C	2:l:338:ASP:OD1	2.59	0.46
1:B:54:SER:OG	1:B:75:ARG:HD2	2.16	0.46
1:F:167:LEU:O	1:F:168:LYS:C	2.57	0.46
1:O:62:PHE:C	1:O:62:PHE:CD1	2.93	0.46
1:Q:167:LEU:O	1:Q:168:LYS:C	2.59	0.46
1:i:357:TYR:O	1:i:358:ASP:C	2.58	0.46
1:i:456:MET:HB2	1:i:456:MET:HE3	1.64	0.46
1:k:452:HIS:HB3	1:k:471:TYR:CE2	2.51	0.46
1:u:452:HIS:HB3	1:u:471:TYR:CE2	2.51	0.46
1:u:481:LEU:CD2	1:u:533:LEU:CG	2.94	0.46
1:y:357:TYR:H	1:y:360:VAL:HG23	1.79	0.46
2:C:31:VAL:CG1	2:C:33:LYS:HE3	2.45	0.46
2:G:8:TYR:HB2	2:G:9:PRO:CD	2.45	0.46
2:G:164:LEU:HD13	2:G:213:LEU:HD12	1.96	0.46
2:J:48:THR:OG1	2:J:51:VAL:HG23	2.16	0.46
2:R:48:THR:OG1	2:R:51:VAL:HG23	2.16	0.46
2:R:169:GLU:HA	2:R:217:ILE:CD1	2.45	0.46
2:V:1:OZT:H17	2:V:33:LYS:HZ1	1.81	0.46
2:2:86:MET:HE3	2:2:86:MET:HB2	1.73	0.46
2:c:430:ASN:HD22	2:c:431:ILE:N	2.13	0.46
2:z:313:VAL:HG21	2:z:464:LEU:HD23	1.98	0.46
1:D:57:TYR:CB	1:D:60:VAL:HG13	2.46	0.46
1:o:481:LEU:HD21	1:o:530:LEU:CD1	2.46	0.46
1:q:357:TYR:O	1:q:358:ASP:C	2.59	0.46
1:u:423:CYS:HA	1:u:439:TYR:O	2.15	0.46
2:E:40:TYR:HD2	2:E:107:TYR:HB3	1.80	0.46
2:X:83:LEU:HD13	2:X:123:PHE:CZ	2.51	0.46
2:Z:37:THR:OG1	2:Z:41:THR:OG1	2.30	0.46
2:e:456:GLN:OE1	2:e:465:ARG:NH2	2.49	0.46
2:z:348:THR:OG1	2:z:351:VAL:HG23	2.16	0.46
1:A:24:ILE:HG22	1:A:157:GLY:HA2	1.97	0.46
1:A:178:THR:HG23	1:A:179:ASP:N	2.30	0.46
1:Q:10:GLU:HB2	1:Y:15:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:217:ARG:HH21	1:1:223:ARG:HG3	1.81	0.46
1:f:324:ILE:CD1	1:f:420:VAL:O	2.62	0.46
1:o:441:ILE:HD12	1:o:441:ILE:N	2.31	0.46
1:w:456:MET:HB2	1:w:456:MET:HE3	1.63	0.46
2:R:37:THR:OG1	2:R:41:THR:OG1	2.30	0.46
2:T:31:VAL:HG12	2:T:33:LYS:HG3	1.98	0.46
2:T:198:ASP:N	2:T:198:ASP:OD1	2.49	0.46
2:Z:45:ILE:N	2:Z:45:ILE:HD12	2.30	0.46
2:Z:58:LEU:HD12	2:Z:58:LEU:O	2.15	0.46
2:h:403:LEU:HD23	2:h:403:LEU:HA	1.79	0.46
2:e:365:HIS:CE1	2:e:369:LEU:HD11	2.51	0.46
2:e:386:MET:HE3	2:e:386:MET:HB2	1.75	0.46
2:t:337:THR:HG21	2:t:343:THR:HG23	1.96	0.46
2:v:519:GLU:O	2:v:522:SER:O	2.33	0.46
1:F:111:PHE:O	1:F:111:PHE:CG	2.68	0.46
1:Q:30:VAL:HG22	1:Q:43:ALA:HB1	1.98	0.46
1:1:57:TYR:OH	1:1:86:GLY:HA3	2.16	0.46
1:i:526:THR:O	1:i:530:LEU:N	2.39	0.46
1:o:340:LEU:CD1	1:o:512:VAL:HG12	2.46	0.46
1:q:335:TYR:CE2	1:q:477:LEU:HD13	2.51	0.46
1:3:341:PHE:CB	1:3:353:ILE:HD13	2.43	0.46
2:h:464:LEU:HD13	2:h:513:LEU:CD1	2.46	0.46
2:4:496:ILE:HG13	2:4:505:VAL:CG2	2.46	0.46
1:F:57:TYR:CB	1:F:60:VAL:HG13	2.47	0.45
1:U:156:MET:HB2	1:U:156:MET:HE3	1.72	0.45
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.98	0.45
1:Y:173:GLU:HG3	1:Y:174:ASN:CG	2.38	0.45
1:b:340:LEU:HD12	1:b:341:PHE:N	2.31	0.45
1:f:428:ALA:HB2	1:f:434:LYS:HB3	1.98	0.45
1:q:340:LEU:HD12	1:q:512:VAL:HG12	1.98	0.45
1:3:333:LEU:HD23	1:3:333:LEU:H	1.79	0.45
2:Z:38:ASP:OD1	2:Z:41:THR:N	2.48	0.45
2:2:191:PHE:HB3	2:2:192:PRO:HD2	1.98	0.45
2:e:409:ILE:H	2:e:409:ILE:HG12	1.46	0.45
2:g:487:VAL:CG1	2:v:521:ARG:CB	2.91	0.45
2:n:313:VAL:HG21	2:n:464:LEU:HD23	1.98	0.45
2:n:338:ASP:OD2	2:n:379:LYS:NZ	2.46	0.45
2:x:478:ASP:OD1	2:4:324:ASN:HB3	2.16	0.45
2:x:513:LEU:O	2:x:517:ILE:HG13	2.16	0.45
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.64	0.45
1:A:217:ARG:NH1	1:A:223:ARG:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD21	1:D:181:LEU:HD13	1.99	0.45
1:D:74:LEU:HD23	1:D:74:LEU:HA	1.60	0.45
1:F:35:TYR:CD2	1:F:38:GLY:O	2.69	0.45
1:K:70:GLU:HB3	1:K:118:TYR:CD2	2.51	0.45
1:U:181:LEU:HD23	1:U:233:LEU:C	2.40	0.45
1:Y:178:THR:CA	1:Y:233:LEU:HG	2.47	0.45
1:o:356:LEU:HD13	1:o:399:LEU:HD13	1.97	0.45
1:q:514:ASP:CG	1:q:523:ARG:HH21	2.24	0.45
1:y:383:ASP:OD2	2:z:365:HIS:CD2	2.69	0.45
2:J:164:LEU:HD13	2:J:213:LEU:HD12	1.98	0.45
2:N:38:ASP:OD1	2:N:41:THR:N	2.48	0.45
2:N:83:LEU:HD13	2:N:123:PHE:CE1	2.51	0.45
2:P:37:THR:OG1	2:P:41:THR:OG1	2.32	0.45
2:P:156:GLN:OE1	2:P:165:ARG:NH2	2.50	0.45
2:V:130:ASN:HD22	2:V:130:ASN:C	2.23	0.45
2:t:331:VAL:HG11	2:t:333:LYS:HE3	1.98	0.45
2:z:337:THR:CG2	2:z:359:TYR:HD2	2.28	0.45
2:4:485:ASP:OD1	2:4:488:ARG:HB2	2.16	0.45
1:B:130:TYR:CE1	1:B:216:ASN:O	2.69	0.45
1:I:10:GLU:HB3	1:I:13:MET:HB2	1.98	0.45
1:I:151:PRO:HD2	1:I:152:HIS:H	1.81	0.45
1:Y:33:LEU:HD11	1:Y:180:ALA:HB1	1.98	0.45
1:k:330:VAL:HG22	1:k:343:ALA:HB1	1.98	0.45
1:o:396:GLY:O	1:o:397:ARG:C	2.59	0.45
1:s:527:GLY:O	1:s:531:GLN:HG2	2.13	0.45
1:y:449:ASP:O	1:y:449:ASP:CG	2.60	0.45
1:3:509:GLU:OE1	1:3:524:ARG:NH2	2.50	0.45
2:L:83:LEU:HD13	2:L:123:PHE:CZ	2.51	0.45
2:T:6:LEU:C	2:T:6:LEU:HD12	2.40	0.45
2:j:401:LEU:HA	2:j:402:PRO:HD3	1.68	0.45
2:t:468:VAL:HG12	2:t:517:ILE:HD12	1.98	0.45
1:D:93:ASP:OD1	2:R:66:TYR:OH	2.24	0.45
1:D:217:ARG:HA	1:D:218:PRO:HD3	1.85	0.45
1:F:217:ARG:HA	1:F:218:PRO:HD3	1.84	0.45
1:K:35:TYR:CE1	1:K:37:GLY:N	2.84	0.45
1:K:182:ARG:HH12	1:K:234:LEU:C	2.25	0.45
1:M:35:TYR:CD2	1:M:38:GLY:O	2.69	0.45
1:M:62:PHE:CD1	1:M:62:PHE:C	2.94	0.45
1:M:167:LEU:O	1:M:168:LYS:C	2.58	0.45
1:Q:35:TYR:CE2	1:Q:40:LEU:HB2	2.51	0.45
1:1:18:GLU:OE1	1:1:18:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:467:LEU:O	1:a:468:LYS:C	2.58	0.45
1:b:443:TYR:CD2	1:b:444:ASP:N	2.85	0.45
1:d:442:THR:OG1	1:d:444:ASP:OD1	2.34	0.45
1:f:390:ASP:OD2	1:f:393:ASP:N	2.50	0.45
1:k:390:ASP:OD2	1:k:393:ASP:N	2.50	0.45
1:q:463:ILE:HG23	1:q:487:ALA:O	2.16	0.45
1:s:467:LEU:O	1:s:468:LYS:C	2.59	0.45
1:w:369:ASN:HB3	1:y:404:ALA:HB1	1.99	0.45
1:y:354:SER:CB	1:y:375:ARG:HD2	2.46	0.45
2:C:213:LEU:O	2:C:217:ILE:HG13	2.17	0.45
2:G:218:ILE:HG22	2:G:219:GLU:N	2.31	0.45
2:X:191:PHE:HB3	2:X:192:PRO:HD2	1.98	0.45
2:c:331:VAL:HG11	2:c:333:LYS:HE3	1.98	0.45
2:j:308:TYR:HB2	2:j:309:PRO:CD	2.46	0.45
2:4:313:VAL:HG21	2:4:464:LEU:HD23	1.98	0.45
1:F:74:LEU:HA	1:F:74:LEU:HD23	1.46	0.45
1:Q:107:LEU:HD12	1:Q:141:ILE:CG2	2.47	0.45
1:S:54:SER:CB	1:S:75:ARG:HD2	2.46	0.45
1:U:35:TYR:CE2	1:U:38:GLY:O	2.70	0.45
1:U:181:LEU:CD2	1:U:233:LEU:CB	2.95	0.45
1:f:441:ILE:HD12	1:f:441:ILE:N	2.31	0.45
1:k:456:MET:HE3	1:k:456:MET:HB2	1.72	0.45
1:u:356:LEU:HG	1:u:362:PHE:HB2	1.98	0.45
1:y:356:LEU:HG	1:y:362:PHE:HB2	1.97	0.45
2:2:1:OZT:H17	2:2:33:LYS:HZ1	1.81	0.45
2:j:325:MET:HG2	2:r:445:PHE:HZ	1.81	0.45
2:p:491:PHE:HB3	2:p:492:PRO:HD2	1.97	0.45
2:x:465:ARG:HG3	2:x:513:LEU:HD22	1.98	0.45
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.51	0.45
1:U:175:ALA:C	1:U:176:SER:O	2.60	0.45
1:1:35:TYR:CD1	1:1:37:GLY:N	2.85	0.45
1:b:441:ILE:N	1:b:441:ILE:CD1	2.76	0.45
1:d:444:ASP:OD1	1:d:446:SER:OG	2.30	0.45
1:f:330:VAL:HG22	1:f:343:ALA:HB1	1.98	0.45
1:o:313:MET:HE3	1:o:313:MET:N	2.30	0.45
2:H:1:OZT:H27	2:H:33:LYS:CE	2.47	0.45
2:E:191:PHE:HB3	2:E:192:PRO:HD2	1.99	0.45
2:L:211:ALA:HB1	2:L:215:ARG:NH2	2.32	0.45
2:N:103:LEU:HD23	2:N:103:LEU:HA	1.84	0.45
2:R:101:LEU:HA	2:R:102:PRO:HD3	1.69	0.45
2:2:156:GLN:OE1	2:2:165:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:383:LEU:HD13	2:h:423:PHE:CZ	2.52	0.45
2:g:301:OZT:H17	2:g:317:ASP:CG	2.41	0.45
2:l:407:TYR:HB2	2:l:497:ILE:HG22	1.99	0.45
2:v:485:ASP:OD1	2:v:488:ARG:HB2	2.17	0.45
1:B:36:ALA:HA	1:B:174:ASN:HD22	1.82	0.45
1:F:35:TYR:HD1	1:F:37:GLY:H	1.65	0.45
1:F:161:GLU:H	1:F:161:GLU:CD	2.25	0.45
1:K:20:ALA:O	1:K:24:ILE:HG13	2.17	0.45
1:M:15:GLU:OE1	2:j:519:GLU:CD	2.60	0.45
1:O:83:ASP:OD2	2:P:65:HIS:HD2	1.99	0.45
1:k:358:ASP:HB3	1:k:519:ARG:O	2.17	0.45
1:m:362:PHE:CD1	1:m:362:PHE:C	2.95	0.45
1:y:341:PHE:HB2	1:y:353:ILE:HD13	1.91	0.45
2:H:45:ILE:N	2:H:45:ILE:HD12	2.32	0.45
2:H:49:ALA:O	2:H:53:VAL:CG2	2.65	0.45
2:L:10:GLY:HA2	2:L:114:PRO:O	2.17	0.45
2:L:217:ILE:O	2:L:221:ARG:HG3	2.17	0.45
2:T:220:SER:O	2:T:220:SER:OG	2.35	0.45
2:X:109:ILE:H	2:X:109:ILE:HG12	1.52	0.45
2:Z:169:GLU:HA	2:Z:217:ILE:CD1	2.46	0.45
2:g:314:MET:CE	2:g:403:LEU:HD13	2.47	0.45
2:g:345:ILE:HD12	2:g:345:ILE:N	2.32	0.45
2:g:456:GLN:OE1	2:g:465:ARG:NH2	2.50	0.45
2:j:313:VAL:HG21	2:j:464:LEU:HD23	1.98	0.45
2:j:331:VAL:CG1	2:j:333:LYS:HE3	2.46	0.45
2:p:313:VAL:HG21	2:p:464:LEU:HD23	1.99	0.45
2:p:338:ASP:C	2:p:338:ASP:OD1	2.60	0.45
2:z:336:ILE:CG2	2:z:338:ASP:O	2.65	0.45
2:4:464:LEU:HD13	2:4:513:LEU:CD1	2.46	0.45
1:M:41:PHE:CB	1:M:53:ILE:HD13	2.45	0.45
1:M:127:VAL:HG12	1:M:128:ALA:N	2.31	0.45
1:Q:56:LEU:HD23	1:Q:56:LEU:HA	1.79	0.45
1:U:217:ARG:HH21	1:U:223:ARG:HG3	1.80	0.45
1:a:357:TYR:OH	1:a:386:GLY:HA3	2.16	0.45
1:b:428:ALA:HB2	1:b:434:LYS:HB3	1.98	0.45
1:k:362:PHE:C	1:k:362:PHE:CD1	2.95	0.45
1:k:467:LEU:O	1:k:468:LYS:C	2.60	0.45
1:u:356:LEU:HG	1:u:362:PHE:CB	2.47	0.45
2:H:185:ASP:OD1	2:H:188:ARG:HB2	2.17	0.45
2:G:49:ALA:O	2:G:53:VAL:CG2	2.65	0.45
2:G:101:LEU:HA	2:G:102:PRO:HD3	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:54:GLU:HA	2:Z:54:GLU:OE1	2.16	0.45
2:Z:198:ASP:OD1	2:Z:198:ASP:N	2.50	0.45
2:2:216:ALA:O	2:2:220:SER:HB3	2.16	0.45
2:e:491:PHE:HB3	2:e:492:PRO:HD2	1.99	0.45
2:j:432:GLU:HG3	2:j:437:GLN:HB2	1.98	0.45
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.85	0.45
1:M:57:TYR:O	1:M:58:ASP:C	2.59	0.45
1:O:225:ILE:CG2	1:O:229:ALA:HB1	2.47	0.45
1:Q:141:ILE:HD12	1:Q:141:ILE:N	2.32	0.45
1:S:172:ALA:O	1:S:175:ALA:HB2	2.17	0.45
1:W:115:ALA:HB3	1:Y:112:THR:CG2	2.32	0.45
1:a:335:TYR:CD2	1:a:338:GLY:O	2.70	0.45
1:d:358:ASP:OD1	1:d:519:ARG:NH1	2.50	0.45
1:i:389:TYR:CD1	2:c:374:LEU:HD21	2.49	0.45
1:k:330:VAL:HG12	1:k:331:VAL:N	2.32	0.45
1:k:430:TYR:CE1	1:k:516:ASN:O	2.70	0.45
1:s:357:TYR:OH	1:s:386:GLY:HA3	2.17	0.45
2:G:140:GLY:O	2:G:143:SER:HB3	2.17	0.45
2:L:132:GLU:HG3	2:L:137:GLN:HB2	1.98	0.45
2:R:103:LEU:HD23	2:R:103:LEU:HA	1.85	0.45
2:g:307:LYS:HE3	2:g:418:GLY:O	2.17	0.45
2:j:338:ASP:C	2:j:338:ASP:OD1	2.59	0.45
2:v:472:TYR:CE1	2:v:518:ILE:HG12	2.52	0.45
2:4:349:ALA:O	2:4:353:VAL:CG2	2.65	0.45
1:A:58:ASP:HB3	1:A:219:ARG:O	2.17	0.45
1:D:16:ARG:HB3	1:D:117:PRO:CG	2.47	0.45
1:K:56:LEU:HD23	1:K:56:LEU:HA	1.77	0.45
1:M:127:VAL:HG23	1:M:213:LEU:CD2	2.47	0.45
1:S:233:LEU:HA	1:S:233:LEU:HD23	1.70	0.45
1:W:69:ASN:HB3	1:Y:104:ALA:HB1	1.97	0.45
1:W:123:CYS:HA	1:W:139:TYR:O	2.17	0.45
1:1:30:VAL:HG22	1:1:43:ALA:HB1	1.99	0.45
1:m:355:GLU:HB2	1:m:522:PHE:CD2	2.52	0.45
1:o:467:LEU:O	1:o:468:LYS:C	2.60	0.45
1:u:333:LEU:HD23	1:u:340:LEU:O	2.17	0.45
1:w:331:VAL:HG12	1:w:333:LEU:HD23	1.99	0.45
2:G:44:GLY:C	2:G:45:ILE:HD12	2.42	0.45
2:N:171:LEU:HD23	2:N:171:LEU:HA	1.77	0.45
2:R:31:VAL:HG11	2:R:33:LYS:HE3	1.98	0.45
2:X:37:THR:HG23	2:X:43:THR:HG23	1.99	0.45
2:g:407:TYR:HB2	2:g:497:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:331:VAL:HG11	2:p:333:LYS:HE3	1.98	0.45
2:t:305:ALA:HB2	2:t:314:MET:HE2	1.99	0.45
1:Q:57:TYR:OH	1:Q:86:GLY:HA3	2.17	0.44
1:W:156:MET:HE3	1:W:156:MET:HB2	1.71	0.44
1:l:226:THR:CG2	1:l:227:GLY:N	2.80	0.44
1:b:383:ASP:OD2	2:c:365:HIS:HD2	1.99	0.44
1:k:534:LEU:HD12	1:k:534:LEU:N	2.32	0.44
1:m:456:MET:HE3	1:m:456:MET:HB2	1.70	0.44
1:o:362:PHE:CD1	1:o:362:PHE:C	2.94	0.44
1:q:330:VAL:HG13	1:q:343:ALA:HB2	1.99	0.44
1:w:340:LEU:HD13	1:w:512:VAL:CG1	2.45	0.44
2:C:49:ALA:O	2:C:53:VAL:HG23	2.17	0.44
2:T:31:VAL:CG1	2:T:33:LYS:HE3	2.47	0.44
2:V:48:THR:OG1	2:V:51:VAL:HG23	2.17	0.44
2:V:83:LEU:HD13	2:V:123:PHE:CE1	2.52	0.44
2:X:83:LEU:HD13	2:X:123:PHE:CE1	2.52	0.44
2:X:156:GLN:OE1	2:X:165:ARG:NH2	2.51	0.44
2:h:358:LEU:HD12	2:h:358:LEU:O	2.17	0.44
2:z:337:THR:HG21	2:z:359:TYR:CD2	2.49	0.44
1:I:161:GLU:N	1:I:162:PRO:CD	2.80	0.44
1:S:230:LEU:HD23	1:S:231:GLN:CA	2.46	0.44
1:W:163:ILE:HG23	1:W:187:ALA:C	2.42	0.44
1:b:314:ARG:HG3	1:b:314:ARG:NH1	2.31	0.44
1:b:463:ILE:HG23	1:b:487:ALA:O	2.17	0.44
1:u:356:LEU:CD1	1:u:362:PHE:HB2	2.47	0.44
2:R:36:ILE:CG2	2:R:38:ASP:O	2.65	0.44
2:R:38:ASP:OD1	2:R:41:THR:N	2.50	0.44
2:T:156:GLN:OE1	2:T:165:ARG:NH2	2.50	0.44
2:V:64:GLU:O	2:V:65:HIS:C	2.59	0.44
2:Z:156:GLN:OE1	2:Z:165:ARG:NH2	2.51	0.44
2:2:31:VAL:HG11	2:2:33:LYS:HE3	2.00	0.44
2:c:338:ASP:OD1	2:c:341:THR:OG1	2.30	0.44
2:n:401:LEU:HA	2:n:402:PRO:HD3	1.67	0.44
2:t:331:VAL:HG12	2:t:333:LYS:HG3	1.99	0.44
2:t:383:LEU:HD13	2:t:423:PHE:CE1	2.52	0.44
2:t:464:LEU:HD11	2:t:505:VAL:HG11	1.99	0.44
2:x:301:OZT:C7	2:x:319:ARG:O	2.65	0.44
2:4:491:PHE:HB3	2:4:492:PRO:HD2	1.99	0.44
1:M:15:GLU:CD	2:j:519:GLU:HG2	2.43	0.44
1:S:35:TYR:CD1	1:S:35:TYR:C	2.95	0.44
1:a:330:VAL:HG13	1:a:343:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:310:GLU:O	1:o:314:ARG:HG3	2.17	0.44
2:H:101:LEU:HA	2:H:102:PRO:HD3	1.63	0.44
2:H:145:PHE:CE1	2:E:144:LEU:HD13	2.52	0.44
2:L:49:ALA:O	2:L:53:VAL:CG2	2.65	0.44
2:N:1:OZT:H27	2:N:33:LYS:NZ	2.31	0.44
2:N:129:TRP:CD1	2:N:129:TRP:H	2.34	0.44
2:N:168:VAL:HG12	2:N:217:ILE:CD1	2.47	0.44
2:P:101:LEU:HA	2:P:102:PRO:HD3	1.65	0.44
2:Z:107:TYR:CB	2:Z:197:ILE:CG2	2.94	0.44
2:j:434:GLU:OE2	2:t:329:ARG:NH1	2.50	0.44
2:t:401:LEU:HA	2:t:402:PRO:HD3	1.69	0.44
2:v:331:VAL:HG11	2:v:333:LYS:HE3	1.98	0.44
2:z:331:VAL:CG1	2:z:333:LYS:HE3	2.48	0.44
1:A:59:ARG:NH2	1:A:221:ALA:HB2	2.32	0.44
1:A:80:GLN:O	1:A:81:PHE:C	2.60	0.44
1:A:161:GLU:H	1:A:161:GLU:CD	2.25	0.44
1:F:79:ILE:O	1:F:80:GLN:C	2.60	0.44
1:I:129:HIS:HB2	1:I:132:GLU:HG2	1.99	0.44
1:K:30:VAL:HG22	1:K:43:ALA:HB1	1.98	0.44
1:M:156:MET:HE3	1:M:156:MET:HB2	1.61	0.44
1:O:225:ILE:CG2	1:O:229:ALA:CB	2.95	0.44
1:W:57:TYR:O	1:W:58:ASP:C	2.60	0.44
1:Y:62:PHE:CD1	1:Y:62:PHE:C	2.95	0.44
1:w:354:SER:CB	1:w:375:ARG:HD2	2.48	0.44
1:y:355:GLU:HB2	1:y:522:PHE:CB	2.46	0.44
1:y:478:THR:N	1:y:533:LEU:HD21	2.33	0.44
1:3:451:PRO:HB3	3:3:110:HOH:O	2.17	0.44
2:G:107:TYR:HB2	2:G:197:ILE:HG22	1.99	0.44
2:G:132:GLU:HG3	2:G:137:GLN:HB2	1.99	0.44
2:N:58:LEU:O	2:N:58:LEU:HD12	2.17	0.44
2:T:205:VAL:HA	2:T:206:PRO:HD3	1.85	0.44
2:X:132:GLU:HG3	2:X:137:GLN:HB2	1.99	0.44
2:h:505:VAL:HA	2:h:506:PRO:HD3	1.84	0.44
2:l:413:ASP:HA	2:l:414:PRO:HD3	1.83	0.44
2:v:383:LEU:HD13	2:v:423:PHE:CZ	2.53	0.44
2:z:349:ALA:O	2:z:353:VAL:HG23	2.16	0.44
2:4:432:GLU:HG3	2:4:437:GLN:HB2	1.99	0.44
1:F:212:VAL:HG23	1:F:212:VAL:O	2.17	0.44
1:S:49:SER:HB2	1:1:97:ARG:CG	2.46	0.44
1:o:336:ALA:N	1:o:474:ASN:HA	2.32	0.44
1:q:357:TYR:OH	1:q:386:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:467:LEU:O	1:q:468:LYS:C	2.61	0.44
1:u:481:LEU:HD22	1:u:533:LEU:HG	1.99	0.44
2:L:31:VAL:CG1	2:L:33:LYS:HE3	2.48	0.44
2:L:185:ASP:OD1	2:L:188:ARG:HB2	2.17	0.44
2:R:45:ILE:N	2:R:45:ILE:HD12	2.32	0.44
2:V:109:ILE:H	2:V:109:ILE:HG12	1.47	0.44
2:h:432:GLU:HG3	2:h:437:GLN:HB2	1.99	0.44
2:g:514:ALA:O	2:g:515:ARG:C	2.59	0.44
2:x:456:GLN:OE1	2:x:465:ARG:NH2	2.49	0.44
2:x:491:PHE:HB3	2:x:492:PRO:HD2	1.98	0.44
1:B:23:GLY:HA3	1:B:119:GLU:OE2	2.18	0.44
1:F:38:GLY:HA3	1:F:213:LEU:O	2.18	0.44
1:K:11:GLN:HE22	2:j:513:LEU:HD21	1.82	0.44
1:Q:31:VAL:CG1	1:Q:33:LEU:CD2	2.94	0.44
1:a:330:VAL:HG22	1:a:343:ALA:CB	2.48	0.44
1:f:467:LEU:O	1:f:468:LYS:C	2.60	0.44
1:i:438:LEU:HD12	1:i:438:LEU:N	2.32	0.44
1:y:331:VAL:HG12	1:y:333:LEU:HD23	1.98	0.44
1:y:467:LEU:O	1:y:468:LYS:C	2.60	0.44
2:L:213:LEU:O	2:L:217:ILE:HG13	2.17	0.44
2:h:345:ILE:HD12	2:h:345:ILE:N	2.33	0.44
2:c:386:MET:HE3	2:c:386:MET:HB2	1.72	0.44
2:l:301:OZT:O	2:l:440:GLY:HA3	2.17	0.44
2:v:308:TYR:HB2	2:v:309:PRO:CD	2.48	0.44
2:4:505:VAL:HA	2:4:506:PRO:HD3	1.83	0.44
1:F:71:PHE:CD1	1:F:71:PHE:C	2.95	0.44
1:F:207:SER:O	1:F:208:LEU:HD23	2.18	0.44
1:M:17:SER:HA	1:M:143:TYR:CE2	2.53	0.44
1:Q:230:LEU:HD23	1:Q:231:GLN:N	2.32	0.44
1:l:79:ILE:HD12	2:2:69:LEU:HD23	2.00	0.44
1:d:357:TYR:CD1	1:d:382:ALA:HB1	2.53	0.44
1:k:509:GLU:OE1	1:k:524:ARG:NH2	2.51	0.44
1:s:330:VAL:HG12	1:s:331:VAL:N	2.31	0.44
1:u:341:PHE:CB	1:u:353:ILE:HD13	2.43	0.44
1:3:467:LEU:O	1:3:468:LYS:C	2.61	0.44
1:3:526:THR:CG2	1:3:527:GLY:N	2.78	0.44
2:H:48:THR:OG1	2:H:51:VAL:HG23	2.16	0.44
2:E:31:VAL:CG1	2:E:33:LYS:HE3	2.48	0.44
2:P:86:MET:HE3	2:P:86:MET:HB2	1.71	0.44
2:X:49:ALA:O	2:X:53:VAL:HG23	2.17	0.44
2:X:103:LEU:HD23	2:X:103:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:194:ALA:HB3	2:Z:210:ILE:HD11	1.99	0.44
2:l:314:MET:HE2	2:l:403:LEU:HD13	1.99	0.44
2:l:491:PHE:CD1	2:l:491:PHE:N	2.85	0.44
2:n:339:ASP:O	2:n:502:ALA:N	2.50	0.44
2:p:331:VAL:CG1	2:p:333:LYS:HE3	2.48	0.44
2:r:383:LEU:HD13	2:r:423:PHE:CE1	2.52	0.44
2:x:409:ILE:H	2:x:409:ILE:HG12	1.48	0.44
1:O:217:ARG:HH21	1:O:223:ARG:HG3	1.78	0.44
1:Q:12:ALA:O	1:Q:16:ARG:HG3	2.17	0.44
1:U:167:LEU:O	1:U:168:LYS:C	2.60	0.44
1:W:30:VAL:HG13	1:W:43:ALA:HB2	2.00	0.44
1:Y:138:LEU:HD12	1:Y:138:LEU:N	2.33	0.44
1:k:534:LEU:CD1	1:k:534:LEU:N	2.81	0.44
1:m:341:PHE:CB	1:m:353:ILE:HD13	2.45	0.44
1:m:370:GLU:HB3	1:m:418:TYR:CD2	2.52	0.44
1:s:452:HIS:HB3	1:s:471:TYR:CE2	2.53	0.44
1:3:330:VAL:HG13	1:3:343:ALA:HB2	1.99	0.44
2:H:13:VAL:HG21	2:H:164:LEU:HD23	1.99	0.44
2:E:107:TYR:CB	2:E:197:ILE:HG22	2.38	0.44
2:T:19:ARG:HH11	2:T:26:ILE:CD1	2.31	0.44
2:h:306:LEU:C	2:h:306:LEU:HD12	2.43	0.44
2:j:403:LEU:HD23	2:j:403:LEU:HA	1.89	0.44
2:p:383:LEU:HD13	2:p:423:PHE:CE1	2.53	0.44
2:4:440:GLY:O	2:4:443:SER:HB3	2.18	0.44
1:F:48:ARG:HH22	1:W:135:ARG:NH1	2.16	0.44
1:F:135:ARG:O	1:F:136:PRO:C	2.61	0.44
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.53	0.44
1:K:97:ARG:NH1	3:K:249:HOH:O	2.50	0.44
1:U:178:THR:HB	1:U:233:LEU:CD2	2.48	0.44
1:1:56:LEU:HD23	1:1:56:LEU:HA	1.84	0.44
1:a:456:MET:HE3	1:a:456:MET:HB2	1.77	0.44
1:b:456:MET:HE3	1:b:456:MET:HB2	1.68	0.44
1:i:330:VAL:HG13	1:i:343:ALA:HB2	2.00	0.44
1:o:449:ASP:CG	1:o:449:ASP:O	2.61	0.44
1:w:349:SER:HB3	1:y:437:GLU:OE2	2.18	0.44
2:H:6:LEU:C	2:H:6:LEU:HD12	2.42	0.44
2:E:61:VAL:O	2:E:61:VAL:HG12	2.17	0.44
2:L:75:THR:O	2:L:76:PHE:C	2.58	0.44
2:T:109:ILE:H	2:T:109:ILE:HG12	1.43	0.44
2:T:132:GLU:HG3	2:T:137:GLN:HB2	2.00	0.44
2:g:513:LEU:HD23	2:g:513:LEU:HA	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:468:VAL:HG12	2:p:517:ILE:HD12	2.00	0.44
2:t:335:TYR:CZ	2:t:353:VAL:HG13	2.53	0.44
2:t:456:GLN:OE1	2:t:465:ARG:NH2	2.51	0.44
1:D:60:VAL:HG21	1:D:99:LEU:CD1	2.48	0.43
1:D:75:ARG:O	1:D:79:ILE:HG13	2.17	0.43
1:F:35:TYR:CD2	1:F:40:LEU:HB2	2.53	0.43
1:F:181:LEU:HD12	1:F:181:LEU:HA	1.76	0.43
1:M:15:GLU:HB2	2:j:519:GLU:CB	2.36	0.43
1:S:163:ILE:HG23	1:S:187:ALA:O	2.18	0.43
1:a:527:GLY:HA2	1:a:530:LEU:HB3	1.99	0.43
1:b:414:GLN:HE21	1:b:414:GLN:HB3	1.60	0.43
1:f:311:GLN:CG	1:f:314:ARG:NH2	2.72	0.43
1:o:330:VAL:HG22	1:o:343:ALA:CB	2.48	0.43
1:o:357:TYR:HB3	1:o:360:VAL:HG13	1.98	0.43
1:s:481:LEU:HD22	1:s:533:LEU:HD12	2.00	0.43
1:w:421:GLU:HG2	1:w:456:MET:HG2	1.99	0.43
2:P:65:HIS:CE1	2:P:69:LEU:HD11	2.53	0.43
2:e:407:TYR:HB2	2:e:497:ILE:HG22	2.00	0.43
2:j:365:HIS:CE1	2:j:369:LEU:HD11	2.53	0.43
2:t:383:LEU:HD13	2:t:423:PHE:CZ	2.53	0.43
1:B:53:ILE:HG22	1:B:54:SER:N	2.33	0.43
1:B:56:LEU:CD1	1:B:62:PHE:HB2	2.48	0.43
1:B:130:TYR:HE1	1:B:216:ASN:O	2.00	0.43
1:I:208:LEU:HD23	1:I:208:LEU:HA	1.69	0.43
1:Q:57:TYR:O	1:Q:58:ASP:C	2.61	0.43
1:S:57:TYR:O	1:S:58:ASP:C	2.58	0.43
1:Y:163:ILE:HG23	1:Y:187:ALA:HB1	2.00	0.43
1:l:114:GLN:HE21	1:l:114:GLN:HB3	1.60	0.43
1:a:428:ALA:HB2	1:a:434:LYS:HB3	1.99	0.43
1:f:330:VAL:HG13	1:f:343:ALA:HB2	1.99	0.43
1:f:452:HIS:CD2	1:f:471:TYR:HE2	2.36	0.43
1:s:331:VAL:HG12	1:s:333:LEU:HD22	2.00	0.43
2:H:86:MET:HE3	2:H:86:MET:HB2	1.72	0.43
2:E:132:GLU:OE1	2:E:132:GLU:HA	2.18	0.43
2:T:37:THR:HG23	2:T:43:THR:HG23	1.97	0.43
2:V:54:GLU:OE1	2:V:54:GLU:HA	2.18	0.43
2:c:401:LEU:HA	2:c:402:PRO:HD3	1.68	0.43
2:v:444:LEU:HD22	2:v:444:LEU:HA	1.85	0.43
1:A:45:ASN:HD22	1:A:209:GLU:HG3	1.83	0.43
1:D:126:GLU:HG2	1:D:127:VAL:N	2.33	0.43
1:U:210:VAL:HG12	1:U:225:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:312:ALA:O	1:a:316:ARG:HG3	2.17	0.43
1:a:362:PHE:CD1	1:a:362:PHE:C	2.95	0.43
1:a:429:HIS:O	1:a:430:TYR:C	2.59	0.43
1:d:310:GLU:OE1	1:d:310:GLU:CA	2.67	0.43
1:k:528:SER:O	1:k:531:GLN:N	2.51	0.43
2:J:198:ASP:OD1	2:J:198:ASP:N	2.51	0.43
2:N:65:HIS:CE1	2:N:69:LEU:HD11	2.53	0.43
2:N:191:PHE:HB3	2:N:192:PRO:HD2	2.00	0.43
2:h:338:ASP:C	2:h:338:ASP:OD1	2.61	0.43
2:n:456:GLN:OE1	2:n:465:ARG:NH2	2.51	0.43
1:A:86:GLY:HA2	1:A:90:ASP:O	2.17	0.43
1:D:220:ARG:NH2	2:E:67:GLU:OE1	2.48	0.43
1:K:149:ASP:CG	1:K:149:ASP:O	2.61	0.43
1:M:152:HIS:CG	1:M:171:TYR:HE2	2.37	0.43
1:O:114:GLN:HE21	1:O:114:GLN:HB3	1.57	0.43
1:f:414:GLN:HE21	1:f:414:GLN:HB3	1.59	0.43
1:o:531:GLN:HA	1:o:534:LEU:HD12	1.99	0.43
1:s:430:TYR:CD2	1:s:430:TYR:C	2.97	0.43
1:u:533:LEU:HA	1:u:533:LEU:HD12	1.74	0.43
1:w:335:TYR:CD1	1:w:336:ALA:N	2.86	0.43
1:y:356:LEU:HD13	1:y:399:LEU:HD13	1.99	0.43
2:N:44:GLY:C	2:N:45:ILE:HD12	2.44	0.43
2:Z:86:MET:HE3	2:Z:86:MET:HB2	1.75	0.43
2:2:211:ALA:O	2:2:212:GLU:C	2.61	0.43
2:r:337:THR:HG21	2:r:343:THR:HG23	1.99	0.43
2:v:313:VAL:HG21	2:v:464:LEU:HD23	2.00	0.43
1:B:205:VAL:HG22	1:B:207:SER:OG	2.18	0.43
1:D:94:VAL:HA	1:D:98:GLN:NE2	2.33	0.43
1:U:123:CYS:HA	1:U:139:TYR:O	2.18	0.43
1:a:357:TYR:O	1:a:358:ASP:C	2.59	0.43
1:a:526:THR:HG23	1:a:527:GLY:H	1.84	0.43
1:b:517:ARG:HH21	1:b:523:ARG:HG3	1.83	0.43
1:o:331:VAL:HG12	1:o:333:LEU:HD23	2.00	0.43
1:o:463:ILE:HG23	1:o:487:ALA:C	2.43	0.43
1:u:484:ALA:O	1:u:488:LEU:HG	2.18	0.43
2:C:31:VAL:HG12	2:C:33:LYS:HG3	2.00	0.43
2:E:50:ALA:HB2	2:R:129:TRP:O	2.18	0.43
2:N:113:ASP:HA	2:N:114:PRO:HD3	1.86	0.43
2:h:301:OZT:H27	2:h:333:LYS:HE2	1.99	0.43
2:h:354:GLU:OE1	2:h:354:GLU:HA	2.18	0.43
2:j:486:LEU:CD2	2:j:491:PHE:CZ	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:345:ILE:N	2:n:345:ILE:HD12	2.33	0.43
2:r:386:MET:HE3	2:r:386:MET:HB2	1.66	0.43
2:v:333:LYS:O	2:v:344:GLY:HA2	2.18	0.43
2:z:383:LEU:HD13	2:z:423:PHE:CZ	2.53	0.43
2:z:485:ASP:OD1	2:z:488:ARG:HB2	2.19	0.43
1:A:56:LEU:HD11	1:A:62:PHE:HB2	1.98	0.43
1:I:40:LEU:CD1	1:I:212:VAL:HG12	2.49	0.43
1:K:89:TYR:CD1	2:E:82:ARG:HD3	2.54	0.43
1:b:330:VAL:HG22	1:b:343:ALA:HB1	2.01	0.43
1:b:451:PRO:HD2	1:b:452:HIS:H	1.84	0.43
1:k:522:PHE:CE2	1:k:524:ARG:HG2	2.54	0.43
1:q:356:LEU:HD23	1:q:356:LEU:HA	1.75	0.43
1:s:331:VAL:HG12	1:s:333:LEU:HD23	2.00	0.43
1:u:414:GLN:HE21	1:u:414:GLN:HB3	1.57	0.43
1:u:456:MET:HB2	1:u:456:MET:HE3	1.72	0.43
2:E:76:PHE:CE2	2:E:80:ILE:HD11	2.53	0.43
2:e:307:LYS:HD3	3:e:48:HOH:O	2.17	0.43
2:l:386:MET:HE3	2:l:386:MET:HB2	1.74	0.43
2:l:459:ASP:OD1	2:l:459:ASP:N	2.51	0.43
2:t:409:ILE:H	2:t:409:ILE:HG12	1.53	0.43
2:x:383:LEU:HD13	2:x:423:PHE:CE1	2.53	0.43
1:A:151:PRO:HD2	3:A:249:HOH:O	2.19	0.43
1:B:181:LEU:HA	1:B:181:LEU:HD12	1.80	0.43
1:I:83:ASP:OD2	2:J:65:HIS:CD2	2.69	0.43
1:K:156:MET:HE3	1:K:156:MET:HB2	1.71	0.43
1:M:212:VAL:HG23	1:M:223:ARG:HB3	2.01	0.43
1:O:57:TYR:O	1:O:58:ASP:C	2.61	0.43
1:S:141:ILE:N	1:S:141:ILE:HD12	2.34	0.43
1:W:209:GLU:OE1	1:W:224:ARG:NH2	2.52	0.43
1:Y:58:ASP:OD1	1:Y:219:ARG:NH1	2.51	0.43
1:Y:208:LEU:HD23	1:Y:208:LEU:HA	1.75	0.43
1:a:526:THR:HG22	1:a:528:SER:H	1.84	0.43
1:b:429:HIS:O	1:b:430:TYR:C	2.62	0.43
1:q:525:ILE:HG22	1:q:530:LEU:HG	2.00	0.43
1:y:421:GLU:HG2	1:y:456:MET:HG2	2.00	0.43
1:3:335:TYR:CE1	1:3:338:GLY:N	2.87	0.43
2:N:31:VAL:HG12	2:N:33:LYS:HG3	2.01	0.43
2:T:45:ILE:HD12	2:T:45:ILE:N	2.34	0.43
2:v:386:MET:HE3	2:v:386:MET:HB2	1.71	0.43
2:v:430:ASN:HD22	2:v:430:ASN:C	2.24	0.43
2:x:383:LEU:HD13	2:x:423:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:498:ASP:OD1	2:z:500:ASP:HB2	2.19	0.43
1:M:129:HIS:HB2	1:M:132:GLU:CG	2.48	0.43
1:S:90:ASP:OD2	1:S:93:ASP:N	2.52	0.43
1:l:18:GLU:O	1:l:22:LYS:HG3	2.18	0.43
1:a:517:ARG:HH21	1:a:523:ARG:HG3	1.81	0.43
1:b:310:GLU:O	1:b:312:ALA:N	2.52	0.43
1:d:330:VAL:HG12	1:d:331:VAL:N	2.33	0.43
1:m:359:ARG:HA	1:m:359:ARG:HD2	1.94	0.43
1:m:390:ASP:OD2	1:m:393:ASP:N	2.51	0.43
1:q:330:VAL:HG22	1:q:343:ALA:HB1	2.01	0.43
1:u:354:SER:CB	1:u:375:ARG:HD2	2.49	0.43
1:w:508:LEU:HA	1:w:508:LEU:HD23	1.69	0.43
1:3:485:VAL:O	1:3:489:ARG:HG3	2.19	0.43
2:C:101:LEU:HA	2:C:102:PRO:HD3	1.63	0.43
2:J:101:LEU:HA	2:J:102:PRO:HD3	1.65	0.43
2:T:144:LEU:HD22	2:T:144:LEU:HA	1.88	0.43
2:V:129:TRP:CD1	2:V:129:TRP:H	2.37	0.43
2:X:35:TYR:CZ	2:X:53:VAL:HG13	2.53	0.43
2:X:134:GLU:OE2	2:Z:29:ARG:NH1	2.51	0.43
2:Z:37:THR:HG21	2:Z:43:THR:CG2	2.47	0.43
2:2:101:LEU:HA	2:2:102:PRO:HD3	1.71	0.43
2:2:205:VAL:HA	2:2:206:PRO:HD3	1.83	0.43
2:r:331:VAL:HG12	2:r:333:LYS:HG3	2.00	0.43
2:v:341:THR:HG22	2:v:406:GLY:HA3	2.00	0.43
2:x:348:THR:OG1	2:x:351:VAL:HG23	2.19	0.43
2:x:401:LEU:HA	2:x:402:PRO:HD3	1.71	0.43
1:A:56:LEU:HG	1:A:62:PHE:CB	2.49	0.43
1:D:111:PHE:HD1	1:D:117:PRO:HB3	1.84	0.43
1:K:49:SER:O	1:K:51:GLN:OE1	2.36	0.43
1:U:178:THR:HB	1:U:233:LEU:HD22	2.00	0.43
1:b:513:LEU:HD12	1:b:513:LEU:HA	1.75	0.43
1:d:335:TYR:CD1	1:d:336:ALA:N	2.87	0.43
1:o:322:LYS:O	1:o:326:ARG:HG3	2.19	0.43
1:s:514:ASP:OD2	1:s:516:ASN:CB	2.66	0.43
1:u:478:THR:HG23	1:u:479:ASP:N	2.34	0.43
2:E:19:ARG:HG3	2:E:20:SER:H	1.83	0.43
2:N:54:GLU:OE1	2:N:54:GLU:HA	2.18	0.43
2:N:156:GLN:OE1	2:N:165:ARG:NH2	2.52	0.43
2:T:164:LEU:HD13	2:T:213:LEU:HD11	2.00	0.43
2:Z:31:VAL:HG11	2:Z:33:LYS:HE3	1.99	0.43
2:2:8:TYR:HB2	2:2:9:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:386:MET:HE3	2:h:386:MET:HB2	1.77	0.43
2:h:464:LEU:HD13	2:h:513:LEU:HD11	2.00	0.43
2:x:354:GLU:OE1	2:x:354:GLU:HA	2.18	0.43
2:z:432:GLU:OE1	2:z:432:GLU:HA	2.19	0.43
2:4:308:TYR:HB2	2:4:309:PRO:CD	2.49	0.43
1:K:56:LEU:HD13	1:K:99:LEU:HD13	2.01	0.43
1:O:121:GLU:HG2	1:O:156:MET:HG2	2.01	0.43
1:Q:142:THR:O	1:Q:143:TYR:C	2.62	0.43
1:S:210:VAL:HG12	1:S:225:ILE:HD12	2.01	0.43
1:U:11:GLN:HA	1:U:11:GLN:NE2	2.21	0.43
1:W:129:HIS:O	1:W:130:TYR:C	2.61	0.43
1:b:310:GLU:O	1:b:311:GLN:C	2.61	0.43
1:f:357:TYR:OH	1:f:386:GLY:HA3	2.19	0.43
1:i:443:TYR:CD2	1:i:443:TYR:C	2.97	0.43
1:i:485:VAL:HG21	1:i:534:LEU:CD1	2.49	0.43
1:s:514:ASP:OD2	1:s:516:ASN:CA	2.66	0.43
1:u:333:LEU:CD1	1:u:480:ALA:HB1	2.48	0.43
2:H:76:PHE:HE2	2:H:80:ILE:HD11	1.82	0.43
2:C:3:ILE:HG22	2:C:4:VAL:N	2.34	0.43
2:E:29:ARG:NH1	2:R:134:GLU:OE2	2.52	0.43
2:E:129:TRP:CD1	2:E:129:TRP:H	2.36	0.43
2:G:38:ASP:OD1	2:G:41:THR:N	2.52	0.43
2:R:37:THR:HG21	2:R:43:THR:CG2	2.49	0.43
2:T:107:TYR:HB2	2:T:197:ILE:HG22	2.00	0.43
2:V:144:LEU:HD22	2:V:144:LEU:HA	1.81	0.43
2:V:191:PHE:CD1	2:V:191:PHE:N	2.86	0.43
2:X:37:THR:HG21	2:X:59:TYR:CD2	2.47	0.43
2:c:313:VAL:HG21	2:c:464:LEU:HD23	2.00	0.43
2:t:319:ARG:NH1	2:t:326:ILE:HD13	2.34	0.43
2:4:456:GLN:OE1	2:4:465:ARG:NH2	2.51	0.43
1:D:219:ARG:NH2	1:D:220:ARG:CD	2.69	0.42
1:M:90:ASP:OD2	1:M:93:ASP:N	2.52	0.42
1:Q:90:ASP:OD2	1:Q:93:ASP:N	2.52	0.42
1:b:318:GLU:CG	1:b:322:LYS:HE3	2.49	0.42
1:b:421:GLU:HG2	1:b:456:MET:HG2	2.01	0.42
1:b:526:THR:O	1:b:530:LEU:N	2.45	0.42
1:d:356:LEU:HG	1:d:362:PHE:CB	2.48	0.42
1:i:428:ALA:HB2	1:i:434:LYS:HB3	2.00	0.42
1:k:508:LEU:HD23	1:k:508:LEU:HA	1.64	0.42
1:u:508:LEU:HD23	1:u:508:LEU:HA	1.69	0.42
1:w:330:VAL:HG22	1:w:343:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:330:VAL:HG22	1:3:343:ALA:HB1	2.01	0.42
2:G:164:LEU:HD23	2:G:164:LEU:HA	1.91	0.42
2:L:101:LEU:HA	2:L:102:PRO:HD3	1.72	0.42
2:N:107:TYR:HB2	2:N:197:ILE:HG22	2.00	0.42
2:T:14:MET:HE1	2:T:103:LEU:O	2.18	0.42
2:Z:109:ILE:H	2:Z:109:ILE:HG12	1.51	0.42
2:j:383:LEU:HD13	2:j:423:PHE:CE1	2.55	0.42
2:j:386:MET:HE3	2:j:386:MET:HB2	1.81	0.42
2:z:403:LEU:HD23	2:z:403:LEU:HA	1.89	0.42
1:A:130:TYR:HE1	1:A:216:ASN:O	2.00	0.42
1:A:135:ARG:HB3	1:A:135:ARG:CZ	2.48	0.42
1:K:50:LEU:C	1:K:51:GLN:OE1	2.61	0.42
1:O:208:LEU:HD23	1:O:208:LEU:HA	1.66	0.42
1:Q:190:ALA:C	1:i:479:ASP:OD1	2.62	0.42
1:Q:208:LEU:HA	1:Q:208:LEU:HD23	1.71	0.42
1:S:181:LEU:CD2	1:S:233:LEU:HB3	2.49	0.42
1:W:30:VAL:HG22	1:W:43:ALA:CB	2.50	0.42
1:Y:156:MET:HE3	1:Y:156:MET:HB2	1.66	0.42
1:a:520:ARG:C	3:a:50:HOH:O	2.61	0.42
1:d:444:ASP:OD1	1:d:446:SER:N	2.30	0.42
1:3:311:GLN:HG3	1:3:314:ARG:HD3	2.01	0.42
2:C:151:LYS:HE2	2:R:221:ARG:HH12	1.83	0.42
2:J:144:LEU:HD22	2:J:144:LEU:HA	1.88	0.42
2:R:156:GLN:OE1	2:R:165:ARG:NH2	2.52	0.42
2:2:49:ALA:O	2:2:53:VAL:CG2	2.67	0.42
2:j:345:ILE:HD12	2:j:345:ILE:N	2.35	0.42
2:p:383:LEU:HD13	2:p:423:PHE:CZ	2.54	0.42
2:v:401:LEU:HA	2:v:402:PRO:HD3	1.69	0.42
2:x:301:OZT:O	2:x:440:GLY:HA3	2.20	0.42
1:A:33:LEU:HD23	1:A:40:LEU:HB3	2.01	0.42
1:A:72:ASP:O	1:A:73:ASN:C	2.60	0.42
1:F:111:PHE:HD1	1:F:117:PRO:HB3	1.85	0.42
1:M:57:TYR:OH	1:M:86:GLY:HA3	2.19	0.42
1:O:30:VAL:HG13	1:O:43:ALA:HB2	2.02	0.42
1:Q:10:GLU:HB2	1:Y:15:GLU:CD	2.44	0.42
1:Q:96:GLY:O	1:Q:97:ARG:C	2.62	0.42
1:i:357:TYR:OH	1:i:386:GLY:HA3	2.19	0.42
1:q:333:LEU:HD23	1:q:333:LEU:H	1.84	0.42
1:y:473:GLU:O	1:y:474:ASN:HB2	2.19	0.42
2:E:101:LEU:HA	2:E:102:PRO:HD3	1.70	0.42
2:T:185:ASP:OD1	2:T:188:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:348:THR:OG1	2:j:351:VAL:HG23	2.18	0.42
2:n:429:TRP:CD1	2:n:429:TRP:H	2.36	0.42
1:A:205:VAL:HG23	1:A:206:ALA:H	1.79	0.42
1:D:45:ASN:HD22	1:D:209:GLU:HG3	1.84	0.42
1:I:30:VAL:HG13	1:I:43:ALA:HB2	2.00	0.42
1:K:32:ALA:HA	1:K:40:LEU:O	2.19	0.42
1:K:67:LYS:O	1:K:71:PHE:CD2	2.73	0.42
1:Y:35:TYR:CD1	1:Y:35:TYR:C	2.98	0.42
1:Y:123:CYS:HA	1:Y:139:TYR:O	2.19	0.42
1:l:90:ASP:HA	3:l:6:HOH:O	2.19	0.42
1:a:313:MET:HE1	1:a:316:ARG:CD	2.49	0.42
1:b:390:ASP:OD2	1:b:393:ASP:N	2.52	0.42
1:k:438:LEU:HD12	1:k:438:LEU:N	2.34	0.42
1:q:479:ASP:O	1:q:483:ILE:HG13	2.19	0.42
1:w:471:TYR:CD1	1:w:472:ALA:N	2.87	0.42
1:3:430:TYR:CE1	1:3:516:ASN:O	2.72	0.42
2:C:109:ILE:H	2:C:109:ILE:HG12	1.58	0.42
2:l:306:LEU:C	2:l:306:LEU:HD12	2.45	0.42
2:l:444:LEU:HD13	2:p:445:PHE:CE1	2.54	0.42
2:r:459:ASP:OD1	2:r:462:SER:HB3	2.18	0.42
2:v:429:TRP:CD1	2:v:429:TRP:H	2.38	0.42
2:v:472:TYR:HE1	2:v:518:ILE:HG12	1.84	0.42
1:D:85:ARG:HH21	1:D:93:ASP:CG	2.26	0.42
1:I:18:GLU:O	1:I:19:LEU:C	2.62	0.42
1:I:48:ARG:NH2	1:S:137:GLU:OE2	2.52	0.42
1:K:90:ASP:OD2	1:K:93:ASP:N	2.52	0.42
1:M:35:TYR:CE1	1:M:37:GLY:C	2.96	0.42
1:M:35:TYR:CZ	1:M:37:GLY:HA3	2.40	0.42
1:S:233:LEU:O	1:S:234:LEU:C	2.62	0.42
1:W:96:GLY:O	1:W:97:ARG:C	2.62	0.42
1:a:508:LEU:HD23	1:a:508:LEU:HA	1.68	0.42
1:3:427:VAL:HG13	1:3:428:ALA:N	2.33	0.42
2:H:144:LEU:HD22	2:H:144:LEU:HA	1.86	0.42
2:E:13:VAL:HG21	2:E:164:LEU:HD23	2.01	0.42
2:G:58:LEU:HD12	2:G:58:LEU:O	2.20	0.42
2:R:31:VAL:CG1	2:R:33:LYS:HE3	2.50	0.42
2:2:65:HIS:CE1	2:2:69:LEU:HD11	2.55	0.42
2:j:376:PHE:CE2	2:j:380:ILE:HD11	2.55	0.42
2:l:431:ILE:HG23	3:l:25:HOH:O	2.18	0.42
2:l:461:ASP:CG	2:l:509:ARG:HH21	2.27	0.42
2:n:516:ALA:O	2:n:520:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:306:LEU:C	2:r:306:LEU:HD12	2.43	0.42
2:r:349:ALA:O	2:r:353:VAL:HG23	2.20	0.42
2:x:337:THR:HG21	2:x:343:THR:CG2	2.48	0.42
2:x:337:THR:HG23	2:x:343:THR:HG23	2.00	0.42
2:z:301:OZT:O	2:z:440:GLY:HA3	2.20	0.42
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.92	0.42
1:A:79:ILE:HD12	2:H:69:LEU:HD23	2.01	0.42
1:D:74:LEU:HD13	1:D:122:LEU:HD21	2.02	0.42
1:M:163:ILE:HD13	1:M:188:LEU:HD23	2.01	0.42
1:Y:36:ALA:HB2	1:Y:174:ASN:CA	2.42	0.42
1:Y:149:ASP:CG	1:Y:149:ASP:O	2.63	0.42
1:1:90:ASP:OD2	1:1:93:ASP:N	2.52	0.42
1:f:348:ARG:NH2	1:w:437:GLU:HG3	2.28	0.42
1:f:359:ARG:NH1	1:f:519:ARG:O	2.47	0.42
1:k:367:LYS:O	1:k:371:PHE:CD2	2.72	0.42
1:s:414:GLN:HE21	1:s:414:GLN:HB3	1.60	0.42
2:C:37:THR:HG23	2:C:43:THR:HG23	2.01	0.42
2:E:37:THR:CG2	2:E:43:THR:HG23	2.48	0.42
2:L:164:LEU:HD13	2:L:213:LEU:HD12	2.02	0.42
2:V:1:OZT:H27	2:V:33:LYS:HE2	2.02	0.42
2:V:37:THR:HG21	2:V:43:THR:CG2	2.49	0.42
2:V:82:ARG:HA	2:V:82:ARG:HD2	1.84	0.42
2:2:129:TRP:CD1	2:2:129:TRP:H	2.37	0.42
2:h:491:PHE:HB3	2:h:492:PRO:HD2	2.01	0.42
2:l:401:LEU:HA	2:l:402:PRO:HD3	1.73	0.42
2:r:331:VAL:CG1	2:r:333:LYS:HE3	2.50	0.42
1:D:141:ILE:HD12	1:D:141:ILE:N	2.34	0.42
1:K:35:TYR:CE2	1:K:38:GLY:O	2.72	0.42
1:O:156:MET:HB2	1:O:156:MET:HE3	1.72	0.42
1:Q:156:MET:HB2	1:Q:156:MET:HE3	1.70	0.42
1:a:396:GLY:O	1:a:397:ARG:C	2.62	0.42
1:d:467:LEU:O	1:d:468:LYS:C	2.63	0.42
1:f:421:GLU:HG2	1:f:456:MET:HG2	2.02	0.42
1:s:330:VAL:HG22	1:s:343:ALA:CB	2.49	0.42
1:w:513:LEU:HD12	1:w:513:LEU:HA	1.87	0.42
1:w:517:ARG:NH2	1:w:523:ARG:HG3	2.33	0.42
1:y:430:TYR:CD2	1:y:430:TYR:O	2.73	0.42
2:C:129:TRP:CD1	2:C:129:TRP:H	2.37	0.42
2:C:214:ALA:O	2:C:218:ILE:HG13	2.20	0.42
2:L:54:GLU:OE1	2:L:54:GLU:HA	2.20	0.42
2:T:130:ASN:HD22	2:T:130:ASN:C	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:45:ILE:N	2:X:45:ILE:HD12	2.34	0.42
2:Z:80:ILE:CD1	2:Z:121:VAL:HG21	2.49	0.42
2:Z:211:ALA:O	2:Z:212:GLU:C	2.62	0.42
2:2:31:VAL:HG12	2:2:33:LYS:HG3	2.01	0.42
2:h:318:ARG:HD2	2:h:331:VAL:O	2.20	0.42
2:c:345:ILE:HG21	2:c:400:ALA:HB1	2.02	0.42
2:l:364:GLU:O	2:l:365:HIS:C	2.63	0.42
2:p:386:MET:HE3	2:p:386:MET:HB2	1.74	0.42
2:r:365:HIS:CE1	2:r:369:LEU:HD11	2.55	0.42
2:r:412:SER:O	2:r:414:PRO:HD3	2.20	0.42
2:t:464:LEU:CD2	2:t:464:LEU:C	2.92	0.42
1:A:56:LEU:HG	1:A:62:PHE:HB2	2.01	0.42
1:A:167:LEU:O	1:A:168:LYS:C	2.61	0.42
1:B:90:ASP:OD1	2:H:78:GLY:HA3	2.19	0.42
1:D:83:ASP:OD2	2:E:65:HIS:CD2	2.73	0.42
1:F:80:GLN:HE21	1:F:80:GLN:HB3	1.62	0.42
1:I:129:HIS:HB2	1:I:132:GLU:CG	2.50	0.42
1:M:129:HIS:ND1	1:M:132:GLU:OE2	2.53	0.42
1:O:138:LEU:HD12	1:O:138:LEU:N	2.35	0.42
1:S:179:ASP:O	1:S:183:ILE:HG13	2.20	0.42
1:S:217:ARG:HA	1:S:218:PRO:HD3	1.86	0.42
1:S:225:ILE:HG22	1:S:230:LEU:CB	2.34	0.42
1:U:163:ILE:HG23	1:U:187:ALA:C	2.45	0.42
1:m:357:TYR:O	1:m:358:ASP:C	2.63	0.42
1:s:438:LEU:N	1:s:438:LEU:HD12	2.35	0.42
1:3:428:ALA:HB2	1:3:434:LYS:HB3	2.01	0.42
2:H:37:THR:HG23	2:H:43:THR:HG23	2.02	0.42
2:H:44:GLY:C	2:H:45:ILE:HD12	2.44	0.42
2:E:103:LEU:HD23	2:E:103:LEU:HA	1.76	0.42
2:E:164:LEU:HD13	2:E:213:LEU:HD12	2.02	0.42
2:E:205:VAL:HA	2:E:206:PRO:HD3	1.82	0.42
2:G:66:TYR:CD2	2:G:66:TYR:C	2.97	0.42
2:P:1:OZT:O	2:P:140:GLY:HA3	2.20	0.42
2:T:20:SER:HB3	2:T:31:VAL:HG21	2.01	0.42
2:X:178:ASP:OD1	2:2:24:ASN:HB3	2.19	0.42
2:l:403:LEU:HD23	2:l:403:LEU:HA	1.81	0.42
2:z:382:ARG:HA	2:z:382:ARG:HD2	1.85	0.42
1:B:217:ARG:HB3	1:B:217:ARG:NH1	2.29	0.42
1:B:220:ARG:HH22	2:C:67:GLU:CD	2.28	0.42
1:K:35:TYR:CG	1:K:38:GLY:O	2.71	0.42
1:M:153:PHE:CD1	1:M:167:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:56:LEU:HB2	1:1:60:VAL:HG22	2.02	0.42
1:1:163:ILE:HG23	1:1:187:ALA:C	2.45	0.42
1:f:513:LEU:HD12	1:f:513:LEU:HA	1.94	0.42
1:m:335:TYR:CE1	1:m:337:GLY:N	2.87	0.42
1:m:517:ARG:NH2	1:m:523:ARG:CG	2.83	0.42
1:o:421:GLU:HG2	1:o:456:MET:HG2	2.01	0.42
1:y:331:VAL:HG12	1:y:333:LEU:CD2	2.50	0.42
1:3:390:ASP:OD2	1:3:393:ASP:N	2.53	0.42
2:C:13:VAL:HG21	2:C:164:LEU:HD23	2.01	0.42
2:E:40:TYR:O	2:E:106:GLY:HA2	2.20	0.42
2:G:38:ASP:OD1	2:G:39:ASP:N	2.52	0.42
2:T:191:PHE:CE1	2:T:211:ALA:HB2	2.55	0.42
2:V:83:LEU:HD13	2:V:123:PHE:CZ	2.55	0.42
2:V:150:MET:O	2:V:151:LYS:C	2.63	0.42
2:h:413:ASP:HA	2:h:414:PRO:HD3	1.88	0.42
2:c:319:ARG:HG3	2:c:320:SER:H	1.84	0.42
2:l:331:VAL:HG11	2:l:333:LYS:HE3	2.00	0.42
2:n:365:HIS:CE1	2:n:369:LEU:HD11	2.55	0.42
2:v:409:ILE:H	2:v:409:ILE:HG12	1.46	0.42
1:B:71:PHE:CD1	1:B:71:PHE:C	2.98	0.42
1:D:56:LEU:HD11	1:D:62:PHE:HB2	2.01	0.42
1:D:72:ASP:O	1:D:73:ASN:C	2.62	0.42
1:F:130:TYR:CE1	1:F:216:ASN:O	2.73	0.42
1:O:107:LEU:HA	1:O:107:LEU:HD23	1.86	0.42
1:Y:30:VAL:HG22	1:Y:43:ALA:CB	2.50	0.42
1:a:526:THR:HG23	1:a:527:GLY:N	2.35	0.42
1:b:530:LEU:O	1:b:530:LEU:HD23	2.20	0.42
1:s:530:LEU:O	1:s:534:LEU:HG	2.19	0.42
1:w:359:ARG:HA	1:w:359:ARG:HD2	1.85	0.42
1:y:478:THR:HA	1:y:533:LEU:CG	2.50	0.42
1:y:478:THR:HB	1:y:533:LEU:CD1	2.45	0.42
2:H:31:VAL:CG1	2:H:33:LYS:HE3	2.50	0.42
2:H:205:VAL:HA	2:H:206:PRO:HD3	1.81	0.42
2:P:144:LEU:HD22	2:P:144:LEU:HA	1.93	0.42
2:T:49:ALA:O	2:T:53:VAL:HG23	2.20	0.42
2:X:31:VAL:HG12	2:X:33:LYS:HG3	2.02	0.42
2:2:168:VAL:HG12	2:2:217:ILE:HD12	2.02	0.42
2:h:435:GLY:N	3:h:42:HOH:O	2.53	0.42
2:r:440:GLY:O	2:r:443:SER:HB3	2.20	0.42
1:A:156:MET:HB2	1:A:156:MET:HE3	1.53	0.41
1:D:35:TYR:OH	1:D:212:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:213:LEU:HD12	1:Y:213:LEU:HA	1.95	0.41
1:b:333:LEU:N	1:b:333:LEU:HD23	2.35	0.41
1:m:438:LEU:N	1:m:438:LEU:HD12	2.35	0.41
1:q:396:GLY:O	1:q:397:ARG:C	2.62	0.41
1:s:423:CYS:HA	1:s:439:TYR:O	2.19	0.41
1:u:330:VAL:HG12	1:u:331:VAL:N	2.34	0.41
1:w:463:ILE:HG23	1:w:487:ALA:O	2.20	0.41
1:y:438:LEU:HD12	1:y:438:LEU:N	2.35	0.41
2:E:213:LEU:O	2:E:217:ILE:HG13	2.20	0.41
2:L:86:MET:HE3	2:L:86:MET:HB2	1.63	0.41
2:R:65:HIS:CE1	2:R:69:LEU:HD11	2.54	0.41
2:Z:214:ALA:C	2:Z:216:ALA:N	2.78	0.41
2:n:383:LEU:HD13	2:n:423:PHE:CE1	2.55	0.41
2:z:391:LEU:CD1	2:z:427:GLY:HA3	2.50	0.41
1:D:35:TYR:HH	1:D:212:VAL:HB	1.85	0.41
1:M:127:VAL:HG11	1:M:215:ALA:CB	2.45	0.41
1:S:156:MET:HE3	1:S:156:MET:HB2	1.76	0.41
1:S:178:THR:HB	1:S:233:LEU:HD22	2.00	0.41
1:1:123:CYS:HA	1:1:139:TYR:O	2.20	0.41
1:1:214:ASP:OD2	1:1:223:ARG:NH2	2.53	0.41
1:b:356:LEU:HB2	1:b:360:VAL:HG22	2.02	0.41
1:m:441:ILE:N	1:m:441:ILE:HD12	2.35	0.41
1:w:311:GLN:HA	1:w:314:ARG:CG	2.49	0.41
2:C:45:ILE:HD12	2:C:45:ILE:N	2.35	0.41
2:R:218:ILE:O	2:R:218:ILE:CG2	2.68	0.41
2:X:49:ALA:O	2:X:53:VAL:CG2	2.69	0.41
2:2:185:ASP:OD1	2:2:188:ARG:HB2	2.20	0.41
2:e:331:VAL:HG12	2:e:333:LYS:HG3	2.01	0.41
2:t:348:THR:OG1	2:t:351:VAL:HG23	2.20	0.41
2:x:331:VAL:CG1	2:x:333:LYS:HE3	2.50	0.41
2:4:314:MET:HE1	2:4:403:LEU:O	2.19	0.41
1:A:23:GLY:HA3	1:A:119:GLU:OE2	2.19	0.41
1:A:35:TYR:CE2	1:A:38:GLY:O	2.72	0.41
1:A:128:ALA:HB2	1:A:134:LYS:HB3	2.01	0.41
1:I:47:SER:HB2	1:S:149:ASP:OD1	2.20	0.41
1:O:126:GLU:HG2	1:O:127:VAL:N	2.35	0.41
1:Q:71:PHE:CD1	1:Q:71:PHE:C	2.99	0.41
1:S:68:PHE:O	1:S:69:ASN:C	2.62	0.41
1:S:177:LEU:HD12	1:S:177:LEU:C	2.43	0.41
1:U:163:ILE:HD13	1:U:188:LEU:HD23	2.02	0.41
1:Y:35:TYR:CG	1:Y:38:GLY:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:311:GLN:O	1:f:315:GLU:HG3	2.20	0.41
1:f:517:ARG:HH21	1:f:523:ARG:HG3	1.85	0.41
1:i:407:LEU:HD23	1:i:407:LEU:HA	1.93	0.41
1:q:527:GLY:O	1:q:531:GLN:N	2.50	0.41
1:s:509:GLU:OE1	1:s:524:ARG:NH2	2.53	0.41
1:y:330:VAL:HG22	1:y:343:ALA:CB	2.51	0.41
1:3:330:VAL:HG12	1:3:331:VAL:N	2.35	0.41
2:G:37:THR:HG23	2:G:43:THR:HG23	2.01	0.41
2:L:76:PHE:CE2	2:L:80:ILE:HD11	2.55	0.41
2:Z:49:ALA:O	2:Z:53:VAL:HG23	2.20	0.41
2:h:444:LEU:HD22	2:h:444:LEU:HA	1.86	0.41
2:c:464:LEU:HD23	2:c:464:LEU:HA	1.89	0.41
2:j:430:ASN:HD22	2:j:430:ASN:C	2.28	0.41
2:j:464:LEU:HD23	2:j:464:LEU:HA	1.85	0.41
2:l:464:LEU:HD13	2:l:513:LEU:HD12	2.03	0.41
2:v:456:GLN:OE1	2:v:465:ARG:NH2	2.53	0.41
1:A:68:PHE:HA	1:A:71:PHE:CE2	2.56	0.41
1:B:35:TYR:CD1	1:B:37:GLY:N	2.83	0.41
1:M:35:TYR:CE2	1:M:177:LEU:HD13	2.55	0.41
1:f:423:CYS:HA	1:f:439:TYR:O	2.20	0.41
1:f:456:MET:HE3	1:f:456:MET:HB2	1.77	0.41
1:k:330:VAL:HG13	1:k:343:ALA:HB2	2.02	0.41
1:m:330:VAL:HG22	1:m:343:ALA:CB	2.50	0.41
1:q:390:ASP:OD2	1:q:393:ASP:N	2.53	0.41
2:H:1:OZT:H27	2:H:33:LYS:NZ	2.33	0.41
2:H:165:ARG:CG	2:H:213:LEU:HD22	2.43	0.41
2:J:31:VAL:CG1	2:J:33:LYS:HE3	2.49	0.41
2:J:185:ASP:OD1	2:J:188:ARG:HB2	2.21	0.41
2:N:205:VAL:HA	2:N:206:PRO:HD3	1.84	0.41
2:R:37:THR:CG2	2:R:59:TYR:CD2	2.91	0.41
2:R:88:ARG:NH2	3:R:243:HOH:O	2.41	0.41
2:X:198:ASP:OD1	2:X:200:ASP:HB2	2.20	0.41
2:c:331:VAL:HG12	2:c:333:LYS:HG3	2.03	0.41
2:e:407:TYR:CE2	2:e:499:ALA:HA	2.55	0.41
2:g:348:THR:OG1	2:g:351:VAL:HG23	2.21	0.41
2:l:337:THR:HG21	2:l:343:THR:HG23	2.02	0.41
2:p:403:LEU:HD23	2:p:403:LEU:HA	1.73	0.41
2:p:413:ASP:HA	2:p:414:PRO:HD3	1.88	0.41
2:x:335:TYR:CZ	2:x:353:VAL:HG13	2.55	0.41
1:A:10:GLU:N	1:O:15:GLU:OE2	2.53	0.41
1:D:207:SER:O	1:D:208:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:LEU:HD23	1:I:230:LEU:HA	1.80	0.41
1:O:56:LEU:HB2	1:O:60:VAL:HG22	2.03	0.41
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	2.03	0.41
1:Y:35:TYR:CE2	1:Y:38:GLY:O	2.73	0.41
1:Y:229:ALA:O	1:Y:232:ALA:HB3	2.20	0.41
1:a:359:ARG:HA	1:a:359:ARG:HD2	1.93	0.41
1:b:371:PHE:CD1	1:b:371:PHE:C	2.98	0.41
1:o:356:LEU:HG	1:o:362:PHE:CB	2.51	0.41
1:w:407:LEU:HD12	1:w:441:ILE:HG22	2.02	0.41
2:G:33:LYS:O	2:G:44:GLY:HA2	2.20	0.41
2:G:54:GLU:OE1	2:G:54:GLU:HA	2.20	0.41
2:2:45:ILE:N	2:2:45:ILE:HD12	2.34	0.41
2:e:383:LEU:HD13	2:e:423:PHE:CZ	2.55	0.41
2:j:505:VAL:HA	2:j:506:PRO:HD3	1.78	0.41
2:l:491:PHE:HB3	2:l:492:PRO:HD2	2.02	0.41
2:n:307:LYS:HE3	2:n:418:GLY:O	2.19	0.41
2:n:386:MET:HB2	2:n:386:MET:HE3	1.68	0.41
2:n:444:LEU:HD13	2:v:445:PHE:CE1	2.56	0.41
1:I:48:ARG:HH21	1:S:137:GLU:HG2	1.80	0.41
1:W:79:ILE:HD12	2:X:69:LEU:HD23	2.02	0.41
1:Y:178:THR:CG2	1:Y:179:ASP:N	2.83	0.41
1:a:312:ALA:C	1:a:313:MET:HE3	2.44	0.41
1:b:340:LEU:HD13	1:b:512:VAL:CG1	2.50	0.41
1:b:368:PHE:O	1:b:369:ASN:C	2.63	0.41
1:d:335:TYR:HE1	1:d:337:GLY:HA3	1.74	0.41
1:d:390:ASP:OD2	1:d:393:ASP:N	2.54	0.41
1:i:383:ASP:OD2	2:j:365:HIS:HD2	2.04	0.41
1:i:396:GLY:O	1:i:397:ARG:C	2.64	0.41
1:m:356:LEU:HA	1:m:356:LEU:HD23	1.72	0.41
1:y:427:VAL:O	1:y:427:VAL:CG1	2.67	0.41
1:3:335:TYR:CE1	1:3:337:GLY:C	2.99	0.41
2:H:191:PHE:HB3	2:H:192:PRO:CD	2.51	0.41
2:G:113:ASP:HA	2:G:114:PRO:HD3	1.90	0.41
2:G:156:GLN:OE1	2:G:165:ARG:NH2	2.54	0.41
2:J:107:TYR:HB2	2:J:197:ILE:HG22	2.01	0.41
2:P:8:TYR:HB2	2:P:9:PRO:CD	2.51	0.41
2:P:76:PHE:CE2	2:P:80:ILE:HD11	2.56	0.41
2:T:49:ALA:O	2:T:53:VAL:CG2	2.69	0.41
2:c:331:VAL:CG1	2:c:333:LYS:HE3	2.51	0.41
2:n:301:OZT:O	2:n:440:GLY:HA3	2.19	0.41
2:p:507:GLU:O	2:p:508:SER:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:486:LEU:HD23	2:v:486:LEU:HA	1.77	0.41
1:A:10:GLU:HA	1:O:15:GLU:OE2	2.20	0.41
1:D:53:ILE:HG22	1:D:54:SER:N	2.34	0.41
1:D:220:ARG:HH22	2:E:67:GLU:CD	2.28	0.41
1:F:126:GLU:HG2	1:F:127:VAL:N	2.35	0.41
1:F:152:HIS:HB3	1:F:171:TYR:CZ	2.55	0.41
1:O:141:ILE:HD12	1:O:141:ILE:N	2.35	0.41
1:S:35:TYR:HD1	1:S:36:ALA:N	2.19	0.41
1:i:356:LEU:HD23	1:i:356:LEU:HA	1.71	0.41
1:q:383:ASP:OD2	2:r:365:HIS:CD2	2.72	0.41
1:s:421:GLU:HG2	1:s:456:MET:HG2	2.03	0.41
1:s:514:ASP:OD2	1:s:514:ASP:C	2.62	0.41
1:w:354:SER:OG	1:w:355:GLU:N	2.53	0.41
1:w:419:GLU:HG2	3:w:94:HOH:O	2.20	0.41
1:w:477:LEU:HD13	1:w:512:VAL:HG11	2.02	0.41
1:3:430:TYR:HE1	1:3:516:ASN:O	2.03	0.41
2:N:53:VAL:O	2:N:54:GLU:C	2.64	0.41
2:V:101:LEU:HA	2:V:102:PRO:HD3	1.66	0.41
2:X:1:OZT:H17	2:X:33:LYS:NZ	2.35	0.41
2:X:25:MET:HG2	2:2:145:PHE:HZ	1.85	0.41
2:c:432:GLU:OE1	2:c:432:GLU:HA	2.20	0.41
2:c:505:VAL:HA	2:c:506:PRO:HD3	1.83	0.41
2:e:375:THR:O	2:e:376:PHE:C	2.60	0.41
2:g:340:TYR:CD1	2:g:409:ILE:HD13	2.56	0.41
2:r:485:ASP:OD1	2:r:488:ARG:HB2	2.20	0.41
2:r:505:VAL:HA	2:r:506:PRO:HD3	1.90	0.41
2:t:440:GLY:O	2:t:443:SER:HB3	2.21	0.41
1:D:161:GLU:H	1:D:161:GLU:CD	2.28	0.41
1:K:58:ASP:HB3	1:K:219:ARG:O	2.21	0.41
1:M:127:VAL:HG13	1:M:215:ALA:HB2	1.96	0.41
1:U:129:HIS:O	1:U:130:TYR:C	2.64	0.41
1:W:114:GLN:HE21	1:W:114:GLN:HB3	1.59	0.41
1:b:354:SER:CB	1:b:375:ARG:HD2	2.51	0.41
1:b:452:HIS:CD2	1:b:471:TYR:HE2	2.39	0.41
1:k:449:ASP:O	1:k:449:ASP:CG	2.63	0.41
1:m:310:GLU:CD	1:m:312:ALA:HB3	2.46	0.41
1:u:356:LEU:CG	1:u:362:PHE:HB2	2.51	0.41
2:H:45:ILE:CD1	3:H:241:HOH:O	2.69	0.41
2:E:31:VAL:HG12	2:E:33:LYS:HG3	2.03	0.41
2:L:83:LEU:HD13	2:L:123:PHE:CE1	2.55	0.41
2:P:171:LEU:HA	2:P:171:LEU:HD23	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:45:ILE:HG21	2:Z:100:ALA:HB1	2.03	0.41
2:2:1:OZT:C7	2:2:33:LYS:HZ1	2.34	0.41
2:c:469:GLU:CA	2:c:517:ILE:HD13	2.50	0.41
2:e:308:TYR:HB2	2:e:309:PRO:CD	2.50	0.41
2:e:505:VAL:HA	2:e:506:PRO:HD3	1.84	0.41
2:p:380:ILE:CD1	2:p:421:VAL:HG21	2.50	0.41
2:p:513:LEU:HD23	2:p:513:LEU:HA	1.90	0.41
2:x:314:MET:CE	2:x:403:LEU:HB3	2.51	0.41
2:z:366:TYR:CD2	2:z:366:TYR:C	2.98	0.41
1:A:138:LEU:HB2	1:A:150:GLU:O	2.21	0.41
1:A:150:GLU:HA	1:A:151:PRO:HD3	1.83	0.41
1:A:161:GLU:N	1:A:162:PRO:CD	2.84	0.41
1:B:55:GLU:OE2	1:B:220:ARG:HD2	2.21	0.41
1:B:56:LEU:HG	1:B:62:PHE:HB2	2.02	0.41
1:D:10:GLU:HG2	1:Q:19:LEU:HD13	2.03	0.41
1:D:123:CYS:HA	1:D:139:TYR:O	2.20	0.41
1:F:176:SER:OG	1:F:178:THR:HG23	2.21	0.41
1:K:16:ARG:HH12	1:K:115:ALA:C	2.29	0.41
1:K:30:VAL:HG12	1:K:31:VAL:N	2.35	0.41
1:K:56:LEU:HB2	1:K:60:VAL:HG22	2.02	0.41
1:K:147:ILE:HG21	1:K:147:ILE:HD13	1.84	0.41
1:K:163:ILE:HG23	1:K:187:ALA:C	2.46	0.41
1:M:19:LEU:HD21	1:M:116:LYS:HG3	2.03	0.41
1:O:30:VAL:HG22	1:O:43:ALA:HB1	2.03	0.41
1:O:35:TYR:CZ	1:O:177:LEU:HD13	2.56	0.41
1:O:79:ILE:HD13	2:P:68:LYS:HB3	2.01	0.41
1:O:123:CYS:HA	1:O:139:TYR:O	2.21	0.41
1:O:128:ALA:HB2	1:O:134:LYS:HB3	2.03	0.41
1:O:161:GLU:N	1:O:162:PRO:CD	2.84	0.41
1:Q:17:SER:HA	1:Q:143:TYR:HE2	1.85	0.41
1:S:121:GLU:HG2	1:S:156:MET:HG2	2.03	0.41
1:S:227:GLY:CA	1:S:230:LEU:CB	2.77	0.41
1:U:79:ILE:HD13	2:V:68:LYS:HB3	2.01	0.41
1:Y:71:PHE:CD1	1:Y:71:PHE:C	2.99	0.41
1:b:530:LEU:CD2	1:b:530:LEU:C	2.94	0.41
1:d:449:ASP:O	1:d:449:ASP:CG	2.64	0.41
1:f:310:GLU:OE1	1:f:310:GLU:CA	2.68	0.41
1:k:441:ILE:N	1:k:441:ILE:HD12	2.36	0.41
1:m:333:LEU:N	1:m:333:LEU:HD23	2.35	0.41
1:m:517:ARG:HH21	1:m:523:ARG:HD2	1.85	0.41
1:q:359:ARG:HH21	1:q:429:HIS:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:368:PHE:O	1:q:369:ASN:C	2.63	0.41
1:u:340:LEU:HD12	1:u:341:PHE:N	2.36	0.41
1:3:354:SER:CB	1:3:375:ARG:HD2	2.51	0.41
1:3:456:MET:HE3	1:3:456:MET:HB2	1.71	0.41
2:C:164:LEU:HD13	2:C:213:LEU:HD12	2.02	0.41
2:G:187:VAL:HG13	2:V:221:ARG:HB3	2.01	0.41
2:P:31:VAL:HG11	2:P:33:LYS:HE3	2.03	0.41
2:R:191:PHE:CD2	2:R:211:ALA:HA	2.55	0.41
2:T:218:ILE:HG22	2:T:219:GLU:N	2.36	0.41
2:V:38:ASP:OD1	2:V:41:THR:N	2.53	0.41
2:X:205:VAL:HA	2:X:206:PRO:HD3	1.81	0.41
2:Z:205:VAL:HA	2:Z:206:PRO:HD3	1.81	0.41
2:2:38:ASP:OD1	2:2:39:ASP:N	2.54	0.41
2:2:54:GLU:OE1	2:2:54:GLU:HA	2.21	0.41
2:c:348:THR:OG1	2:c:351:VAL:HG23	2.21	0.41
2:e:313:VAL:HG21	2:e:464:LEU:HD23	2.01	0.41
2:g:337:THR:CG2	2:g:359:TYR:HD2	2.34	0.41
2:j:429:TRP:CD1	2:j:429:TRP:H	2.39	0.41
2:l:314:MET:HE1	2:l:403:LEU:O	2.20	0.41
2:l:485:ASP:OD1	2:l:488:ARG:HB2	2.20	0.41
2:p:432:GLU:OE1	2:p:432:GLU:HA	2.21	0.41
2:p:513:LEU:O	2:p:517:ILE:HG13	2.20	0.41
2:r:345:ILE:CG2	2:r:400:ALA:HB1	2.51	0.41
2:r:403:LEU:HD23	2:r:403:LEU:HA	1.83	0.41
2:r:409:ILE:H	2:r:409:ILE:HG12	1.54	0.41
2:v:407:TYR:HB2	2:v:497:ILE:HG22	2.01	0.41
2:z:306:LEU:C	2:z:306:LEU:HD12	2.46	0.41
2:z:338:ASP:OD1	2:z:339:ASP:N	2.53	0.41
2:z:358:LEU:O	2:z:358:LEU:HD12	2.21	0.41
2:4:386:MET:HB2	2:4:386:MET:HE3	1.70	0.41
2:4:409:ILE:H	2:4:409:ILE:HG12	1.53	0.41
1:A:207:SER:O	1:A:208:LEU:HD23	2.21	0.41
1:B:33:LEU:O	1:B:33:LEU:HD23	2.20	0.41
1:B:161:GLU:N	1:B:162:PRO:CD	2.83	0.41
1:D:181:LEU:CD2	1:D:233:LEU:HD21	2.46	0.41
1:O:59:ARG:HA	1:O:59:ARG:HD2	1.98	0.41
1:Q:144:ASP:CG	1:Q:146:SER:OG	2.61	0.41
1:s:533:LEU:HD23	1:s:533:LEU:HA	1.65	0.41
1:u:519:ARG:HH11	1:u:519:ARG:HG2	1.85	0.41
1:w:450:GLU:HA	1:w:451:PRO:HD3	1.92	0.41
1:y:357:TYR:CB	1:y:360:VAL:CG2	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:THR:HG21	2:C:59:TYR:HD2	1.86	0.41
2:L:156:GLN:OE1	2:L:165:ARG:NH2	2.54	0.41
2:N:13:VAL:HG21	2:N:164:LEU:HD23	2.03	0.41
2:e:403:LEU:HD23	2:e:403:LEU:HA	1.90	0.41
2:j:358:LEU:O	2:j:358:LEU:HD12	2.20	0.41
2:n:403:LEU:HA	2:n:403:LEU:HD23	1.79	0.41
2:p:348:THR:OG1	2:p:351:VAL:HG23	2.21	0.41
2:p:456:GLN:OE1	2:p:465:ARG:NH2	2.54	0.41
2:r:444:LEU:HD22	2:r:444:LEU:HA	1.83	0.41
2:t:464:LEU:HD12	2:t:509:ARG:NH1	2.36	0.41
1:K:123:CYS:HA	1:K:139:TYR:O	2.21	0.40
1:Q:129:HIS:O	1:Q:130:TYR:C	2.65	0.40
1:S:30:VAL:HG12	1:S:31:VAL:N	2.36	0.40
1:U:11:GLN:O	1:U:15:GLU:HB2	2.21	0.40
1:U:35:TYR:CE1	1:U:37:GLY:CA	3.04	0.40
1:1:167:LEU:O	1:1:168:LYS:C	2.64	0.40
1:b:330:VAL:HG13	1:b:343:ALA:HB2	2.02	0.40
1:b:415:ALA:HB3	1:i:412:THR:CG2	2.38	0.40
1:d:389:TYR:HD1	2:r:374:LEU:HD21	1.86	0.40
1:i:344:GLU:HA	1:i:508:LEU:HD23	2.03	0.40
1:u:517:ARG:NH1	1:u:520:ARG:O	2.53	0.40
1:u:526:THR:HG22	1:u:527:GLY:H	1.86	0.40
1:w:311:GLN:CB	1:w:314:ARG:CD	2.97	0.40
2:R:40:TYR:CE1	2:R:109:ILE:HD13	2.56	0.40
2:T:144:LEU:HD13	2:X:145:PHE:CE1	2.55	0.40
2:X:54:GLU:OE1	2:X:54:GLU:HA	2.21	0.40
2:Z:214:ALA:O	2:Z:215:ARG:C	2.62	0.40
2:h:383:LEU:HA	2:h:383:LEU:HD23	1.85	0.40
2:j:486:LEU:HD11	2:j:518:ILE:HD13	2.03	0.40
2:n:521:ARG:NH1	3:n:62:HOH:O	2.54	0.40
2:p:376:PHE:CE2	2:p:380:ILE:HD11	2.57	0.40
2:p:409:ILE:H	2:p:409:ILE:HG12	1.44	0.40
2:v:491:PHE:CD2	2:v:511:ALA:HA	2.56	0.40
1:A:130:TYR:CD1	1:A:216:ASN:O	2.74	0.40
1:D:167:LEU:HD23	1:D:167:LEU:HA	1.86	0.40
1:K:68:PHE:O	1:K:69:ASN:C	2.64	0.40
1:U:30:VAL:HG22	1:U:43:ALA:CB	2.50	0.40
1:U:79:ILE:HG23	2:V:68:LYS:HE3	2.03	0.40
1:W:56:LEU:HD23	1:W:56:LEU:HA	1.81	0.40
1:W:161:GLU:N	1:W:162:PRO:CD	2.85	0.40
1:a:310:GLU:HG3	1:a:313:MET:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:478:THR:HA	1:a:533:LEU:CD2	2.51	0.40
1:d:310:GLU:O	1:d:313:MET:HB3	2.21	0.40
1:d:508:LEU:HD23	1:d:508:LEU:HA	1.73	0.40
1:i:335:TYR:CZ	1:i:337:GLY:HA3	2.54	0.40
1:i:422:LEU:N	1:i:422:LEU:CD1	2.85	0.40
1:q:456:MET:HE3	1:q:456:MET:HB2	1.65	0.40
1:u:430:TYR:CE1	1:u:516:ASN:O	2.75	0.40
1:w:526:THR:HG22	1:w:527:GLY:H	1.86	0.40
2:H:65:HIS:CE1	2:H:69:LEU:HD11	2.56	0.40
2:C:49:ALA:O	2:C:53:VAL:CG2	2.69	0.40
2:C:205:VAL:HA	2:C:206:PRO:HD3	1.86	0.40
2:G:35:TYR:CZ	2:G:53:VAL:HG13	2.56	0.40
2:G:75:THR:O	2:G:76:PHE:C	2.62	0.40
2:N:58:LEU:HD12	2:N:58:LEU:C	2.45	0.40
2:N:101:LEU:HA	2:N:102:PRO:HD3	1.69	0.40
2:R:129:TRP:H	2:R:129:TRP:CD1	2.39	0.40
2:V:37:THR:HG23	2:V:43:THR:HG23	2.04	0.40
2:V:103:LEU:HD23	2:V:103:LEU:HA	1.83	0.40
2:e:401:LEU:HA	2:e:402:PRO:HD3	1.72	0.40
2:l:376:PHE:CE2	2:l:380:ILE:HD11	2.56	0.40
2:r:345:ILE:HG21	2:r:400:ALA:HB1	2.02	0.40
2:z:409:ILE:H	2:z:409:ILE:HG12	1.45	0.40
1:M:96:GLY:O	1:M:97:ARG:C	2.65	0.40
1:Q:56:LEU:HD13	1:Q:99:LEU:HD13	2.02	0.40
1:l:152:HIS:CD2	1:l:171:TYR:HE2	2.39	0.40
1:d:438:LEU:N	1:d:438:LEU:HD12	2.36	0.40
1:i:449:ASP:O	1:i:449:ASP:CG	2.64	0.40
1:w:478:THR:HA	1:w:533:LEU:HD11	2.03	0.40
2:G:103:LEU:HA	2:G:103:LEU:HD23	1.79	0.40
2:N:8:TYR:HB2	2:N:9:PRO:CD	2.51	0.40
2:N:130:ASN:HD22	2:N:130:ASN:C	2.30	0.40
2:P:54:GLU:OE1	2:P:54:GLU:HA	2.21	0.40
2:X:101:LEU:HA	2:X:102:PRO:HD3	1.74	0.40
2:X:129:TRP:O	2:Z:50:ALA:HB2	2.21	0.40
2:2:164:LEU:HD13	2:2:213:LEU:HD12	2.02	0.40
2:p:412:SER:O	2:p:414:PRO:HD3	2.22	0.40
2:t:331:VAL:HG12	2:t:333:LYS:HE3	2.02	0.40
2:4:403:LEU:HD23	2:4:403:LEU:HA	1.80	0.40
1:B:31:VAL:HG22	1:B:155:VAL:HG22	2.03	0.40
1:B:126:GLU:HG2	1:B:127:VAL:N	2.37	0.40
1:B:217:ARG:HA	1:B:218:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ALA:O	1:D:153:PHE:HA	2.22	0.40
1:D:61:GLY:N	1:D:213:LEU:HD21	2.37	0.40
1:K:151:PRO:HD2	1:K:152:HIS:H	1.85	0.40
1:O:23:GLY:HA2	1:O:26:ARG:HD3	2.04	0.40
1:S:225:ILE:CG2	1:S:230:LEU:HB2	2.34	0.40
1:W:167:LEU:O	1:W:168:LYS:C	2.63	0.40
1:Y:116:LYS:HA	1:Y:117:PRO:HD2	1.84	0.40
1:1:231:GLN:HG3	1:1:234:LEU:HD12	2.03	0.40
1:b:356:LEU:HG	1:b:362:PHE:HB2	2.03	0.40
1:d:340:LEU:HD12	1:d:512:VAL:HG12	2.03	0.40
1:d:369:ASN:HB3	1:k:404:ALA:HB1	2.02	0.40
1:k:340:LEU:HD12	1:k:512:VAL:HG12	2.03	0.40
1:o:456:MET:HE3	1:o:456:MET:HB2	1.64	0.40
1:q:335:TYR:HD1	1:q:336:ALA:N	2.19	0.40
1:s:461:GLU:N	1:s:462:PRO:CD	2.84	0.40
1:w:467:LEU:O	1:w:468:LYS:C	2.65	0.40
2:C:191:PHE:HB3	2:C:192:PRO:HD2	2.03	0.40
2:E:8:TYR:HB2	2:E:9:PRO:CD	2.52	0.40
2:G:14:MET:HE2	2:G:103:LEU:CD1	2.50	0.40
2:J:129:TRP:CD1	2:J:129:TRP:H	2.38	0.40
2:N:73:PRO:HA	3:N:241:HOH:O	2.21	0.40
2:R:49:ALA:O	2:R:53:VAL:HG23	2.20	0.40
2:R:164:LEU:HD23	2:R:164:LEU:HA	1.95	0.40
2:X:14:MET:HE1	2:X:103:LEU:O	2.22	0.40
2:X:58:LEU:HD12	2:X:58:LEU:O	2.21	0.40
2:2:164:LEU:HD23	2:2:164:LEU:HA	1.92	0.40
2:e:306:LEU:HD12	2:e:306:LEU:C	2.46	0.40
2:e:358:LEU:HD12	2:e:358:LEU:HA	1.67	0.40
2:g:337:THR:HG21	2:g:359:TYR:CD2	2.53	0.40
2:r:413:ASP:HA	2:r:414:PRO:HD3	1.89	0.40
2:t:485:ASP:OD1	2:t:488:ARG:HB2	2.21	0.40
2:v:391:LEU:C	2:v:393:ALA:N	2.80	0.40
2:z:331:VAL:HG12	2:z:333:LYS:HG3	2.04	0.40
2:z:338:ASP:OD1	2:z:341:THR:N	2.54	0.40
1:A:233:LEU:HD12	1:A:233:LEU:N	2.37	0.40
1:M:30:VAL:HG12	1:M:31:VAL:N	2.37	0.40
1:M:83:ASP:OD2	2:N:65:HIS:CD2	2.72	0.40
1:M:152:HIS:CG	1:M:171:TYR:CE2	3.09	0.40
1:Q:79:ILE:HG23	2:R:68:LYS:HE3	2.04	0.40
1:S:30:VAL:HG22	1:S:43:ALA:HB1	2.03	0.40
1:W:48:ARG:NH2	1:Y:137:GLU:CG	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:PHE:O	1:1:69:ASN:C	2.63	0.40
1:a:315:GLU:HG2	1:b:310:GLU:CB	2.52	0.40
1:b:488:LEU:HD23	1:b:488:LEU:HA	1.92	0.40
1:k:481:LEU:CD2	1:k:534:LEU:CD1	2.99	0.40
1:k:520:ARG:HD3	2:l:364:GLU:OE2	2.21	0.40
1:o:442:THR:O	1:o:444:ASP:N	2.55	0.40
1:s:357:TYR:O	1:s:358:ASP:C	2.63	0.40
1:3:340:LEU:HD13	1:3:512:VAL:HG12	2.02	0.40
1:3:421:GLU:HG2	1:3:456:MET:HG2	2.03	0.40
1:3:434:LYS:HG2	1:3:435:ARG:N	2.36	0.40
2:H:191:PHE:CD1	2:H:191:PHE:N	2.89	0.40
2:C:113:ASP:HA	2:C:114:PRO:HD3	1.82	0.40
2:J:31:VAL:HG12	2:J:33:LYS:HG3	2.03	0.40
2:J:103:LEU:HD23	2:J:103:LEU:HA	1.86	0.40
2:N:45:ILE:HD13	3:N:243:HOH:O	2.19	0.40
2:Z:76:PHE:CE2	2:Z:80:ILE:HD11	2.57	0.40
2:Z:80:ILE:HD11	2:Z:121:VAL:HG21	2.04	0.40
2:h:301:OZT:O	2:h:440:GLY:HA3	2.21	0.40
2:n:491:PHE:CD1	2:n:491:PHE:N	2.89	0.40
2:t:319:ARG:HG3	2:t:320:SER:H	1.78	0.40
2:v:382:ARG:HA	2:v:382:ARG:HD2	1.87	0.40
2:z:505:VAL:HA	2:z:506:PRO:HD3	1.82	0.40
2:4:429:TRP:CD1	2:4:429:TRP:H	2.39	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	207/240 (86%)	193 (93%)	13 (6%)	1 (0%)	24	51
1	3	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	24	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/240 (86%)	189 (91%)	18 (9%)	0	100	100
1	B	207/240 (86%)	187 (90%)	19 (9%)	1 (0%)	24	51
1	D	206/240 (86%)	185 (90%)	21 (10%)	0	100	100
1	F	189/240 (79%)	170 (90%)	18 (10%)	1 (0%)	24	51
1	I	208/240 (87%)	199 (96%)	8 (4%)	1 (0%)	24	51
1	K	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	24	51
1	M	201/240 (84%)	190 (94%)	11 (6%)	0	100	100
1	O	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51
1	Q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	S	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	U	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	W	189/240 (79%)	175 (93%)	13 (7%)	1 (0%)	24	51
1	Y	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	24	51
1	a	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51
1	b	207/240 (86%)	193 (93%)	13 (6%)	1 (0%)	24	51
1	d	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	24	51
1	f	207/240 (86%)	190 (92%)	16 (8%)	1 (0%)	24	51
1	i	207/240 (86%)	195 (94%)	11 (5%)	1 (0%)	24	51
1	k	207/240 (86%)	199 (96%)	7 (3%)	1 (0%)	24	51
1	m	204/240 (85%)	190 (93%)	13 (6%)	1 (0%)	24	51
1	o	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	s	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	24	51
1	u	207/240 (86%)	198 (96%)	8 (4%)	1 (0%)	24	51
1	w	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51
1	y	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51
2	2	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	4	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	C	213/240 (89%)	212 (100%)	1 (0%)	0	100	100
2	E	213/240 (89%)	212 (100%)	1 (0%)	0	100	100
2	G	213/240 (89%)	209 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	213/240 (89%)	210 (99%)	3 (1%)	0	100	100
2	J	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	L	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
2	N	213/240 (89%)	210 (99%)	3 (1%)	0	100	100
2	P	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	R	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	T	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	V	214/240 (89%)	209 (98%)	5 (2%)	0	100	100
2	X	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	Z	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	c	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
2	e	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	g	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
2	h	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
2	j	213/240 (89%)	207 (97%)	5 (2%)	1 (0%)	24	51
2	l	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	n	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
2	p	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
2	r	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	t	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	v	215/240 (90%)	212 (99%)	3 (1%)	0	100	100
2	x	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	z	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
All	All	11711/13440 (87%)	11238 (96%)	447 (4%)	26 (0%)	43	70

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	PRO
1	F	151	PRO
1	I	151	PRO
1	b	451	PRO
1	o	451	PRO
1	K	151	PRO

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Mol	Chain	Res	Type
1	O	151	PRO
1	Q	151	PRO
1	S	151	PRO
1	U	151	PRO
1	Y	151	PRO
1	l	151	PRO
1	a	451	PRO
1	d	451	PRO
1	f	451	PRO
1	i	451	PRO
1	k	451	PRO
1	m	451	PRO
1	q	451	PRO
1	s	451	PRO
1	u	451	PRO
1	w	451	PRO
1	3	451	PRO
1	W	151	PRO
1	y	451	PRO
2	j	517	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	162/184 (88%)	152 (94%)	10 (6%)	16	43
1	3	161/184 (88%)	147 (91%)	14 (9%)	9	27
1	A	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	B	162/184 (88%)	140 (86%)	22 (14%)	3	10
1	D	161/184 (88%)	141 (88%)	20 (12%)	4	13
1	F	149/184 (81%)	129 (87%)	20 (13%)	4	11
1	I	163/184 (89%)	147 (90%)	16 (10%)	7	22
1	K	162/184 (88%)	149 (92%)	13 (8%)	11	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	158/184 (86%)	148 (94%)	10 (6%)	16	42
1	O	162/184 (88%)	151 (93%)	11 (7%)	14	39
1	Q	162/184 (88%)	150 (93%)	12 (7%)	13	35
1	S	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	U	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	W	148/184 (80%)	137 (93%)	11 (7%)	13	35
1	Y	161/184 (88%)	147 (91%)	14 (9%)	9	27
1	a	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	b	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	d	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	f	162/184 (88%)	150 (93%)	12 (7%)	13	35
1	i	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	k	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	m	160/184 (87%)	149 (93%)	11 (7%)	14	38
1	o	162/184 (88%)	151 (93%)	11 (7%)	14	39
1	q	162/184 (88%)	146 (90%)	16 (10%)	7	22
1	s	162/184 (88%)	151 (93%)	11 (7%)	14	39
1	u	162/184 (88%)	153 (94%)	9 (6%)	19	47
1	w	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	y	162/184 (88%)	147 (91%)	15 (9%)	8	25
2	2	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	4	161/177 (91%)	149 (92%)	12 (8%)	12	34
2	C	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	E	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	G	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	H	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	J	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	L	161/177 (91%)	143 (89%)	18 (11%)	6	17
2	N	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	P	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	R	161/177 (91%)	146 (91%)	15 (9%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	V	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	X	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	Z	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	c	161/177 (91%)	145 (90%)	16 (10%)	7	22
2	e	161/177 (91%)	149 (92%)	12 (8%)	12	34
2	g	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	h	160/177 (90%)	145 (91%)	15 (9%)	8	24
2	j	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	l	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	n	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	p	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	r	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	t	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	v	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	x	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	z	161/177 (91%)	151 (94%)	10 (6%)	16	43
All	All	9008/10108 (89%)	8244 (92%)	764 (8%)	10	28

All (764) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	19	LEU
1	A	49	SER
1	A	58	ASP
1	A	60	VAL
1	A	62	PHE
1	A	79	ILE
1	A	92	ARG
1	A	112	THR
1	A	122	LEU
1	A	147	ILE
1	A	159	THR
1	A	205	VAL
1	A	207	SER

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Mol	Chain	Res	Type
1	B	10	GLU
1	B	13	MET
1	B	19	LEU
1	B	33	LEU
1	B	49	SER
1	B	60	VAL
1	B	62	PHE
1	B	112	THR
1	B	122	LEU
1	B	127	VAL
1	B	140	ARG
1	B	147	ILE
1	B	159	THR
1	B	174	ASN
1	B	178	THR
1	B	205	VAL
1	B	207	SER
1	B	213	LEU
1	B	217	ARG
1	B	230	LEU
1	B	231	GLN
1	B	234	LEU
1	D	11	GLN
1	D	13	MET
1	D	18	GLU
1	D	21	ARG
1	D	49	SER
1	D	60	VAL
1	D	62	PHE
1	D	112	THR
1	D	122	LEU
1	D	127	VAL
1	D	140	ARG
1	D	147	ILE
1	D	159	THR
1	D	174	ASN
1	D	178	THR
1	D	205	VAL
1	D	207	SER
1	D	213	LEU
1	D	225	ILE
1	D	230	LEU

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Mol	Chain	Res	Type
1	F	44	GLU
1	F	49	SER
1	F	60	VAL
1	F	62	PHE
1	F	80	GLN
1	F	112	THR
1	F	122	LEU
1	F	127	VAL
1	F	140	ARG
1	F	147	ILE
1	F	159	THR
1	F	160	THR
1	F	174	ASN
1	F	178	THR
1	F	205	VAL
1	F	207	SER
1	F	213	LEU
1	F	217	ARG
1	F	230	LEU
1	F	233	LEU
1	I	10	GLU
1	I	11	GLN
1	I	13	MET
1	I	33	LEU
1	I	48	ARG
1	I	58	ASP
1	I	60	VAL
1	I	62	PHE
1	I	112	THR
1	I	147	ILE
1	I	149	ASP
1	I	205	VAL
1	I	216	ASN
1	I	225	ILE
1	I	226	THR
1	I	233	LEU
1	K	60	VAL
1	K	62	PHE
1	K	112	THR
1	K	127	VAL
1	K	133	THR
1	K	135	ARG

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Mol	Chain	Res	Type
1	K	147	ILE
1	K	149	ASP
1	K	205	VAL
1	K	213	LEU
1	K	216	ASN
1	K	228	SER
1	K	234	LEU
1	M	13	MET
1	M	60	VAL
1	M	62	PHE
1	M	112	THR
1	M	133	THR
1	M	147	ILE
1	M	176	SER
1	M	205	VAL
1	M	216	ASN
1	M	228	SER
1	O	13	MET
1	O	60	VAL
1	O	62	PHE
1	O	112	THR
1	O	127	VAL
1	O	147	ILE
1	O	149	ASP
1	O	205	VAL
1	O	216	ASN
1	O	231	GLN
1	O	234	LEU
1	Q	11	GLN
1	Q	13	MET
1	Q	33	LEU
1	Q	60	VAL
1	Q	62	PHE
1	Q	112	THR
1	Q	127	VAL
1	Q	133	THR
1	Q	149	ASP
1	Q	205	VAL
1	Q	216	ASN
1	Q	230	LEU
1	S	11	GLN
1	S	13	MET

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Mol	Chain	Res	Type
1	S	48	ARG
1	S	60	VAL
1	S	62	PHE
1	S	112	THR
1	S	127	VAL
1	S	147	ILE
1	S	149	ASP
1	S	173	GLU
1	S	178	THR
1	S	205	VAL
1	S	230	LEU
1	S	231	GLN
1	U	10	GLU
1	U	11	GLN
1	U	13	MET
1	U	60	VAL
1	U	62	PHE
1	U	112	THR
1	U	127	VAL
1	U	133	THR
1	U	135	ARG
1	U	147	ILE
1	U	149	ASP
1	U	205	VAL
1	U	216	ASN
1	W	33	LEU
1	W	60	VAL
1	W	62	PHE
1	W	112	THR
1	W	127	VAL
1	W	133	THR
1	W	147	ILE
1	W	149	ASP
1	W	179	ASP
1	W	205	VAL
1	W	230	LEU
1	Y	11	GLN
1	Y	13	MET
1	Y	14	ARG
1	Y	60	VAL
1	Y	62	PHE
1	Y	112	THR

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Mol	Chain	Res	Type
1	Y	127	VAL
1	Y	135	ARG
1	Y	147	ILE
1	Y	149	ASP
1	Y	179	ASP
1	Y	205	VAL
1	Y	216	ASN
1	Y	231	GLN
1	1	10	GLU
1	1	60	VAL
1	1	62	PHE
1	1	112	THR
1	1	127	VAL
1	1	133	THR
1	1	147	ILE
1	1	149	ASP
1	1	205	VAL
1	1	216	ASN
1	a	313	MET
1	a	349	SER
1	a	360	VAL
1	a	362	PHE
1	a	412	THR
1	a	427	VAL
1	a	433	THR
1	a	447	ILE
1	a	449	ASP
1	a	505	VAL
1	a	513	LEU
1	a	526	THR
1	a	533	LEU
1	a	534	LEU
1	b	313	MET
1	b	360	VAL
1	b	362	PHE
1	b	412	THR
1	b	427	VAL
1	b	441	ILE
1	b	447	ILE
1	b	449	ASP
1	b	476	SER
1	b	505	VAL

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Mol	Chain	Res	Type
1	b	516	ASN
1	b	526	THR
1	b	530	LEU
1	d	310	GLU
1	d	311	GLN
1	d	313	MET
1	d	333	LEU
1	d	349	SER
1	d	360	VAL
1	d	362	PHE
1	d	412	THR
1	d	427	VAL
1	d	433	THR
1	d	435	ARG
1	d	447	ILE
1	d	449	ASP
1	d	505	VAL
1	f	310	GLU
1	f	313	MET
1	f	360	VAL
1	f	362	PHE
1	f	412	THR
1	f	427	VAL
1	f	435	ARG
1	f	447	ILE
1	f	449	ASP
1	f	505	VAL
1	f	516	ASN
1	f	528	SER
1	i	313	MET
1	i	333	LEU
1	i	349	SER
1	i	360	VAL
1	i	362	PHE
1	i	412	THR
1	i	427	VAL
1	i	433	THR
1	i	447	ILE
1	i	449	ASP
1	i	505	VAL
1	i	516	ASN
1	i	530	LEU

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Mol	Chain	Res	Type
1	k	311	GLN
1	k	313	MET
1	k	314	ARG
1	k	333	LEU
1	k	358	ASP
1	k	360	VAL
1	k	362	PHE
1	k	412	THR
1	k	447	ILE
1	k	449	ASP
1	k	505	VAL
1	k	513	LEU
1	k	530	LEU
1	k	533	LEU
1	m	313	MET
1	m	360	VAL
1	m	362	PHE
1	m	412	THR
1	m	427	VAL
1	m	433	THR
1	m	447	ILE
1	m	449	ASP
1	m	505	VAL
1	m	516	ASN
1	m	531	GLN
1	o	313	MET
1	o	360	VAL
1	o	362	PHE
1	o	412	THR
1	o	427	VAL
1	o	447	ILE
1	o	449	ASP
1	o	479	ASP
1	o	505	VAL
1	o	513	LEU
1	o	526	THR
1	q	313	MET
1	q	333	LEU
1	q	335	TYR
1	q	349	SER
1	q	359	ARG
1	q	360	VAL

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Mol	Chain	Res	Type
1	q	362	PHE
1	q	412	THR
1	q	427	VAL
1	q	433	THR
1	q	441	ILE
1	q	447	ILE
1	q	449	ASP
1	q	505	VAL
1	q	516	ASN
1	q	530	LEU
1	s	313	MET
1	s	333	LEU
1	s	349	SER
1	s	360	VAL
1	s	412	THR
1	s	427	VAL
1	s	447	ILE
1	s	449	ASP
1	s	505	VAL
1	s	514	ASP
1	s	516	ASN
1	u	313	MET
1	u	360	VAL
1	u	362	PHE
1	u	412	THR
1	u	427	VAL
1	u	447	ILE
1	u	449	ASP
1	u	505	VAL
1	u	513	LEU
1	w	313	MET
1	w	335	TYR
1	w	360	VAL
1	w	362	PHE
1	w	412	THR
1	w	427	VAL
1	w	447	ILE
1	w	449	ASP
1	w	474	ASN
1	w	505	VAL
1	w	513	LEU
1	w	533	LEU

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Mol	Chain	Res	Type
1	w	534	LEU
1	y	311	GLN
1	y	313	MET
1	y	333	LEU
1	y	362	PHE
1	y	412	THR
1	y	427	VAL
1	y	432	GLU
1	y	435	ARG
1	y	447	ILE
1	y	449	ASP
1	y	505	VAL
1	y	513	LEU
1	y	516	ASN
1	y	530	LEU
1	y	533	LEU
1	3	310	GLU
1	3	311	GLN
1	3	313	MET
1	3	314	ARG
1	3	360	VAL
1	3	362	PHE
1	3	412	THR
1	3	427	VAL
1	3	447	ILE
1	3	449	ASP
1	3	479	ASP
1	3	505	VAL
1	3	513	LEU
1	3	530	LEU
2	H	4	VAL
2	H	12	VAL
2	H	38	ASP
2	H	53	VAL
2	H	62	GLU
2	H	83	LEU
2	H	101	LEU
2	H	103	LEU
2	H	109	ILE
2	H	144	LEU
2	H	164	LEU
2	H	200	ASP

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Mol	Chain	Res	Type
2	H	207	GLU
2	H	209	ARG
2	H	212	GLU
2	H	220	SER
2	H	222	SER
2	C	4	VAL
2	C	38	ASP
2	C	53	VAL
2	C	62	GLU
2	C	83	LEU
2	C	101	LEU
2	C	103	LEU
2	C	109	ILE
2	C	131	ILE
2	C	144	LEU
2	C	164	LEU
2	C	198	ASP
2	C	208	SER
2	E	4	VAL
2	E	13	VAL
2	E	53	VAL
2	E	62	GLU
2	E	83	LEU
2	E	101	LEU
2	E	103	LEU
2	E	109	ILE
2	E	144	LEU
2	E	164	LEU
2	E	208	SER
2	G	4	VAL
2	G	12	VAL
2	G	19	ARG
2	G	38	ASP
2	G	53	VAL
2	G	62	GLU
2	G	83	LEU
2	G	101	LEU
2	G	103	LEU
2	G	109	ILE
2	G	144	LEU
2	G	164	LEU
2	G	196	ILE

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Mol	Chain	Res	Type
2	G	208	SER
2	J	4	VAL
2	J	12	VAL
2	J	53	VAL
2	J	62	GLU
2	J	83	LEU
2	J	101	LEU
2	J	103	LEU
2	J	109	ILE
2	J	144	LEU
2	J	164	LEU
2	J	208	SER
2	L	4	VAL
2	L	12	VAL
2	L	13	VAL
2	L	19	ARG
2	L	38	ASP
2	L	53	VAL
2	L	62	GLU
2	L	83	LEU
2	L	101	LEU
2	L	103	LEU
2	L	109	ILE
2	L	144	LEU
2	L	164	LEU
2	L	196	ILE
2	L	208	SER
2	L	209	ARG
2	L	210	ILE
2	L	220	SER
2	N	4	VAL
2	N	19	ARG
2	N	53	VAL
2	N	62	GLU
2	N	83	LEU
2	N	101	LEU
2	N	103	LEU
2	N	109	ILE
2	N	144	LEU
2	N	164	LEU
2	N	196	ILE
2	N	203	VAL

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Mol	Chain	Res	Type
2	N	207	GLU
2	N	208	SER
2	N	209	ARG
2	P	4	VAL
2	P	12	VAL
2	P	38	ASP
2	P	53	VAL
2	P	62	GLU
2	P	83	LEU
2	P	101	LEU
2	P	103	LEU
2	P	109	ILE
2	P	144	LEU
2	P	164	LEU
2	P	196	ILE
2	P	208	SER
2	P	220	SER
2	R	4	VAL
2	R	38	ASP
2	R	39	ASP
2	R	53	VAL
2	R	62	GLU
2	R	83	LEU
2	R	101	LEU
2	R	103	LEU
2	R	109	ILE
2	R	144	LEU
2	R	164	LEU
2	R	196	ILE
2	R	208	SER
2	R	212	GLU
2	R	213	LEU
2	T	4	VAL
2	T	12	VAL
2	T	38	ASP
2	T	53	VAL
2	T	62	GLU
2	T	83	LEU
2	T	101	LEU
2	T	103	LEU
2	T	109	ILE
2	T	144	LEU

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Mol	Chain	Res	Type
2	T	164	LEU
2	T	196	ILE
2	T	208	SER
2	T	217	ILE
2	T	220	SER
2	V	4	VAL
2	V	12	VAL
2	V	38	ASP
2	V	53	VAL
2	V	62	GLU
2	V	83	LEU
2	V	101	LEU
2	V	103	LEU
2	V	109	ILE
2	V	144	LEU
2	V	164	LEU
2	V	196	ILE
2	V	208	SER
2	V	221	ARG
2	V	222	SER
2	X	4	VAL
2	X	12	VAL
2	X	19	ARG
2	X	53	VAL
2	X	62	GLU
2	X	83	LEU
2	X	101	LEU
2	X	103	LEU
2	X	109	ILE
2	X	144	LEU
2	X	164	LEU
2	X	208	SER
2	X	220	SER
2	Z	4	VAL
2	Z	12	VAL
2	Z	53	VAL
2	Z	62	GLU
2	Z	83	LEU
2	Z	101	LEU
2	Z	103	LEU
2	Z	109	ILE
2	Z	144	LEU

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Mol	Chain	Res	Type
2	Z	164	LEU
2	Z	209	ARG
2	2	4	VAL
2	2	12	VAL
2	2	19	ARG
2	2	38	ASP
2	2	53	VAL
2	2	62	GLU
2	2	83	LEU
2	2	101	LEU
2	2	103	LEU
2	2	144	LEU
2	2	164	LEU
2	2	208	SER
2	2	209	ARG
2	2	220	SER
2	h	304	VAL
2	h	312	VAL
2	h	313	VAL
2	h	353	VAL
2	h	362	GLU
2	h	383	LEU
2	h	401	LEU
2	h	403	LEU
2	h	409	ILE
2	h	431	ILE
2	h	444	LEU
2	h	464	LEU
2	h	496	ILE
2	h	508	SER
2	h	509	ARG
2	c	304	VAL
2	c	312	VAL
2	c	319	ARG
2	c	338	ASP
2	c	353	VAL
2	c	362	GLU
2	c	383	LEU
2	c	401	LEU
2	c	403	LEU
2	c	409	ILE
2	c	444	LEU

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Mol	Chain	Res	Type
2	c	464	LEU
2	c	503	VAL
2	c	509	ARG
2	c	518	ILE
2	c	520	SER
2	e	304	VAL
2	e	353	VAL
2	e	362	GLU
2	e	383	LEU
2	e	401	LEU
2	e	403	LEU
2	e	409	ILE
2	e	444	LEU
2	e	464	LEU
2	e	496	ILE
2	e	508	SER
2	e	520	SER
2	g	304	VAL
2	g	312	VAL
2	g	319	ARG
2	g	353	VAL
2	g	362	GLU
2	g	383	LEU
2	g	401	LEU
2	g	403	LEU
2	g	409	ILE
2	g	444	LEU
2	g	464	LEU
2	g	496	ILE
2	g	508	SER
2	g	509	ARG
2	j	304	VAL
2	j	312	VAL
2	j	353	VAL
2	j	362	GLU
2	j	383	LEU
2	j	401	LEU
2	j	403	LEU
2	j	409	ILE
2	j	444	LEU
2	j	461	ASP
2	j	464	LEU

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Mol	Chain	Res	Type
2	j	496	ILE
2	j	520	SER
2	l	304	VAL
2	l	319	ARG
2	l	353	VAL
2	l	362	GLU
2	l	383	LEU
2	l	401	LEU
2	l	403	LEU
2	l	409	ILE
2	l	444	LEU
2	l	464	LEU
2	l	496	ILE
2	l	508	SER
2	l	512	GLU
2	l	520	SER
2	n	304	VAL
2	n	312	VAL
2	n	339	ASP
2	n	353	VAL
2	n	362	GLU
2	n	383	LEU
2	n	401	LEU
2	n	403	LEU
2	n	444	LEU
2	n	464	LEU
2	n	496	ILE
2	n	508	SER
2	n	520	SER
2	n	522	SER
2	p	304	VAL
2	p	312	VAL
2	p	353	VAL
2	p	362	GLU
2	p	383	LEU
2	p	401	LEU
2	p	403	LEU
2	p	409	ILE
2	p	444	LEU
2	p	464	LEU
2	p	496	ILE
2	p	500	ASP

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Mol	Chain	Res	Type
2	p	508	SER
2	r	304	VAL
2	r	353	VAL
2	r	362	GLU
2	r	383	LEU
2	r	401	LEU
2	r	403	LEU
2	r	409	ILE
2	r	444	LEU
2	r	464	LEU
2	r	496	ILE
2	r	520	SER
2	t	304	VAL
2	t	312	VAL
2	t	317	ASP
2	t	338	ASP
2	t	353	VAL
2	t	362	GLU
2	t	383	LEU
2	t	401	LEU
2	t	403	LEU
2	t	409	ILE
2	t	444	LEU
2	t	464	LEU
2	t	496	ILE
2	t	508	SER
2	t	520	SER
2	v	304	VAL
2	v	312	VAL
2	v	319	ARG
2	v	338	ASP
2	v	353	VAL
2	v	362	GLU
2	v	383	LEU
2	v	401	LEU
2	v	403	LEU
2	v	409	ILE
2	v	444	LEU
2	v	464	LEU
2	v	496	ILE
2	v	508	SER
2	x	304	VAL

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Mol	Chain	Res	Type
2	x	312	VAL
2	x	317	ASP
2	x	338	ASP
2	x	353	VAL
2	x	362	GLU
2	x	383	LEU
2	x	401	LEU
2	x	403	LEU
2	x	409	ILE
2	x	444	LEU
2	x	464	LEU
2	x	496	ILE
2	x	508	SER
2	x	509	ARG
2	z	304	VAL
2	z	312	VAL
2	z	353	VAL
2	z	362	GLU
2	z	383	LEU
2	z	401	LEU
2	z	403	LEU
2	z	409	ILE
2	z	444	LEU
2	z	464	LEU
2	4	304	VAL
2	4	312	VAL
2	4	319	ARG
2	4	353	VAL
2	4	362	GLU
2	4	383	LEU
2	4	401	LEU
2	4	403	LEU
2	4	409	ILE
2	4	444	LEU
2	4	464	LEU
2	4	508	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	45	ASN

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Mol	Chain	Res	Type
1	A	98	GLN
1	A	129	HIS
1	A	174	ASN
1	B	174	ASN
1	B	231	GLN
1	D	45	ASN
1	D	73	ASN
1	D	98	GLN
1	D	174	ASN
1	F	80	GLN
1	F	129	HIS
1	F	174	ASN
1	I	11	GLN
1	I	98	GLN
1	I	114	GLN
1	I	152	HIS
1	K	73	ASN
1	K	98	GLN
1	K	114	GLN
1	K	129	HIS
1	M	98	GLN
1	M	114	GLN
1	O	98	GLN
1	O	114	GLN
1	O	129	HIS
1	O	152	HIS
1	Q	98	GLN
1	Q	114	GLN
1	Q	152	HIS
1	S	51	GLN
1	S	98	GLN
1	S	114	GLN
1	S	231	GLN
1	U	11	GLN
1	U	98	GLN
1	U	114	GLN
1	U	129	HIS
1	W	51	GLN
1	W	114	GLN
1	Y	11	GLN
1	Y	98	GLN
1	Y	114	GLN

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Mol	Chain	Res	Type
1	Y	152	HIS
1	Y	174	ASN
1	l	98	GLN
1	l	114	GLN
1	l	129	HIS
1	a	398	GLN
1	a	414	GLN
1	a	429	HIS
1	a	452	HIS
1	b	398	GLN
1	b	414	GLN
1	b	429	HIS
1	b	452	HIS
1	d	398	GLN
1	d	414	GLN
1	d	429	HIS
1	d	452	HIS
1	f	311	GLN
1	f	398	GLN
1	f	414	GLN
1	f	452	HIS
1	i	311	GLN
1	i	398	GLN
1	i	414	GLN
1	i	452	HIS
1	i	474	ASN
1	i	531	GLN
1	k	398	GLN
1	k	414	GLN
1	k	452	HIS
1	m	398	GLN
1	m	414	GLN
1	m	452	HIS
1	o	398	GLN
1	o	414	GLN
1	o	429	HIS
1	q	311	GLN
1	q	398	GLN
1	q	414	GLN
1	q	452	HIS
1	s	351	GLN
1	s	398	GLN

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Mol	Chain	Res	Type
1	s	414	GLN
1	s	452	HIS
1	s	516	ASN
1	u	398	GLN
1	u	414	GLN
1	u	452	HIS
1	w	398	GLN
1	w	414	GLN
1	w	429	HIS
1	w	474	ASN
1	y	398	GLN
1	y	414	GLN
1	y	452	HIS
1	3	398	GLN
1	3	414	GLN
1	3	429	HIS
1	3	531	GLN
2	H	65	HIS
2	H	130	ASN
2	C	65	HIS
2	C	110	HIS
2	C	130	ASN
2	E	65	HIS
2	E	130	ASN
2	G	65	HIS
2	G	130	ASN
2	J	65	HIS
2	J	130	ASN
2	L	65	HIS
2	L	130	ASN
2	N	65	HIS
2	N	130	ASN
2	P	65	HIS
2	P	130	ASN
2	R	65	HIS
2	R	130	ASN
2	T	65	HIS
2	T	130	ASN
2	V	65	HIS
2	V	130	ASN
2	X	65	HIS
2	X	130	ASN

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Mol	Chain	Res	Type
2	Z	65	HIS
2	Z	130	ASN
2	2	65	HIS
2	2	130	ASN
2	h	365	HIS
2	h	430	ASN
2	c	365	HIS
2	c	430	ASN
2	e	365	HIS
2	e	430	ASN
2	g	365	HIS
2	g	430	ASN
2	j	365	HIS
2	j	430	ASN
2	l	365	HIS
2	l	430	ASN
2	n	365	HIS
2	n	410	HIS
2	n	430	ASN
2	p	365	HIS
2	p	430	ASN
2	r	365	HIS
2	r	430	ASN
2	t	365	HIS
2	t	430	ASN
2	v	365	HIS
2	v	430	ASN
2	x	365	HIS
2	x	430	ASN
2	z	365	HIS
2	z	430	ASN
2	4	365	HIS
2	4	410	HIS
2	4	430	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OZT	T	1	2	6,9,10	2.75	2 (33%)	9,12,14	2.34	3 (33%)
2	OZT	h	301	2	6,9,10	3.08	2 (33%)	9,12,14	2.41	4 (44%)
2	OZT	X	1	2	6,9,10	3.02	2 (33%)	9,12,14	2.58	4 (44%)
2	OZT	L	1	2	6,9,10	2.74	2 (33%)	9,12,14	2.46	5 (55%)
2	OZT	N	1	2	6,9,10	2.91	2 (33%)	9,12,14	2.28	4 (44%)
2	OZT	z	301	2	6,9,10	3.37	2 (33%)	9,12,14	2.45	3 (33%)
2	OZT	E	1	2	6,9,10	3.28	2 (33%)	9,12,14	2.68	5 (55%)
2	OZT	l	301	2	6,9,10	2.81	2 (33%)	9,12,14	2.51	4 (44%)
2	OZT	t	301	2	6,9,10	2.83	2 (33%)	9,12,14	2.20	4 (44%)
2	OZT	Z	1	2	6,9,10	2.92	2 (33%)	9,12,14	1.72	3 (33%)
2	OZT	g	301	2	6,9,10	2.84	2 (33%)	9,12,14	2.72	4 (44%)
2	OZT	r	301	2	6,9,10	3.00	2 (33%)	9,12,14	2.60	4 (44%)
2	OZT	C	1	2	6,9,10	3.18	2 (33%)	9,12,14	1.77	2 (22%)
2	OZT	2	1	2	6,9,10	2.83	2 (33%)	9,12,14	2.21	3 (33%)
2	OZT	c	301	2	6,9,10	3.04	2 (33%)	9,12,14	2.19	5 (55%)
2	OZT	n	301	2	6,9,10	3.31	2 (33%)	9,12,14	2.25	4 (44%)
2	OZT	v	301	2	6,9,10	3.25	2 (33%)	9,12,14	2.87	3 (33%)
2	OZT	p	301	2	6,9,10	3.20	2 (33%)	9,12,14	2.85	5 (55%)
2	OZT	x	301	2	6,9,10	3.40	2 (33%)	9,12,14	2.36	4 (44%)
2	OZT	4	301	2	6,9,10	3.32	2 (33%)	9,12,14	2.83	5 (55%)
2	OZT	R	1	2	6,9,10	3.25	2 (33%)	9,12,14	3.02	5 (55%)
2	OZT	G	1	2	6,9,10	2.95	2 (33%)	9,12,14	2.32	3 (33%)
2	OZT	e	301	2	6,9,10	3.13	2 (33%)	9,12,14	2.06	4 (44%)
2	OZT	J	1	2	6,9,10	3.16	2 (33%)	9,12,14	2.36	3 (33%)
2	OZT	V	1	2	6,9,10	3.12	2 (33%)	9,12,14	1.96	3 (33%)
2	OZT	j	301	2	6,9,10	2.99	2 (33%)	9,12,14	1.82	5 (55%)
2	OZT	H	1	2	6,9,10	3.30	2 (33%)	9,12,14	2.69	4 (44%)
2	OZT	P	1	2	6,9,10	2.80	2 (33%)	9,12,14	2.66	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	T	1	2	-	0/1/14/16	0/1/1/1
2	OZT	h	301	2	-	0/1/14/16	0/1/1/1
2	OZT	X	1	2	-	0/1/14/16	0/1/1/1
2	OZT	L	1	2	-	0/1/14/16	0/1/1/1
2	OZT	N	1	2	-	0/1/14/16	0/1/1/1
2	OZT	z	301	2	-	0/1/14/16	0/1/1/1
2	OZT	E	1	2	-	0/1/14/16	0/1/1/1
2	OZT	l	301	2	-	0/1/14/16	0/1/1/1
2	OZT	t	301	2	-	1/1/14/16	0/1/1/1
2	OZT	Z	1	2	-	0/1/14/16	0/1/1/1
2	OZT	g	301	2	-	0/1/14/16	0/1/1/1
2	OZT	r	301	2	-	0/1/14/16	0/1/1/1
2	OZT	C	1	2	-	0/1/14/16	0/1/1/1
2	OZT	2	1	2	-	1/1/14/16	0/1/1/1
2	OZT	c	301	2	-	0/1/14/16	0/1/1/1
2	OZT	n	301	2	-	1/1/14/16	0/1/1/1
2	OZT	v	301	2	-	0/1/14/16	0/1/1/1
2	OZT	p	301	2	-	0/1/14/16	0/1/1/1
2	OZT	x	301	2	-	0/1/14/16	0/1/1/1
2	OZT	4	301	2	-	1/1/14/16	0/1/1/1
2	OZT	R	1	2	-	1/1/14/16	0/1/1/1
2	OZT	G	1	2	-	0/1/14/16	0/1/1/1
2	OZT	e	301	2	-	0/1/14/16	0/1/1/1
2	OZT	J	1	2	-	0/1/14/16	0/1/1/1
2	OZT	V	1	2	-	0/1/14/16	0/1/1/1
2	OZT	j	301	2	-	0/1/14/16	0/1/1/1
2	OZT	H	1	2	-	0/1/14/16	0/1/1/1
2	OZT	P	1	2	-	0/1/14/16	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	x	301	OZT	O1-C5	7.69	1.46	1.36
2	z	301	OZT	O1-C5	7.68	1.46	1.36
2	n	301	OZT	O1-C5	7.63	1.46	1.36
2	E	1	OZT	O1-C5	7.49	1.46	1.36
2	4	301	OZT	O1-C5	7.47	1.46	1.36
2	H	1	OZT	O1-C5	7.41	1.46	1.36
2	v	301	OZT	O1-C5	7.23	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	p	301	OZT	O1-C5	7.14	1.45	1.36
2	C	1	OZT	O1-C5	7.12	1.45	1.36
2	V	1	OZT	O1-C5	7.08	1.45	1.36
2	c	301	OZT	O1-C5	7.06	1.45	1.36
2	e	301	OZT	O1-C5	7.03	1.45	1.36
2	J	1	OZT	O1-C5	7.01	1.45	1.36
2	R	1	OZT	O1-C5	6.97	1.45	1.36
2	X	1	OZT	O1-C5	6.79	1.45	1.36
2	h	301	OZT	O1-C5	6.79	1.45	1.36
2	j	301	OZT	O1-C5	6.77	1.45	1.36
2	G	1	OZT	O1-C5	6.67	1.45	1.36
2	r	301	OZT	O1-C5	6.64	1.45	1.36
2	Z	1	OZT	O1-C5	6.57	1.45	1.36
2	N	1	OZT	O1-C5	6.42	1.44	1.36
2	T	1	OZT	O1-C5	6.35	1.44	1.36
2	l	301	OZT	O1-C5	6.33	1.44	1.36
2	2	1	OZT	O1-C5	6.30	1.44	1.36
2	L	1	OZT	O1-C5	6.27	1.44	1.36
2	t	301	OZT	O1-C5	6.26	1.44	1.36
2	P	1	OZT	O1-C5	6.04	1.44	1.36
2	g	301	OZT	O1-C5	6.03	1.44	1.36
2	R	1	OZT	O1-C2	-3.70	1.41	1.46
2	p	301	OZT	O1-C2	-3.12	1.41	1.46
2	v	301	OZT	O1-C2	-3.04	1.42	1.46
2	h	301	OZT	O1-C2	-3.03	1.42	1.46
2	g	301	OZT	O1-C2	-2.99	1.42	1.46
2	J	1	OZT	O1-C2	-2.98	1.42	1.46
2	H	1	OZT	O1-C2	-2.88	1.42	1.46
2	r	301	OZT	O1-C2	-2.86	1.42	1.46
2	N	1	OZT	O1-C2	-2.78	1.42	1.46
2	4	301	OZT	O1-C2	-2.73	1.42	1.46
2	P	1	OZT	O1-C2	-2.72	1.42	1.46
2	E	1	OZT	O1-C2	-2.70	1.42	1.46
2	t	301	OZT	O1-C2	-2.69	1.42	1.46
2	2	1	OZT	O1-C2	-2.64	1.42	1.46
2	j	301	OZT	O1-C2	-2.63	1.42	1.46
2	x	301	OZT	O1-C2	-2.60	1.42	1.46
2	G	1	OZT	O1-C2	-2.58	1.42	1.46
2	C	1	OZT	O1-C2	-2.53	1.42	1.46
2	e	301	OZT	O1-C2	-2.52	1.42	1.46
2	z	301	OZT	O1-C2	-2.50	1.42	1.46
2	n	301	OZT	O1-C2	-2.50	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	1	OZT	O1-C2	-2.49	1.42	1.46
2	V	1	OZT	O1-C2	-2.45	1.43	1.46
2	l	301	OZT	O1-C2	-2.36	1.43	1.46
2	L	1	OZT	O1-C2	-2.16	1.43	1.46
2	c	301	OZT	O1-C2	-2.07	1.43	1.46
2	T	1	OZT	O1-C2	-2.06	1.43	1.46
2	X	1	OZT	O1-C2	-2.05	1.43	1.46

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	301	OZT	C2-O1-C5	-5.91	101.57	110.33
2	r	301	OZT	C2-CA-C	-5.81	106.08	114.16
2	H	1	OZT	CA-N-C5	-5.77	103.83	112.75
2	J	1	OZT	O1-C2-C7	-5.65	101.34	108.68
2	v	301	OZT	C2-CA-C	-5.17	106.98	114.16
2	R	1	OZT	O1-C2-C7	-5.07	102.09	108.68
2	E	1	OZT	O1-C2-CA	4.87	108.15	103.72
2	T	1	OZT	CA-N-C5	-4.83	105.28	112.75
2	z	301	OZT	CA-N-C5	-4.83	105.28	112.75
2	g	301	OZT	C2-CA-C	-4.75	107.55	114.16
2	L	1	OZT	C2-CA-C	-4.66	107.68	114.16
2	g	301	OZT	CA-N-C5	-4.56	105.70	112.75
2	p	301	OZT	O1-C2-C7	-4.49	102.84	108.68
2	l	301	OZT	O1-C2-C7	-4.46	102.88	108.68
2	x	301	OZT	CA-N-C5	-4.43	105.90	112.75
2	p	301	OZT	CA-N-C5	-4.40	105.95	112.75
2	R	1	OZT	C2-CA-C	-4.39	108.06	114.16
2	p	301	OZT	C2-O1-C5	-4.35	103.89	110.33
2	G	1	OZT	CA-N-C5	-4.31	106.08	112.75
2	P	1	OZT	CA-N-C5	-4.28	106.14	112.75
2	X	1	OZT	CA-N-C5	-4.26	106.17	112.75
2	v	301	OZT	C2-O1-C5	-4.25	104.03	110.33
2	v	301	OZT	CA-N-C5	-4.17	106.31	112.75
2	R	1	OZT	C2-O1-C5	-4.13	104.20	110.33
2	H	1	OZT	C2-O1-C5	-4.04	104.35	110.33
2	T	1	OZT	C2-O1-C5	-4.02	104.37	110.33
2	h	301	OZT	C2-O1-C5	-4.01	104.38	110.33
2	4	301	OZT	CA-N-C5	-3.99	106.58	112.75
2	t	301	OZT	C2-CA-C	-3.83	108.83	114.16
2	r	301	OZT	C2-O1-C5	-3.82	104.67	110.33
2	P	1	OZT	C2-O1-C5	-3.80	104.70	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	OZT	C2-CA-C	-3.79	108.89	114.16
2	E	1	OZT	C2-O1-C5	-3.78	104.73	110.33
2	R	1	OZT	CA-N-C5	-3.74	106.97	112.75
2	N	1	OZT	C2-O1-C5	-3.74	104.79	110.33
2	l	301	OZT	C2-O1-C5	-3.73	104.80	110.33
2	X	1	OZT	C2-O1-C5	-3.70	104.84	110.33
2	c	301	OZT	C2-CA-C	-3.66	109.07	114.16
2	z	301	OZT	C2-O1-C5	-3.65	104.93	110.33
2	l	301	OZT	O1-C2-CA	3.64	107.03	103.72
2	h	301	OZT	O1-C2-C7	-3.61	103.98	108.68
2	2	1	OZT	C2-CA-C	-3.61	109.14	114.16
2	P	1	OZT	O1-C5-N	-3.48	107.04	109.87
2	g	301	OZT	C2-O1-C5	-3.42	105.26	110.33
2	N	1	OZT	O1-C2-CA	3.41	106.83	103.72
2	n	301	OZT	C2-CA-C	-3.32	109.55	114.16
2	X	1	OZT	C2-CA-C	-3.25	109.64	114.16
2	P	1	OZT	C2-CA-C	-3.17	109.74	114.16
2	L	1	OZT	C2-O1-C5	-3.17	105.63	110.33
2	E	1	OZT	C2-CA-C	-3.17	109.75	114.16
2	2	1	OZT	C2-O1-C5	-3.15	105.66	110.33
2	t	301	OZT	C2-O1-C5	-3.14	105.67	110.33
2	n	301	OZT	C2-O1-C5	-3.10	105.73	110.33
2	x	301	OZT	C2-O1-C5	-3.09	105.75	110.33
2	n	301	OZT	CA-N-C5	-3.05	108.03	112.75
2	x	301	OZT	C2-CA-C	-3.04	109.93	114.16
2	t	301	OZT	CA-N-C5	-3.01	108.09	112.75
2	V	1	OZT	O1-C2-C7	-2.95	104.85	108.68
2	e	301	OZT	O1-C2-CA	2.89	106.35	103.72
2	C	1	OZT	O1-C5-N	-2.89	107.51	109.87
2	h	301	OZT	CA-N-C5	-2.88	108.30	112.75
2	V	1	OZT	CA-N-C5	-2.87	108.31	112.75
2	e	301	OZT	C2-O1-C5	-2.83	106.14	110.33
2	e	301	OZT	O6-C5-N	-2.80	125.88	129.19
2	H	1	OZT	C2-CA-C	-2.78	110.29	114.16
2	J	1	OZT	C2-O1-C5	-2.78	106.21	110.33
2	L	1	OZT	O1-C2-CA	2.74	106.21	103.72
2	G	1	OZT	C2-O1-C5	-2.71	106.31	110.33
2	c	301	OZT	C2-O1-C5	-2.70	106.33	110.33
2	L	1	OZT	CA-N-C5	-2.69	108.59	112.75
2	2	1	OZT	O1-C2-CA	2.67	106.15	103.72
2	4	301	OZT	O6-C5-N	-2.67	126.03	129.19
2	l	301	OZT	CA-N-C5	-2.66	108.64	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	1	OZT	CA-N-C5	-2.65	108.66	112.75
2	Z	1	OZT	C2-O1-C5	-2.65	106.41	110.33
2	x	301	OZT	O6-C5-N	-2.60	126.11	129.19
2	L	1	OZT	O-C-CA	-2.60	117.99	124.86
2	j	301	OZT	C2-CA-C	-2.59	110.55	114.16
2	g	301	OZT	O1-C5-N	-2.58	107.77	109.87
2	E	1	OZT	O-C-CA	-2.54	118.14	124.86
2	c	301	OZT	O1-C2-C7	2.51	111.93	108.68
2	z	301	OZT	O6-C5-N	-2.49	126.24	129.19
2	V	1	OZT	C2-O1-C5	-2.48	106.66	110.33
2	N	1	OZT	CA-N-C5	-2.48	108.92	112.75
2	j	301	OZT	C2-O1-C5	-2.43	106.73	110.33
2	X	1	OZT	O1-C5-N	-2.38	107.94	109.87
2	c	301	OZT	O-C-CA	-2.37	118.58	124.86
2	C	1	OZT	O-C-CA	-2.36	118.62	124.86
2	T	1	OZT	C2-CA-C	-2.34	110.90	114.16
2	p	301	OZT	O1-C2-CA	2.34	105.85	103.72
2	H	1	OZT	O1-C2-C7	-2.34	105.64	108.68
2	j	301	OZT	O1-C2-CA	2.31	105.82	103.72
2	J	1	OZT	CA-N-C5	-2.30	109.19	112.75
2	r	301	OZT	O1-C2-CA	2.26	105.77	103.72
2	j	301	OZT	O-C-CA	-2.25	118.92	124.86
2	t	301	OZT	O1-C2-C7	-2.24	105.77	108.68
2	N	1	OZT	O1-C5-N	-2.23	108.05	109.87
2	e	301	OZT	C2-CA-C	-2.17	111.14	114.16
2	4	301	OZT	O1-C5-O6	2.17	125.33	121.37
2	E	1	OZT	O6-C5-N	-2.14	126.66	129.19
2	h	301	OZT	O1-C5-N	2.11	111.59	109.87
2	r	301	OZT	O-C-CA	-2.08	119.35	124.86
2	4	301	OZT	O-C-CA	-2.07	119.38	124.86
2	Z	1	OZT	C2-CA-C	-2.07	111.28	114.16
2	R	1	OZT	O1-C2-CA	-2.07	101.84	103.72
2	c	301	OZT	O1-C2-CA	2.04	105.58	103.72
2	p	301	OZT	O-C-CA	-2.03	119.49	124.86
2	j	301	OZT	CA-N-C5	-2.02	109.62	112.75
2	n	301	OZT	O1-C2-CA	2.00	105.54	103.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	1	OZT	O-C-CA-C2

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Mol	Chain	Res	Type	Atoms
2	t	301	OZT	O-C-CA-C2
2	2	1	OZT	O-C-CA-C2
2	n	301	OZT	O-C-CA-C2
2	4	301	OZT	O-C-CA-C2

There are no ring outliers.

23 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	h	301	OZT	2	0
2	X	1	OZT	6	0
2	L	1	OZT	4	0
2	N	1	OZT	2	0
2	z	301	OZT	1	0
2	E	1	OZT	4	0
2	l	301	OZT	1	0
2	t	301	OZT	1	0
2	Z	1	OZT	1	0
2	g	301	OZT	11	0
2	r	301	OZT	1	0
2	C	1	OZT	2	0
2	2	1	OZT	6	0
2	c	301	OZT	1	0
2	n	301	OZT	1	0
2	p	301	OZT	1	0
2	x	301	OZT	2	0
2	4	301	OZT	5	0
2	J	1	OZT	1	0
2	V	1	OZT	3	0
2	j	301	OZT	1	0
2	H	1	OZT	8	0
2	P	1	OZT	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	211/240 (87%)	0.75	23 (10%) 10 9	19, 76, 123, 148	0
1	3	210/240 (87%)	0.49	9 (4%) 40 32	26, 72, 119, 146	0
1	A	211/240 (87%)	0.41	9 (4%) 40 32	20, 58, 105, 155	0
1	B	211/240 (87%)	0.14	3 (1%) 73 66	16, 48, 93, 141	0
1	D	210/240 (87%)	1.78	75 (35%) 1 1	36, 98, 148, 167	0
1	F	193/240 (80%)	0.30	6 (3%) 51 42	21, 55, 103, 136	0
1	I	212/240 (88%)	0.40	4 (1%) 66 58	23, 55, 101, 116	0
1	K	211/240 (87%)	1.12	31 (14%) 6 4	30, 74, 114, 166	0
1	M	205/240 (85%)	1.27	45 (21%) 2 2	27, 82, 142, 204	0
1	O	211/240 (87%)	0.50	13 (6%) 26 20	15, 67, 114, 137	0
1	Q	211/240 (87%)	2.00	97 (45%) 0 0	52, 111, 152, 185	0
1	S	211/240 (87%)	0.59	12 (5%) 29 23	23, 64, 113, 134	0
1	U	211/240 (87%)	0.60	7 (3%) 49 40	11, 69, 117, 140	0
1	W	193/240 (80%)	1.40	45 (23%) 2 2	31, 89, 134, 158	0
1	Y	210/240 (87%)	1.30	49 (23%) 2 2	29, 80, 125, 142	0
1	a	211/240 (87%)	0.34	5 (2%) 59 50	21, 61, 114, 153	0
1	b	211/240 (87%)	0.47	11 (5%) 33 26	20, 61, 110, 129	0
1	d	211/240 (87%)	0.68	12 (5%) 29 23	25, 76, 124, 160	0
1	f	211/240 (87%)	0.89	24 (11%) 10 8	25, 80, 124, 150	0
1	i	211/240 (87%)	0.37	7 (3%) 49 40	18, 56, 105, 131	0
1	k	211/240 (87%)	0.37	4 (1%) 66 58	20, 58, 105, 159	0
1	m	208/240 (86%)	0.70	12 (5%) 29 22	21, 76, 124, 159	0
1	o	211/240 (87%)	0.73	17 (8%) 18 15	22, 74, 123, 158	0
1	q	211/240 (87%)	1.15	25 (11%) 9 8	36, 88, 132, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	s	211/240 (87%)	0.48	9 (4%)	40 32	16, 64, 108, 133	0
1	u	211/240 (87%)	0.71	11 (5%)	33 26	21, 76, 117, 138	0
1	w	211/240 (87%)	1.57	62 (29%)	1 1	41, 96, 138, 187	0
1	y	211/240 (87%)	1.51	71 (33%)	1 1	41, 83, 126, 145	0
2	2	216/240 (90%)	-0.21	3 (1%)	73 66	16, 38, 90, 124	0
2	4	216/240 (90%)	-0.11	2 (0%)	81 75	15, 42, 88, 112	0
2	C	216/240 (90%)	0.17	3 (1%)	73 66	19, 51, 92, 122	0
2	E	216/240 (90%)	0.35	5 (2%)	61 52	16, 55, 92, 154	0
2	G	216/240 (90%)	-0.17	3 (1%)	73 66	14, 41, 86, 149	0
2	H	216/240 (90%)	0.08	3 (1%)	73 66	21, 47, 89, 125	0
2	J	216/240 (90%)	0.20	5 (2%)	61 52	21, 51, 94, 143	0
2	L	216/240 (90%)	0.15	4 (1%)	66 58	21, 45, 86, 140	0
2	N	216/240 (90%)	-0.21	2 (0%)	81 75	16, 33, 76, 114	0
2	P	216/240 (90%)	-0.27	2 (0%)	81 75	13, 34, 77, 121	0
2	R	216/240 (90%)	0.59	6 (2%)	55 46	26, 62, 100, 135	0
2	T	216/240 (90%)	0.01	4 (1%)	66 58	14, 42, 90, 114	0
2	V	217/240 (90%)	-0.32	3 (1%)	73 66	11, 32, 80, 126	0
2	X	216/240 (90%)	0.07	4 (1%)	66 58	22, 42, 85, 119	0
2	Z	216/240 (90%)	0.44	6 (2%)	55 46	28, 55, 100, 145	0
2	c	214/240 (89%)	-0.01	4 (1%)	66 58	20, 45, 83, 130	0
2	e	216/240 (90%)	0.05	3 (1%)	73 66	18, 46, 90, 122	0
2	g	216/240 (90%)	0.01	3 (1%)	73 66	21, 46, 89, 152	0
2	h	213/240 (88%)	-0.20	2 (0%)	81 75	14, 39, 75, 119	0
2	j	216/240 (90%)	0.03	3 (1%)	73 66	15, 47, 88, 127	0
2	l	216/240 (90%)	-0.07	3 (1%)	73 66	18, 39, 84, 128	0
2	n	216/240 (90%)	-0.20	2 (0%)	81 75	13, 38, 87, 120	0
2	p	216/240 (90%)	-0.31	4 (1%)	66 58	13, 33, 73, 140	0
2	r	216/240 (90%)	0.19	2 (0%)	81 75	21, 50, 93, 124	0
2	t	216/240 (90%)	0.07	5 (2%)	61 52	18, 48, 90, 121	0
2	v	218/240 (90%)	-0.21	5 (2%)	61 52	13, 36, 85, 123	0
2	x	216/240 (90%)	0.08	4 (1%)	66 58	24, 45, 92, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	z	216/240 (90%)	0.09	2 (0%) 81 75	22, 49, 98, 130	0
All	All	11907/13440 (88%)	0.41	795 (6%) 24 19	11, 56, 117, 204	0

All (795) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	LEU	6.0
1	k	472	ALA	5.7
1	M	19	LEU	5.1
1	D	35	TYR	4.9
1	w	443	TYR	4.8
1	w	338	GLY	4.7
1	w	477	LEU	4.6
1	W	226	THR	4.6
1	K	35	TYR	4.5
2	L	99	LEU	4.5
1	A	131	GLY	4.5
1	y	337	GLY	4.4
2	Z	99	LEU	4.4
2	P	99	LEU	4.4
1	Q	39	VAL	4.3
1	Q	177	LEU	4.3
1	D	40	LEU	4.2
1	f	317	SER	4.2
1	Q	50	LEU	4.2
1	q	526	THR	4.2
1	w	488	LEU	4.2
2	Z	100	ALA	4.1
2	n	400	ALA	4.1
1	W	143	TYR	4.1
1	Y	38	GLY	4.1
2	n	399	LEU	4.0
2	h	400	ALA	4.0
1	Q	162	PRO	4.0
1	Q	181	LEU	4.0
1	D	136	PRO	4.0
1	y	518	PRO	4.0
1	D	180	ALA	4.0
2	C	99	LEU	4.0
1	D	175	ALA	3.9
1	y	338	GLY	3.9
1	Y	177	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	m	530	LEU	3.9
2	2	100	ALA	3.9
1	F	35	TYR	3.9
1	K	38	GLY	3.9
1	W	230	LEU	3.9
1	D	12	ALA	3.9
1	f	320	ALA	3.9
1	Q	13	MET	3.8
1	Y	130	TYR	3.8
1	D	181	LEU	3.8
1	W	177	LEU	3.8
1	Y	230	LEU	3.8
1	q	455	VAL	3.8
2	J	100	ALA	3.8
2	L	100	ALA	3.8
1	D	233	LEU	3.8
2	p	399	LEU	3.8
1	Q	159	THR	3.8
1	M	13	MET	3.8
1	w	453	PHE	3.8
1	w	441	ILE	3.8
2	l	400	ALA	3.8
1	W	188	LEU	3.8
2	X	99	LEU	3.8
1	D	226	THR	3.8
1	y	478	THR	3.8
1	D	10	GLU	3.7
1	f	314	ARG	3.7
2	H	99	LEU	3.7
1	w	505	VAL	3.7
1	b	472	ALA	3.7
1	w	475	ALA	3.7
2	g	393	ALA	3.7
1	Q	143	TYR	3.7
1	i	505	VAL	3.7
1	o	531	GLN	3.7
2	x	399	LEU	3.7
2	v	400	ALA	3.7
1	O	19	LEU	3.6
1	w	454	VAL	3.6
1	Q	153	PHE	3.6
1	M	24	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	w	467	LEU	3.6
1	W	180	ALA	3.6
1	Y	36	ALA	3.6
1	u	484	ALA	3.6
1	D	44	GLU	3.6
1	y	505	VAL	3.6
1	Q	178	THR	3.6
1	D	13	MET	3.6
2	N	99	LEU	3.6
1	W	27	ALA	3.6
1	Q	171	TYR	3.6
1	y	516	ASN	3.6
2	x	400	ALA	3.5
1	Q	33	LEU	3.5
1	Q	175	ALA	3.5
1	W	190	ALA	3.5
1	y	475	ALA	3.5
2	N	100	ALA	3.5
1	M	228	SER	3.5
1	Q	185	VAL	3.5
2	E	99	LEU	3.5
2	X	100	ALA	3.5
2	j	400	ALA	3.5
1	M	17	SER	3.5
2	e	399	LEU	3.5
1	Q	41	PHE	3.5
1	Q	52	LYS	3.5
1	Y	134	LYS	3.5
1	Y	133	THR	3.5
2	r	400	ALA	3.5
1	Q	61	GLY	3.4
1	l	13	MET	3.4
2	l	399	LEU	3.4
2	P	100	ALA	3.4
1	d	337	GLY	3.4
1	Q	64	ALA	3.4
1	D	143	TYR	3.4
2	z	399	LEU	3.4
1	Q	25	ALA	3.4
1	Q	65	ALA	3.4
1	o	472	ALA	3.4
1	Q	62	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	y	341	PHE	3.4
2	V	99	LEU	3.4
2	Z	38	ASP	3.4
1	Q	56	LEU	3.3
1	Q	127	VAL	3.3
1	U	205	VAL	3.3
1	A	150	GLU	3.3
1	3	472	ALA	3.3
2	p	400	ALA	3.3
1	K	205	VAL	3.3
1	Q	156	MET	3.3
1	q	505	VAL	3.3
1	f	318	GLU	3.3
1	M	172	ALA	3.3
1	y	336	ALA	3.3
2	L	93	ALA	3.3
1	D	41	PHE	3.3
1	M	153	PHE	3.3
2	j	399	LEU	3.3
1	M	21	ARG	3.3
1	a	311	GLN	3.3
1	D	183	ILE	3.3
1	Q	163	ILE	3.3
2	E	100	ALA	3.3
1	u	333	LEU	3.3
1	Q	31	VAL	3.3
1	y	430	TYR	3.2
1	K	172	ALA	3.2
1	W	172	ALA	3.2
2	V	100	ALA	3.2
1	Q	213	LEU	3.2
1	M	42	VAL	3.2
1	D	37	GLY	3.2
1	Q	136	PRO	3.2
1	Q	165	ASN	3.2
1	Q	20	ALA	3.2
2	2	99	LEU	3.2
1	w	321	ARG	3.2
1	m	338	GLY	3.2
1	D	163	ILE	3.2
1	Q	24	ILE	3.2
1	q	477	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	16	ARG	3.2
1	K	16	ARG	3.2
1	M	177	LEU	3.2
1	Q	164	ALA	3.2
2	x	415	GLN	3.2
1	D	38	GLY	3.2
1	D	157	GLY	3.2
1	y	471	TYR	3.1
1	Y	187	ALA	3.1
1	q	490	ALA	3.1
1	y	472	ALA	3.1
1	a	505	VAL	3.1
1	D	156	MET	3.1
2	v	399	LEU	3.1
1	M	229	ALA	3.1
1	Q	34	ALA	3.1
2	z	400	ALA	3.1
1	W	174	ASN	3.1
1	D	171	TYR	3.1
2	H	100	ALA	3.1
1	Y	205	VAL	3.1
1	y	411	PHE	3.1
1	M	231	GLN	3.1
1	f	311	GLN	3.1
1	D	134	LYS	3.1
1	W	215	ALA	3.1
1	M	111	PHE	3.1
1	Q	42	VAL	3.1
1	D	90	ASP	3.1
1	y	525	ILE	3.1
2	T	99	LEU	3.1
1	U	172	ALA	3.0
1	Y	41	PHE	3.0
1	D	19	LEU	3.0
1	q	513	LEU	3.0
2	t	399	LEU	3.0
1	D	115	ALA	3.0
1	M	20	ALA	3.0
1	l	172	ALA	3.0
1	i	472	ALA	3.0
1	M	205	VAL	3.0
1	Y	127	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	Y	171	TYR	3.0
1	Q	158	GLY	3.0
1	o	311	GLN	3.0
1	w	463	ILE	3.0
1	D	33	LEU	3.0
1	Y	33	LEU	3.0
1	o	344	GLU	3.0
1	b	433	THR	3.0
1	I	172	ALA	3.0
1	Q	155	VAL	3.0
1	y	434	LYS	3.0
1	D	174	ASN	3.0
1	w	355	GLU	3.0
1	w	459	THR	3.0
1	k	313	MET	3.0
1	Q	144	ASP	3.0
1	y	432	GLU	3.0
2	2	93	ALA	3.0
1	W	205	VAL	3.0
1	K	143	TYR	2.9
1	M	171	TYR	2.9
1	Q	35	TYR	2.9
1	y	488	LEU	2.9
1	y	474	ASN	2.9
1	Q	49	SER	2.9
1	M	164	ALA	2.9
1	Q	190	ALA	2.9
1	m	472	ALA	2.9
1	w	312	ALA	2.9
2	g	400	ALA	2.9
1	D	31	VAL	2.9
1	3	344	GLU	2.9
1	Y	174	ASN	2.9
1	D	155	VAL	2.9
1	Q	30	VAL	2.9
1	w	325	ALA	2.9
1	W	181	LEU	2.9
1	3	530	LEU	2.9
1	Q	38	GLY	2.9
1	K	171	TYR	2.9
1	O	15	GLU	2.9
2	R	198	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	185	VAL	2.9
1	F	172	ALA	2.9
1	Y	184	ALA	2.9
2	c	400	ALA	2.9
2	l	393	ALA	2.9
2	t	393	ALA	2.9
1	o	526	THR	2.9
1	D	24	ILE	2.9
1	l	163	ILE	2.9
1	M	188	LEU	2.9
1	D	114	GLN	2.9
1	y	455	VAL	2.9
1	3	486	ALA	2.9
1	K	14	ARG	2.9
1	Y	228	SER	2.9
1	D	151	PRO	2.8
2	E	64	GLU	2.8
1	W	175	ALA	2.8
1	m	529	ALA	2.8
2	G	93	ALA	2.8
1	a	514	ASP	2.8
1	f	319	LEU	2.8
2	J	99	LEU	2.8
1	D	162	PRO	2.8
1	Q	44	GLU	2.8
1	A	172	ALA	2.8
1	Q	135	ARG	2.8
1	Q	187	ALA	2.8
1	b	505	VAL	2.8
1	w	490	ALA	2.8
1	y	342	VAL	2.8
2	v	524	ALA	2.8
1	Q	188	LEU	2.8
2	h	399	LEU	2.8
1	Y	226	THR	2.8
1	q	478	THR	2.8
1	M	157	GLY	2.8
1	Y	126	GLU	2.8
1	S	189	ARG	2.8
1	W	171	TYR	2.8
1	Y	180	ALA	2.8
1	q	486	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	y	425	ALA	2.8
2	C	100	ALA	2.8
2	R	100	ALA	2.8
1	y	534	LEU	2.8
1	W	133	THR	2.8
2	T	222	SER	2.8
1	q	431	GLY	2.8
1	Y	55	GLU	2.8
1	W	184	ALA	2.8
1	m	484	ALA	2.8
2	G	100	ALA	2.8
1	Q	40	LEU	2.8
1	Y	129	HIS	2.8
1	D	159	THR	2.8
1	M	159	THR	2.8
1	w	437	GLU	2.7
1	M	185	VAL	2.7
1	O	205	VAL	2.7
1	Q	205	VAL	2.7
1	W	206	ALA	2.7
2	t	400	ALA	2.7
1	y	467	LEU	2.7
2	4	399	LEU	2.7
1	o	419	GLU	2.7
1	o	505	VAL	2.7
1	K	111	PHE	2.7
1	Q	68	PHE	2.7
1	d	312	ALA	2.7
1	m	490	ALA	2.7
1	s	472	ALA	2.7
1	w	320	ALA	2.7
1	y	333	LEU	2.7
1	y	423	CYS	2.7
1	D	178	THR	2.7
1	y	479	ASP	2.7
2	j	522	SER	2.7
1	K	121	GLU	2.7
1	O	206	ALA	2.7
1	Q	183	ILE	2.7
1	f	334	ALA	2.7
2	R	93	ALA	2.7
2	V	216	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	g	399	LEU	2.7
2	4	400	ALA	2.7
1	Q	112	THR	2.7
1	D	149	ASP	2.7
1	S	179	ASP	2.7
1	f	449	ASP	2.7
1	W	176	SER	2.7
1	W	154	VAL	2.7
1	f	467	LEU	2.7
1	w	333	LEU	2.7
1	w	438	LEU	2.7
2	c	399	LEU	2.7
1	f	490	ALA	2.7
1	q	472	ALA	2.7
1	Q	118	TYR	2.7
1	K	179	ASP	2.7
1	y	358	ASP	2.7
1	Y	188	LEU	2.7
1	Y	229	ALA	2.6
1	y	522	PHE	2.6
1	q	313	MET	2.6
1	W	112	THR	2.6
1	D	214	ASP	2.6
1	M	28	LYS	2.6
1	Y	58	ASP	2.6
1	w	455	VAL	2.6
1	Y	172	ALA	2.6
1	A	14	ARG	2.6
1	f	443	TYR	2.6
1	w	439	TYR	2.6
1	y	435	ARG	2.6
1	d	336	ALA	2.6
1	y	448	ALA	2.6
1	l	17	SER	2.6
1	W	130	TYR	2.6
1	Y	218	PRO	2.6
1	w	436	PRO	2.6
1	y	431	GLY	2.6
1	w	331	VAL	2.6
1	3	526	THR	2.6
2	R	99	LEU	2.6
1	B	11	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	m	311	GLN	2.6
2	Z	64	GLU	2.6
1	w	466	ALA	2.6
1	I	14	ARG	2.6
1	K	182	ARG	2.6
1	f	321	ARG	2.6
1	M	181	LEU	2.6
1	y	513	LEU	2.6
1	d	505	VAL	2.6
1	M	18	GLU	2.6
1	D	65	ALA	2.6
1	M	25	ALA	2.6
1	O	172	ALA	2.6
1	l	12	ALA	2.6
1	q	475	ALA	2.6
1	y	515	ALA	2.6
2	Z	92	ALA	2.6
1	q	514	ASP	2.6
2	L	204	ASP	2.6
1	U	49	SER	2.5
1	W	228	SER	2.5
1	y	533	LEU	2.5
1	M	163	ILE	2.5
1	D	95	THR	2.5
1	Q	160	THR	2.5
1	W	159	THR	2.5
1	s	459	THR	2.5
1	y	311	GLN	2.5
1	D	164	ALA	2.5
1	l	175	ALA	2.5
1	u	472	ALA	2.5
1	K	214	ASP	2.5
1	Y	220	ARG	2.5
1	Q	207	SER	2.5
1	Y	176	SER	2.5
1	D	167	LEU	2.5
1	Q	19	LEU	2.5
1	Q	208	LEU	2.5
1	S	38	GLY	2.5
1	b	530	LEU	2.5
1	w	337	GLY	2.5
2	G	99	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	225	ILE	2.5
1	Q	225	ILE	2.5
1	y	339	VAL	2.5
1	U	169	GLU	2.5
1	Q	184	ALA	2.5
1	l	148	ALA	2.5
1	y	532	ALA	2.5
2	T	100	ALA	2.5
2	p	393	ALA	2.5
1	Q	28	LYS	2.5
1	d	468	LYS	2.5
1	D	176	SER	2.5
1	Q	29	SER	2.5
1	A	13	MET	2.5
1	l	205	VAL	2.5
1	W	111	PHE	2.5
1	W	153	PHE	2.5
1	q	344	GLU	2.5
1	D	27	ALA	2.5
1	Q	172	ALA	2.5
1	Q	206	ALA	2.5
1	Q	215	ALA	2.5
1	Q	16	ARG	2.5
1	W	50	LEU	2.5
1	w	319	LEU	2.5
1	y	340	LEU	2.5
1	y	477	LEU	2.5
1	u	476	SER	2.5
1	w	451	PRO	2.5
1	y	476	SER	2.5
1	Q	212	VAL	2.5
1	Y	35	TYR	2.5
1	Y	209	GLU	2.5
1	D	97	ARG	2.5
1	K	128	ALA	2.5
1	M	180	ALA	2.5
1	Q	36	ALA	2.5
1	Q	63	ALA	2.5
1	m	475	ALA	2.5
1	K	152	HIS	2.5
1	D	179	ASP	2.4
1	u	477	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	q	324	ILE	2.4
1	w	462	PRO	2.4
2	Z	131	ILE	2.4
1	M	131	GLY	2.4
1	W	227	GLY	2.4
2	J	222	SER	2.4
1	Q	224	ARG	2.4
1	y	519	ARG	2.4
1	l	166	ALA	2.4
1	l	171	TYR	2.4
1	k	526	THR	2.4
1	y	433	THR	2.4
1	Y	216	ASN	2.4
1	D	188	LEU	2.4
1	D	110	ILE	2.4
1	Q	210	VAL	2.4
1	Q	140	ARG	2.4
1	Y	135	ARG	2.4
1	D	222	PHE	2.4
1	W	137	GLU	2.4
1	w	318	GLU	2.4
1	w	419	GLU	2.4
1	M	206	ALA	2.4
1	w	484	ALA	2.4
1	y	480	ALA	2.4
1	Q	139	TYR	2.4
1	f	457	GLY	2.4
1	w	457	GLY	2.4
1	y	331	VAL	2.4
1	b	326	ARG	2.4
1	f	315	GLU	2.4
1	q	329	SER	2.4
1	w	310	GLU	2.4
1	Y	128	ALA	2.4
1	a	472	ALA	2.4
2	J	92	ALA	2.4
1	W	35	TYR	2.4
1	o	319	LEU	2.4
1	K	58	ASP	2.4
1	f	444	ASP	2.4
1	M	150	GLU	2.4
1	w	469	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	3	437	GLU	2.4
1	D	190	ALA	2.4
1	W	64	ALA	2.4
1	f	472	ALA	2.4
1	w	464	ALA	2.4
1	D	29	SER	2.4
1	w	414	GLN	2.4
2	t	522	SER	2.4
1	b	526	THR	2.4
1	q	335	TYR	2.4
1	K	177	LEU	2.4
1	Q	167	LEU	2.4
1	o	488	LEU	2.4
1	Y	42	VAL	2.3
1	w	322	LYS	2.3
1	y	314	ARG	2.3
1	y	489	ARG	2.3
1	Q	71	PHE	2.3
1	M	137	GLU	2.3
1	q	332	ALA	2.3
1	w	515	ALA	2.3
1	Y	138	LEU	2.3
1	m	333	LEU	2.3
1	y	439	TYR	2.3
1	y	452	HIS	2.3
1	M	16	ARG	2.3
1	Q	120	VAL	2.3
1	f	505	VAL	2.3
1	Q	69	ASN	2.3
1	Y	227	GLY	2.3
1	D	166	ALA	2.3
1	Y	148	ALA	2.3
1	d	472	ALA	2.3
1	Q	51	GLN	2.3
1	l	156	MET	2.3
1	w	311	GLN	2.3
1	Q	122	LEU	2.3
1	l	177	LEU	2.3
1	y	530	LEU	2.3
2	c	522	SER	2.3
2	p	522	SER	2.3
1	F	159	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	159	THR	2.3
1	O	226	THR	2.3
1	l	226	THR	2.3
1	u	459	THR	2.3
1	w	416	LYS	2.3
1	D	182	ARG	2.3
1	M	151	PRO	2.3
1	W	31	VAL	2.3
1	W	155	VAL	2.3
1	q	342	VAL	2.3
1	Q	66	GLY	2.3
1	s	338	GLY	2.3
1	D	184	ALA	2.3
1	K	150	GLU	2.3
1	O	229	ALA	2.3
1	Y	125	ALA	2.3
1	o	355	GLU	2.3
1	q	358	ASP	2.3
1	w	456	MET	2.3
1	u	488	LEU	2.3
1	K	17	SER	2.3
1	Q	47	SER	2.3
1	w	476	SER	2.3
1	y	349	SER	2.3
1	m	459	THR	2.3
1	s	462	PRO	2.3
1	Q	174	ASN	2.3
1	D	221	ALA	2.3
1	D	229	ALA	2.3
1	M	15	GLU	2.3
1	M	175	ALA	2.3
1	W	169	GLU	2.3
1	Y	175	ALA	2.3
1	q	334	ALA	2.3
2	e	434	GLU	2.3
1	f	333	LEU	2.3
1	o	477	LEU	2.3
1	y	481	LEU	2.3
2	R	38	ASP	2.3
1	D	207	SER	2.3
1	Q	151	PRO	2.3
1	y	427	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	158	GLY	2.3
1	w	411	PHE	2.2
1	K	206	ALA	2.2
1	M	125	ALA	2.2
1	S	229	ALA	2.2
1	o	473	GLU	2.2
2	R	219	GLU	2.2
1	S	188	LEU	2.2
1	S	234	LEU	2.2
1	y	517	ARG	2.2
2	v	509	ARG	2.2
1	D	170	SER	2.2
1	K	136	PRO	2.2
1	Q	89	TYR	2.2
1	m	337	GLY	2.2
1	Q	222	PHE	2.2
1	m	313	MET	2.2
1	F	110	ILE	2.2
1	f	471	TYR	2.2
1	S	131	GLY	2.2
1	f	313	MET	2.2
1	D	232	ALA	2.2
1	K	134	LYS	2.2
1	M	44	GLU	2.2
1	M	65	ALA	2.2
1	Q	148	ALA	2.2
1	Q	169	GLU	2.2
1	l	167	LEU	2.2
1	y	529	ALA	2.2
2	H	93	ALA	2.2
2	c	391	LEU	2.2
1	K	97	ARG	2.2
1	U	231	GLN	2.2
1	Y	219	ARG	2.2
1	d	444	ASP	2.2
1	y	514	ASP	2.2
1	D	127	VAL	2.2
1	Q	60	VAL	2.2
1	w	342	VAL	2.2
1	l	142	THR	2.2
1	W	170	SER	2.2
1	q	471	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	28	LYS	2.2
1	s	530	LEU	2.2
1	w	407	LEU	2.2
1	w	481	LEU	2.2
1	w	530	LEU	2.2
1	Q	32	ALA	2.2
1	S	172	ALA	2.2
1	W	36	ALA	2.2
1	Y	164	ALA	2.2
1	l	113	GLU	2.2
1	i	469	GLU	2.2
2	e	400	ALA	2.2
1	Q	21	ARG	2.2
1	l	147	ILE	2.2
1	y	523	ARG	2.2
1	B	205	VAL	2.2
1	3	505	VAL	2.2
2	E	38	ASP	2.2
1	U	226	THR	2.2
1	y	526	THR	2.2
1	I	134	LYS	2.2
1	i	527	GLY	2.2
1	w	328	LYS	2.2
1	d	471	TYR	2.2
1	i	530	LEU	2.2
1	y	470	SER	2.2
2	t	508	SER	2.2
1	D	20	ALA	2.2
1	M	121	GLU	2.2
1	Q	115	ALA	2.2
1	f	327	ALA	2.2
1	s	450	GLU	2.2
1	D	59	ARG	2.1
1	M	183	ILE	2.1
1	Y	225	ILE	2.1
1	u	454	VAL	2.1
1	K	28	LYS	2.1
1	d	526	THR	2.1
1	Q	234	LEU	2.1
1	W	208	LEU	2.1
1	w	340	LEU	2.1
1	M	190	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	186	ALA	2.1
1	w	487	ALA	2.1
1	w	421	GLU	2.1
1	D	141	ILE	2.1
1	W	231	GLN	2.1
1	q	474	ASN	2.1
1	k	328	LYS	2.1
1	d	479	ASP	2.1
1	y	449	ASP	2.1
1	D	133	THR	2.1
1	D	160	THR	2.1
1	W	38	GLY	2.1
1	a	527	GLY	2.1
1	y	361	GLY	2.1
1	y	453	PHE	2.1
1	K	135	ARG	2.1
1	M	143	TYR	2.1
1	b	515	ALA	2.1
1	i	314	ARG	2.1
1	o	435	ARG	2.1
1	q	482	ARG	2.1
1	w	471	TYR	2.1
2	r	393	ALA	2.1
1	K	209	GLU	2.1
1	Y	10	GLU	2.1
1	Y	183	ILE	2.1
1	b	450	GLU	2.1
1	y	437	GLU	2.1
2	E	222	SER	2.1
1	1	152	HIS	2.1
1	W	120	VAL	2.1
1	W	185	VAL	2.1
1	3	313	MET	2.1
1	1	162	PRO	2.1
1	y	451	PRO	2.1
1	D	145	GLY	2.1
1	O	188	LEU	2.1
1	U	38	GLY	2.1
1	f	488	LEU	2.1
1	o	533	LEU	2.1
1	w	527	GLY	2.1
2	v	523	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	178	THR	2.1
1	S	226	THR	2.1
2	x	500	ASP	2.1
1	K	140	ARG	2.1
1	Y	215	ALA	2.1
1	A	10	GLU	2.1
1	A	18	GLU	2.1
1	w	447	ILE	2.1
1	y	335	TYR	2.1
1	3	528	SER	2.1
2	C	222	SER	2.1
1	s	531	GLN	2.1
1	A	28	LYS	2.1
1	d	313	MET	2.1
1	I	205	VAL	2.1
1	u	331	VAL	2.1
1	u	505	VAL	2.1
1	K	151	PRO	2.1
1	y	356	LEU	2.1
1	F	111	PHE	2.1
1	O	153	PHE	2.1
1	S	157	GLY	2.1
1	s	337	GLY	2.1
1	w	366	GLY	2.1
1	M	97	ARG	2.1
1	O	133	THR	2.1
1	Y	149	ASP	2.1
2	X	38	ASP	2.1
1	K	20	ALA	2.1
1	Y	221	ALA	2.1
1	w	353	ILE	2.1
1	y	466	ALA	2.1
1	A	44	GLU	2.1
1	D	209	GLU	2.1
1	y	450	GLU	2.1
1	y	509	GLU	2.1
1	l	35	TYR	2.1
1	K	13	MET	2.0
1	s	476	SER	2.0
1	D	60	VAL	2.0
1	f	534	LEU	2.0
1	u	534	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	21	ARG	2.0
1	D	96	GLY	2.0
1	Q	157	GLY	2.0
1	i	338	GLY	2.0
1	Q	142	THR	2.0
1	b	412	THR	2.0
1	w	460	THR	2.0
1	O	12	ALA	2.0
1	Q	214	ASP	2.0
1	l	72	ASP	2.0
1	f	448	ALA	2.0
2	J	198	ASP	2.0
2	T	93	ALA	2.0
2	X	198	ASP	2.0
1	D	119	GLU	2.0
1	K	137	GLU	2.0
1	Q	161	GLU	2.0
1	l	169	GLU	2.0
1	o	315	GLU	2.0
1	D	130	TYR	2.0
1	D	42	VAL	2.0
1	M	146	SER	2.0
1	W	42	VAL	2.0
1	W	207	SER	2.0
1	o	452	HIS	2.0
1	w	349	SER	2.0
1	y	351	GLN	2.0
1	W	213	LEU	2.0
1	Y	97	ARG	2.0
1	w	369	ASN	2.0
1	y	520	ARG	2.0
1	W	157	GLY	2.0
1	l	38	GLY	2.0
1	b	431	GLY	2.0
1	o	457	GLY	2.0
1	Q	43	ALA	2.0
1	S	190	ALA	2.0
1	b	442	THR	2.0
1	q	532	ALA	2.0
1	O	44	GLU	2.0
1	Q	58	ASP	2.0
1	d	310	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	y	355	GLU	2.0
1	Y	13	MET	2.0
1	w	424	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OZT	R	1	9/10	0.91	0.11	18,44,69,87	0
2	OZT	c	301	9/10	0.91	0.13	39,63,87,89	0
2	OZT	E	1	9/10	0.92	0.11	37,49,92,109	0
2	OZT	l	301	9/10	0.93	0.12	24,38,76,81	0
2	OZT	e	301	9/10	0.94	0.10	26,57,76,88	0
2	OZT	r	301	9/10	0.94	0.09	23,32,68,69	0
2	OZT	t	301	9/10	0.94	0.10	28,37,51,63	0
2	OZT	z	301	9/10	0.94	0.08	26,36,64,66	0
2	OZT	J	1	9/10	0.95	0.08	22,28,50,52	0
2	OZT	L	1	9/10	0.95	0.10	30,51,75,78	0
2	OZT	x	301	9/10	0.95	0.07	26,34,49,61	0
2	OZT	C	1	9/10	0.95	0.09	26,53,60,67	0
2	OZT	4	301	9/10	0.95	0.09	11,23,37,60	0
2	OZT	V	1	9/10	0.96	0.08	18,39,47,73	0
2	OZT	v	301	9/10	0.96	0.09	26,50,58,58	0
2	OZT	g	301	9/10	0.96	0.09	21,28,60,70	0
2	OZT	X	1	9/10	0.96	0.08	5,31,53,62	0
2	OZT	T	1	9/10	0.96	0.07	15,22,49,54	0
2	OZT	Z	1	9/10	0.97	0.07	7,30,54,97	0
2	OZT	n	301	9/10	0.97	0.07	3,38,52,53	0
2	OZT	p	301	9/10	0.97	0.07	14,42,57,61	0
2	OZT	2	1	9/10	0.97	0.07	10,20,43,65	0
2	OZT	h	301	9/10	0.97	0.07	14,36,46,49	0
2	OZT	N	1	9/10	0.97	0.06	3,25,42,54	0
2	OZT	P	1	9/10	0.97	0.07	10,26,35,48	0
2	OZT	H	1	9/10	0.97	0.07	0,26,62,100	0
2	OZT	j	301	9/10	0.97	0.07	6,46,65,76	0
2	OZT	G	1	9/10	0.98	0.06	18,32,46,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.