



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 02:07 PM BST

PDB ID : 3HF9  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

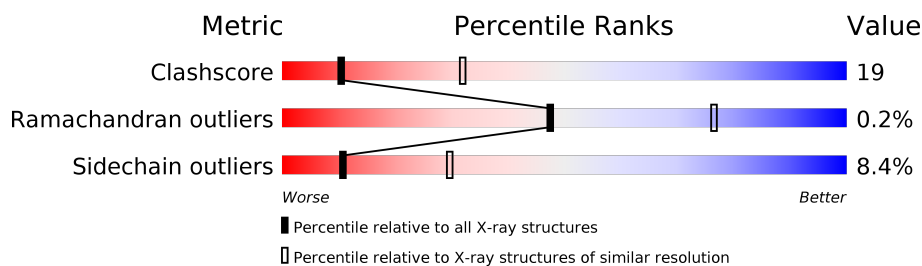
# 1 Overall quality at a glance

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))
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)















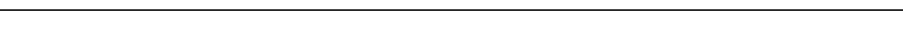




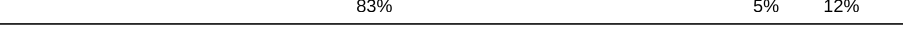





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	240	57% 30% • 12%
1	3	240	61% 24% • 13%
1	A	240	50% 34% • 12%
1	B	240	50% 33% 5% 12%
1	D	240	43% 41% • 13%
1	F	240	48% 27% 6% 20%
1	I	240	60% 25% • 12%
1	K	240	55% 30% • 12%
























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Mol	Chain	Length	Quality of chain
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	
2	C	240	
2	E	240	
2	G	240	

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Mol	Chain	Length	Quality of chain
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	
2	z	240	

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 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

*Continued on next page...*

*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

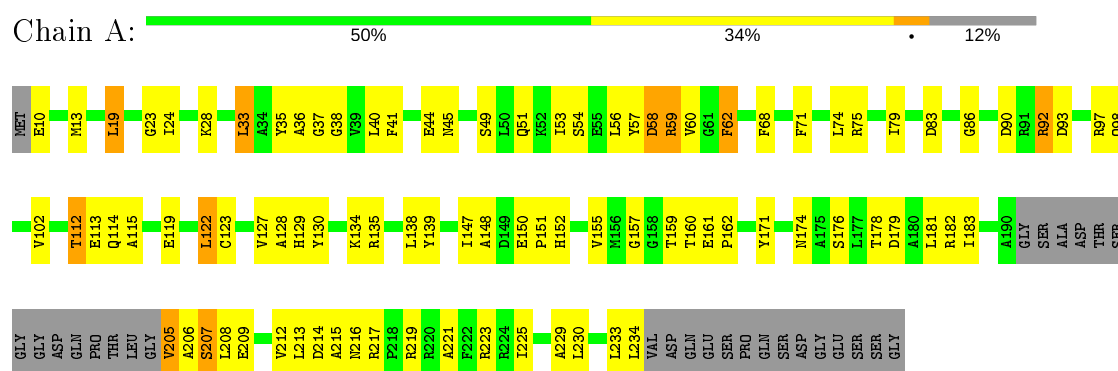


### 3 Residue-property plots [i](#)

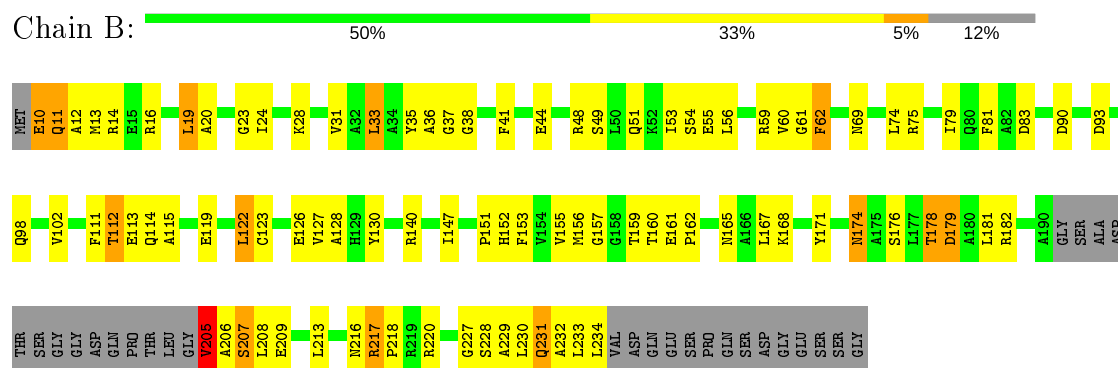
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

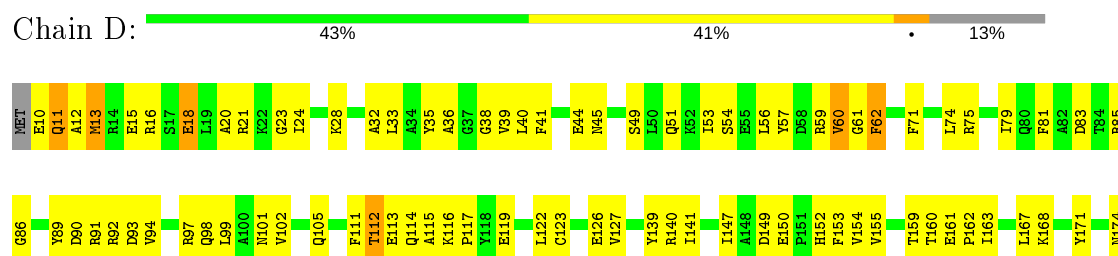
- Molecule 1: Proteasome (Alpha subunit) PrcA

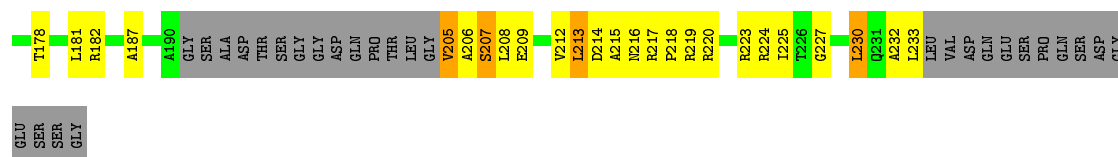


- Molecule 1: Proteasome (Alpha subunit) PrcA

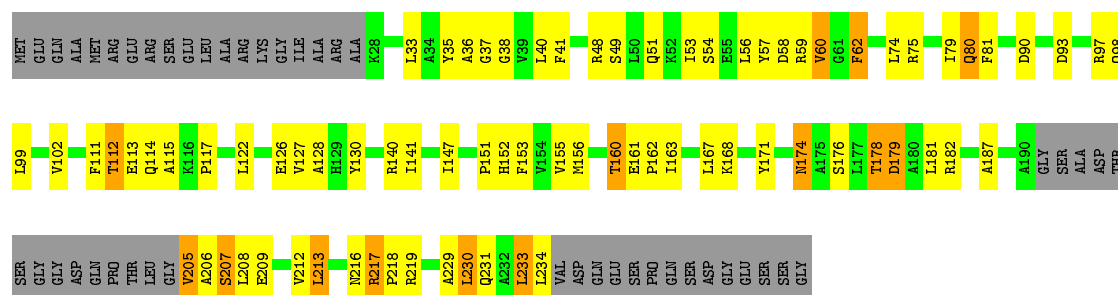


- Molecule 1: Proteasome (Alpha subunit) PrcA

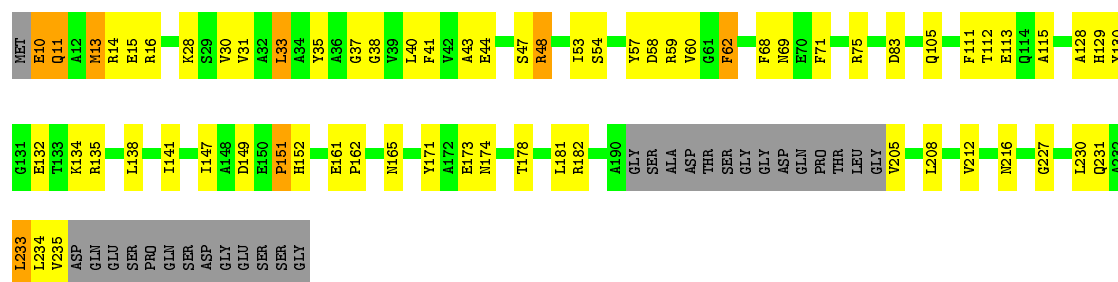




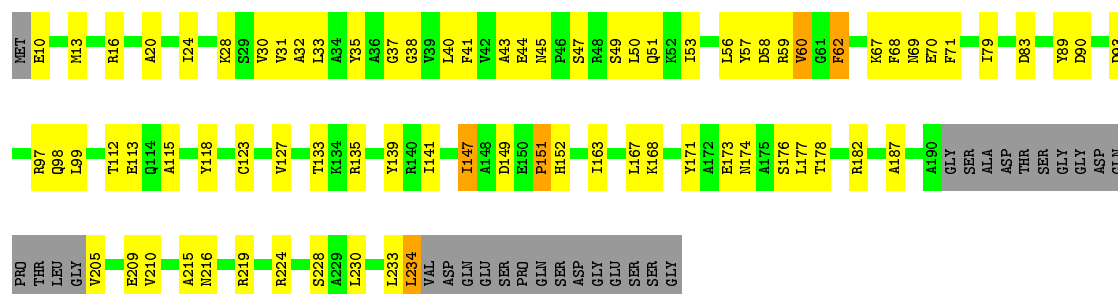
• Molecule 1: Proteasome (Alpha subunit) PrcA



• Molecule 1: Proteasome (Alpha subunit) PrcA

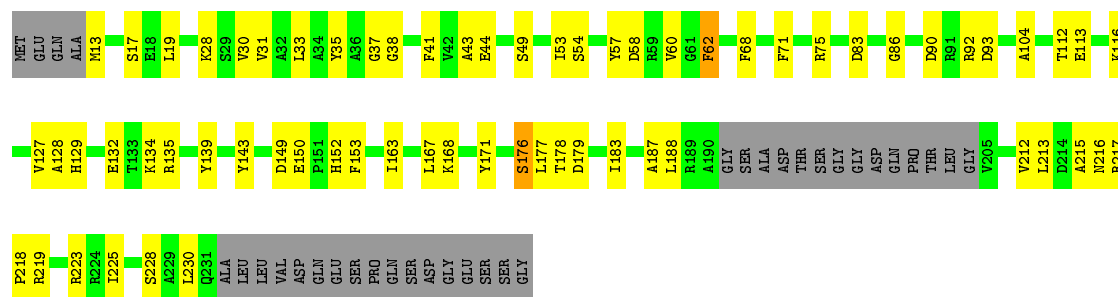


• Molecule 1: Proteasome (Alpha subunit) PrcA



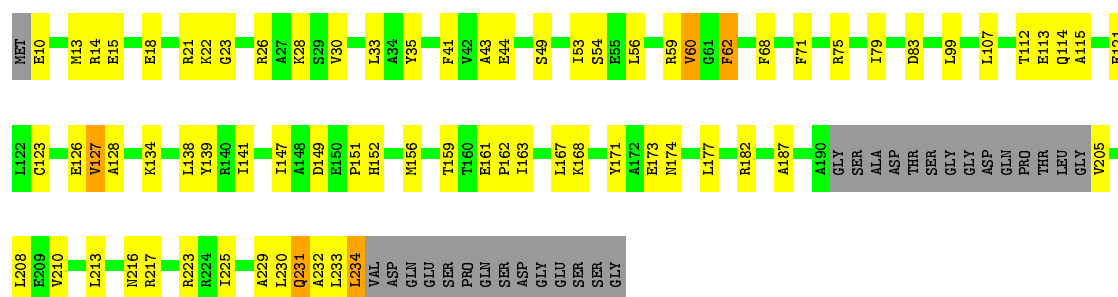
• Molecule 1: Proteasome (Alpha subunit) PrcA





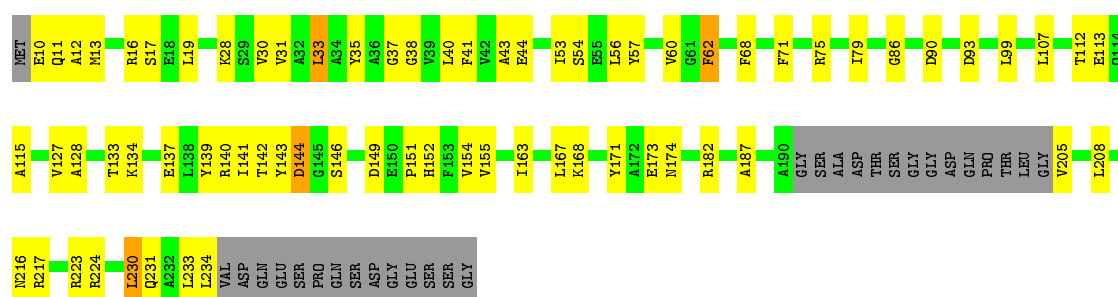
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain O: 57% 29% 12%



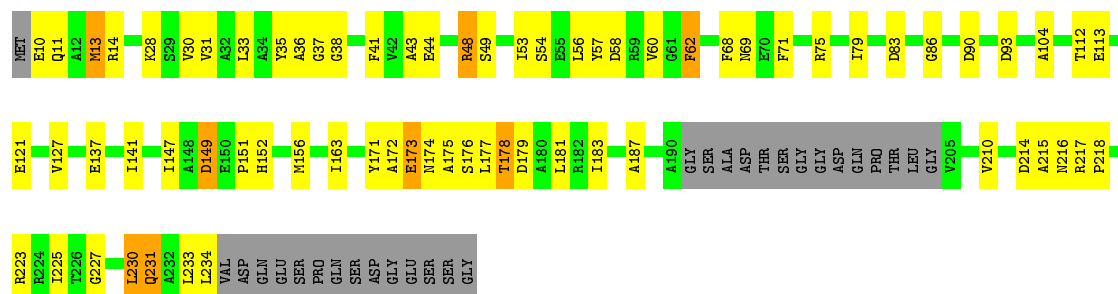
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain Q: 58% 28% 12%

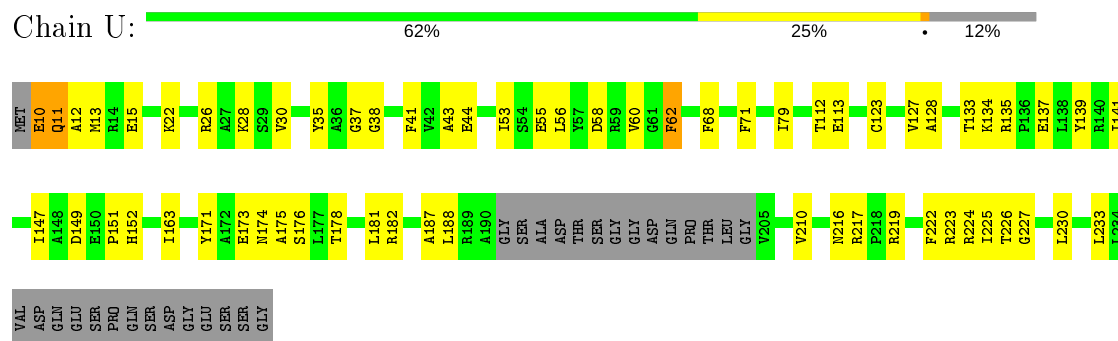


• Molecule 1: Proteasome (Alpha subunit) PrcA

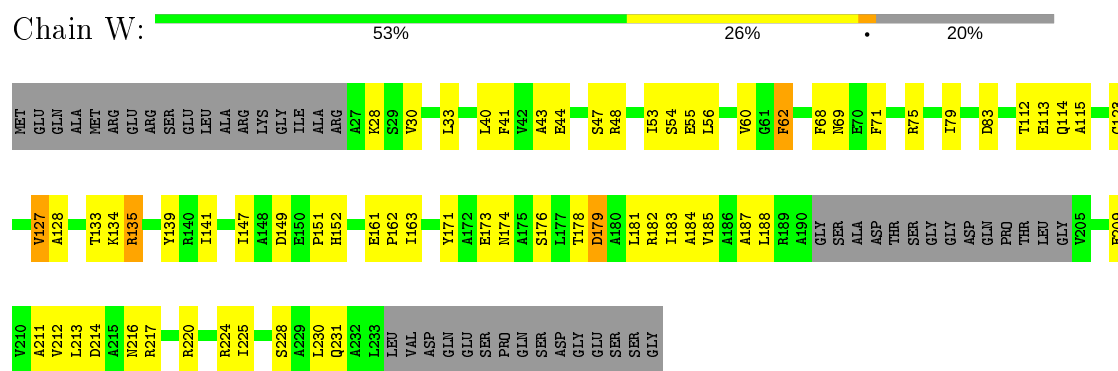
Chain S: 58% 26% 12%



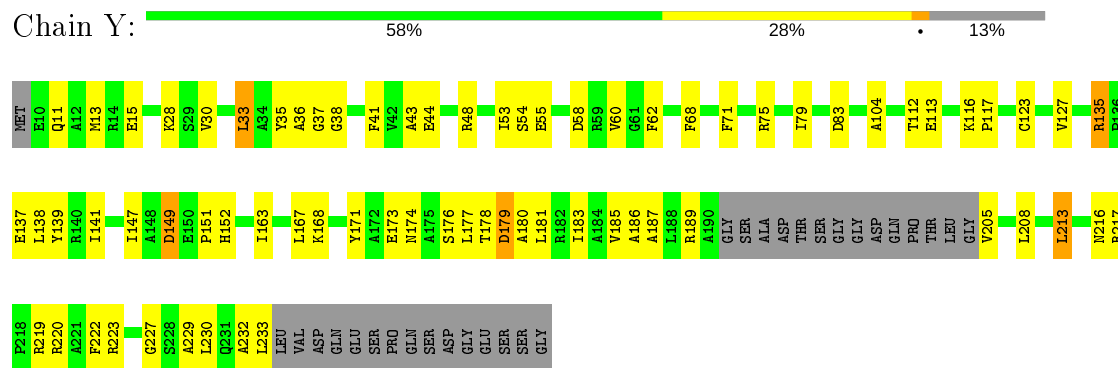
- Molecule 1: Proteasome (Alpha subunit) PrcA



- Molecule 1: Proteasome (Alpha subunit) PrcA

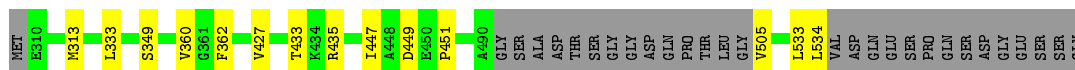
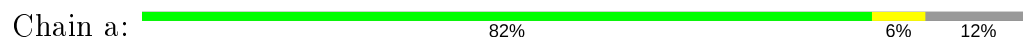


- Molecule 1: Proteasome (Alpha subunit) PrcA

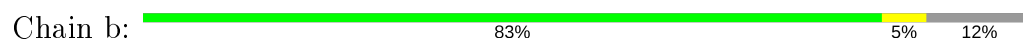




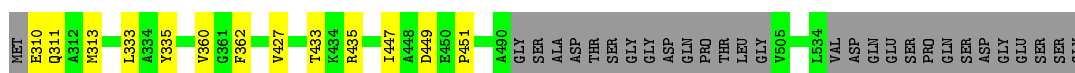
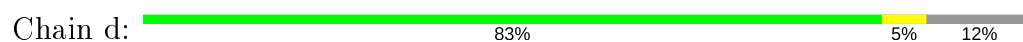
- Molecule 1: Proteasome (Alpha subunit) PrcA



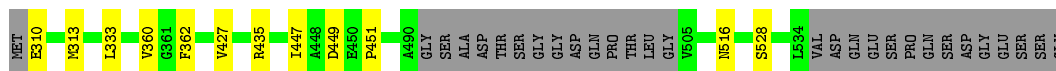
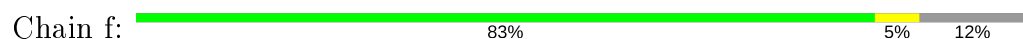
- Molecule 1: Proteasome (Alpha subunit) PrcA



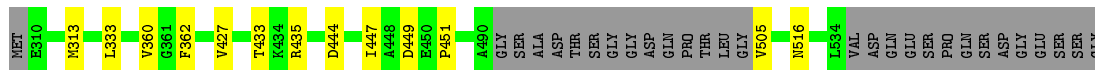
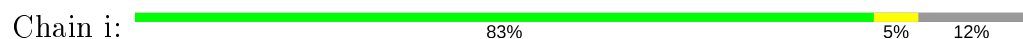
- Molecule 1: Proteasome (Alpha subunit) PrcA



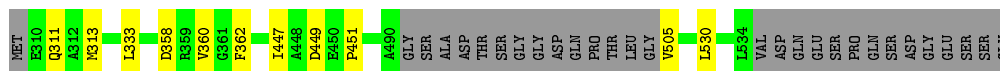
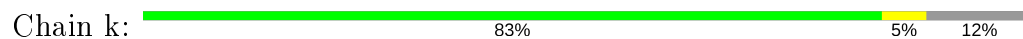
- Molecule 1: Proteasome (Alpha subunit) PrcA



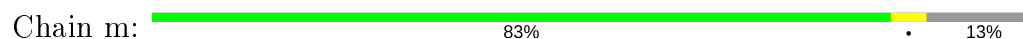
- Molecule 1: Proteasome (Alpha subunit) PrcA

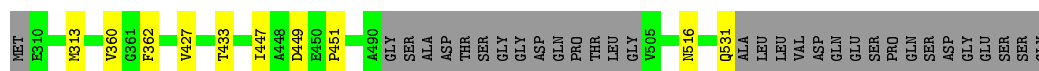


- Molecule 1: Proteasome (Alpha subunit) PrcA

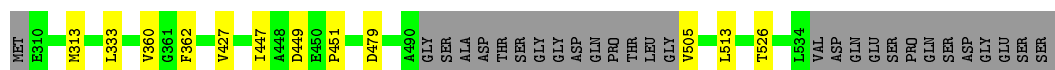
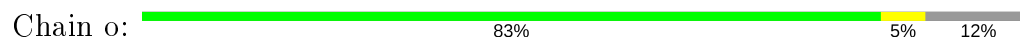


- Molecule 1: Proteasome (Alpha subunit) PrcA

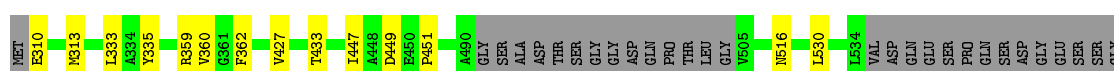
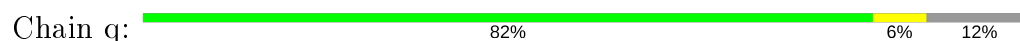




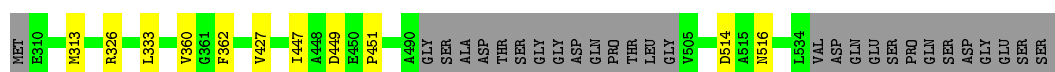
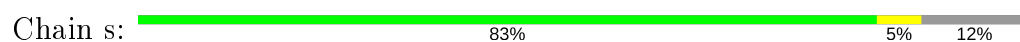
- Molecule 1: Proteasome (Alpha subunit) PrcA



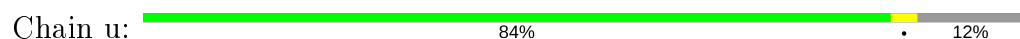
- Molecule 1: Proteasome (Alpha subunit) PrcA



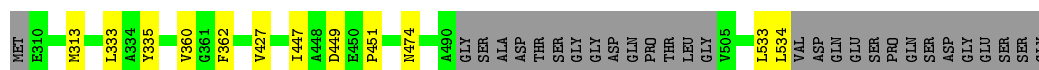
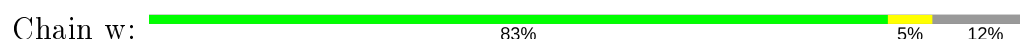
- Molecule 1: Proteasome (Alpha subunit) PrcA



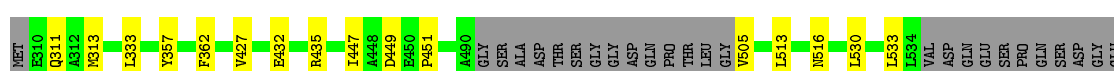
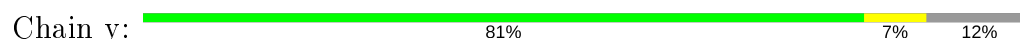
- Molecule 1: Proteasome (Alpha subunit) PrcA



- Molecule 1: Proteasome (Alpha subunit) PrcA

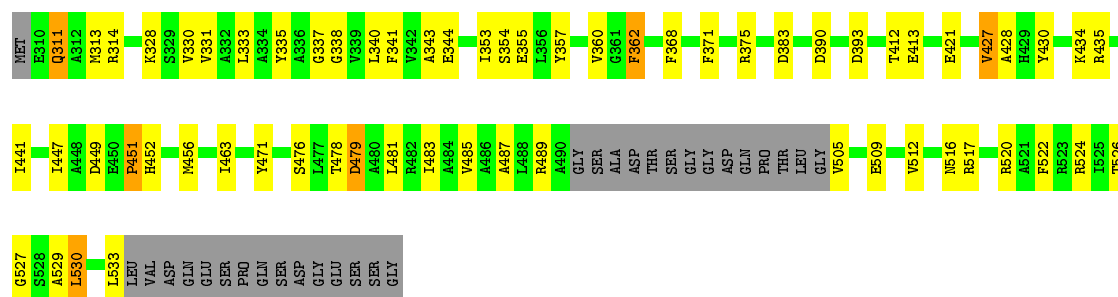


- Molecule 1: Proteasome (Alpha subunit) PrcA



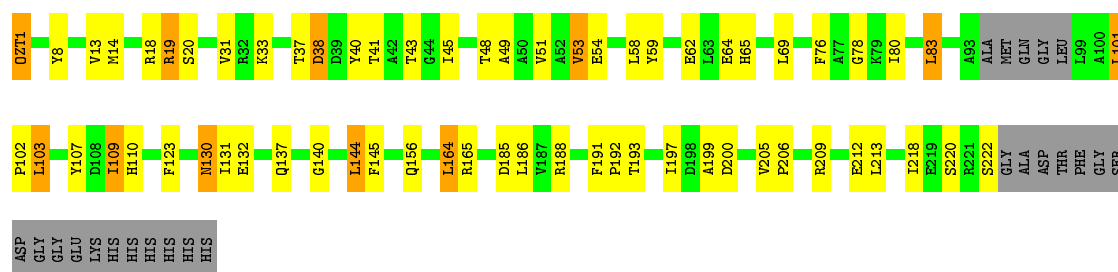
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain 3: 



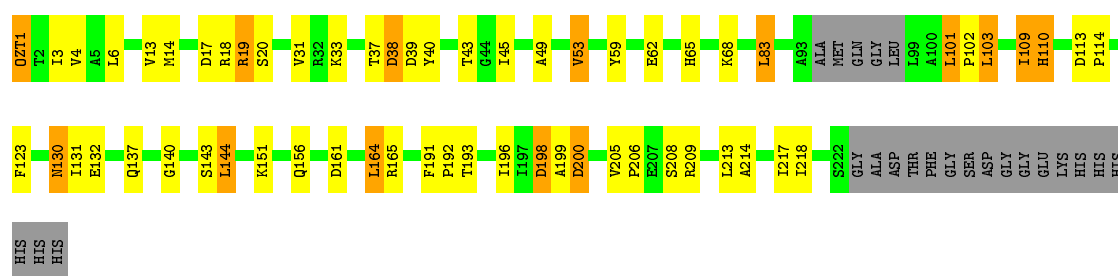
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain H: 



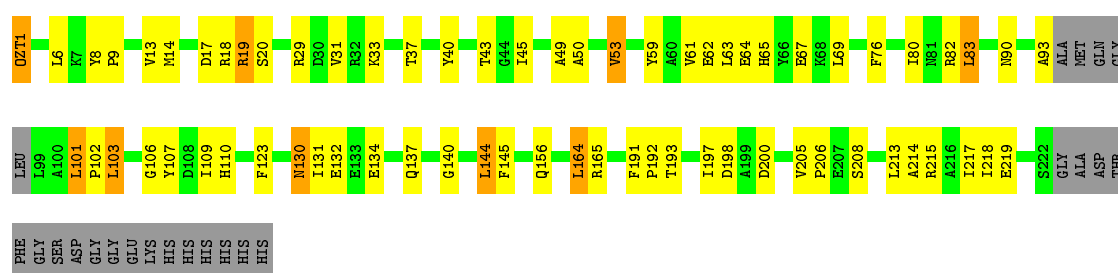
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain C: 



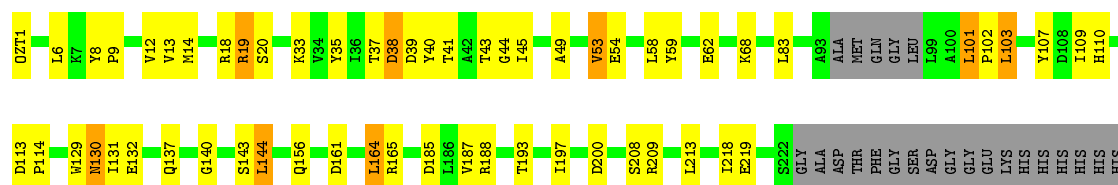
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain E: 



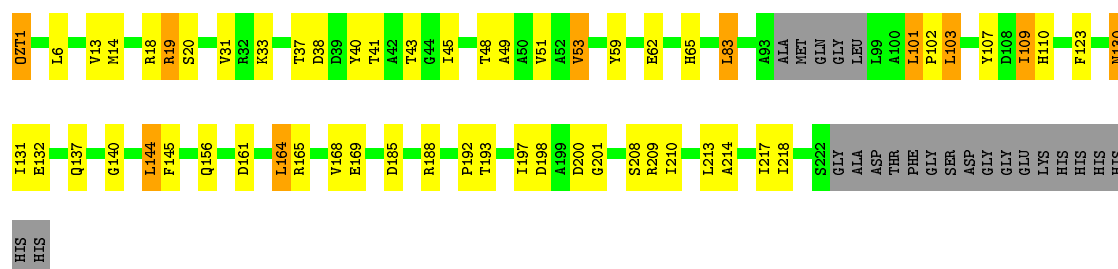
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain G:  66% 21% • 10%



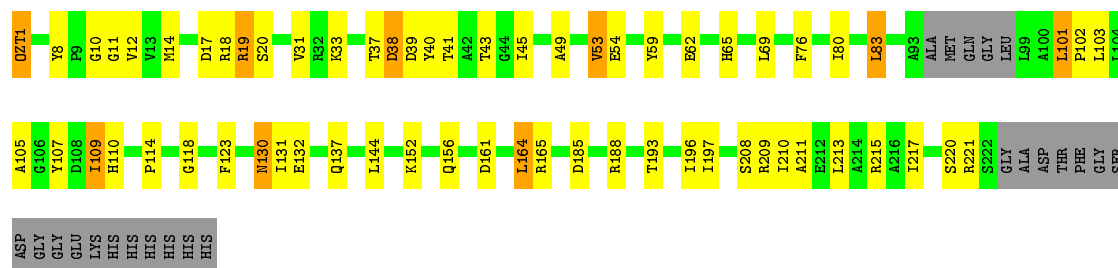
- Molecule 2: Proteasome (Beta subunit) PrCB

Chain J:  66% 20% 10%



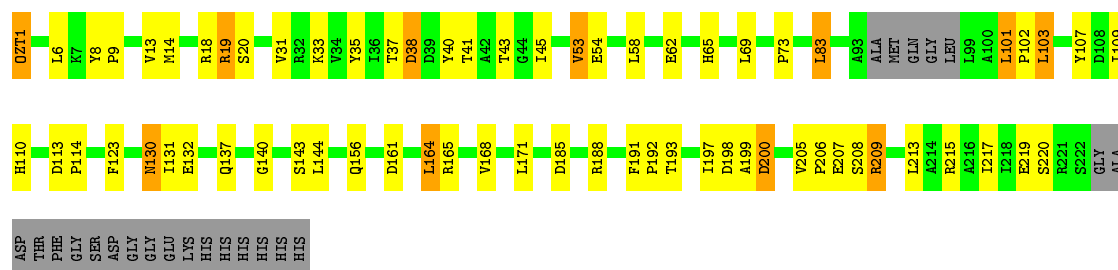
- Molecule 2: Proteasome (Beta subunit) PrCB

Chain L:  64% 23% • 10%



- Molecule 2: Proteasome (Beta subunit) PrCB

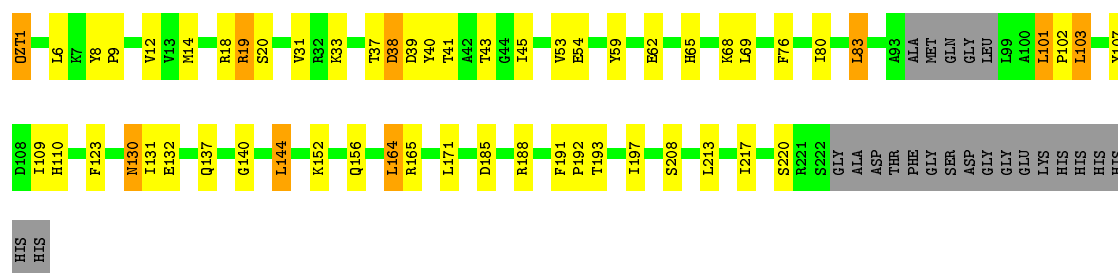
Chain N:  63% 23% 5% 10%



- Molecule 2: Proteasome (Beta subunit) PrcB

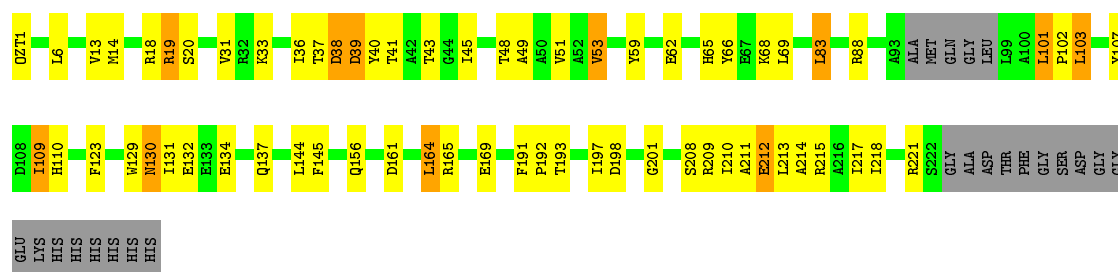
Chain P:  67% 20% 10%





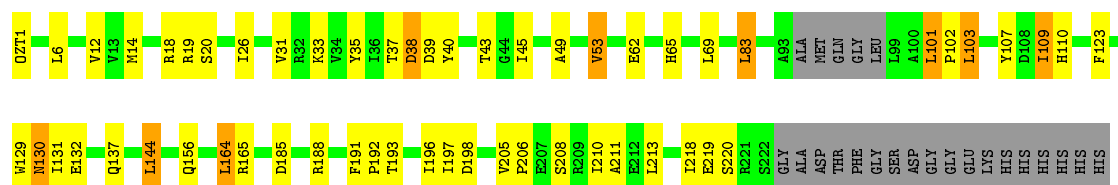
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain R: 63% 23% 5% 10%



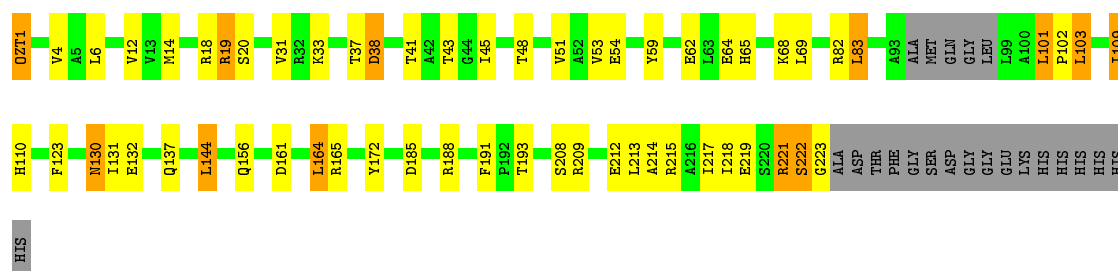
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain T: 67% 20% 10% 3%



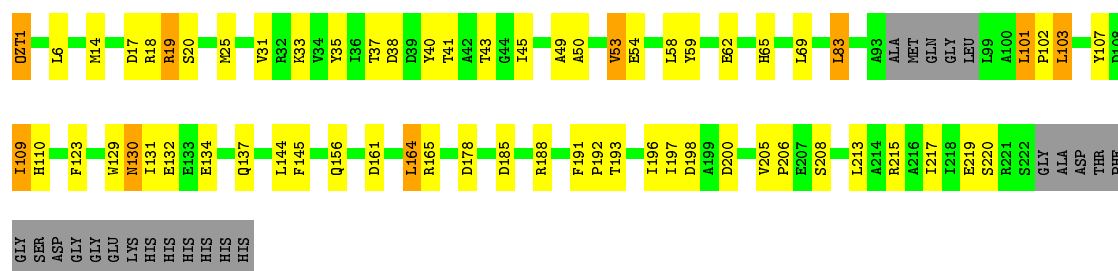
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain V: 66% 20% 5% 9%

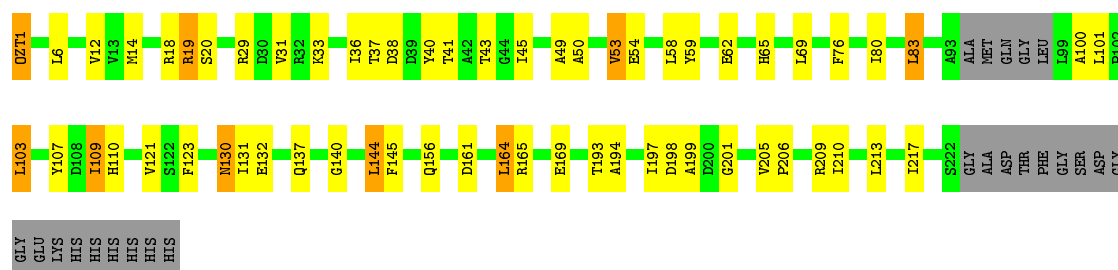


• Molecule 2: Proteasome (Beta subunit) PrcB

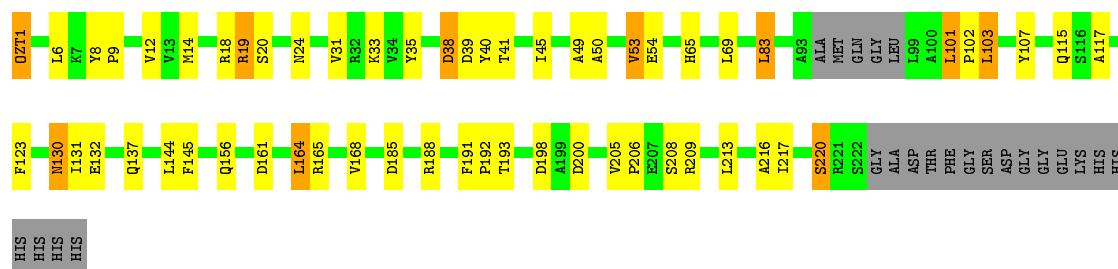
Chain X: 64% 23% 10% 3%



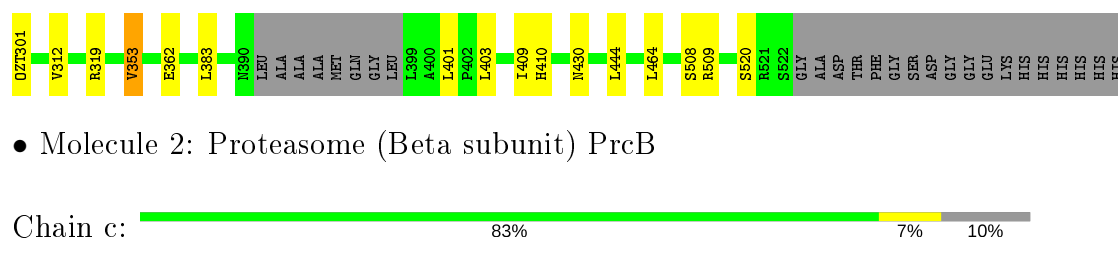
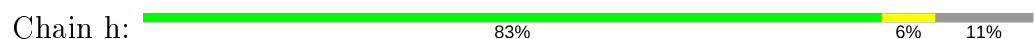
• Molecule 2: Proteasome (Beta subunit) PrcB



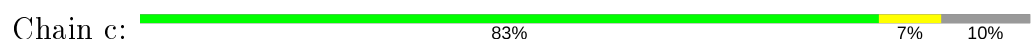
• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB




• Molecule 2: Proteasome (Beta subunit) PrcB




HIS  
HIS

## • Molecule 2: Proteasome (Beta subunit) PrcB

Chain e:  84% 6% 10%


O2T301	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	L464	D500	S508	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	SER	ASP	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## • Molecule 2: Proteasome (Beta subunit) PrcB

Chain g:  84% 6% 10%

O2T301	V304	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	P402	L403	I409	H410	N430	L444	L464	S508	R509	S522	GLY	ALA	ASP	THR	PHE	GLY	SER	ASP	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----


## • Molecule 2: Proteasome (Beta subunit) PrcB

Chain j:  83% 8% 10%

O2T301	V304	V312	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	D461	L464	I496	B517	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----


HIS  
HIS

## • Molecule 2: Proteasome (Beta subunit) PrcB

Chain l:  84% 7% 10%


O2T301	R319	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	L464	I496	S508	E512	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## • Molecule 2: Proteasome (Beta subunit) PrcB

Chain n:  83% 7% 10%

O2T301	V312	R319	D339	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	N430	L444	D461	L464	I496	S508	S520	R521	S522	GLY	ALA	ASP	THR	PHE	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

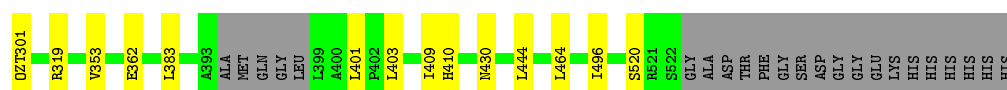
## • Molecule 2: Proteasome (Beta subunit) PrcB

Chain p:  85% 6% 10%

O2T301	V353	E362	L383	A393	ALA	MET	GLN	GLY	LEU	L399	A400	L401	P402	L403	I409	H410	N430	L444	L464	I496	D500	S508	S522	GLY	ALA	ASP	THR	PHE	GLY	SER	ASP	GLY	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS
--------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

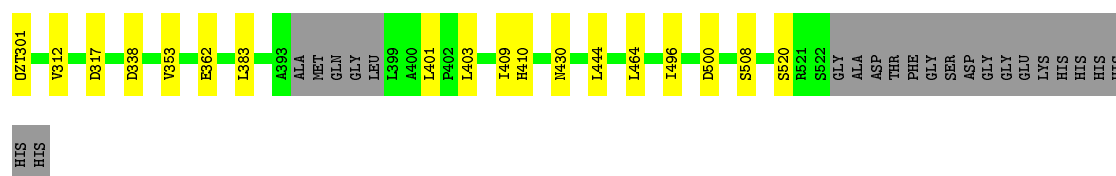
- Molecule 2: Proteasome (Beta subunit) PrCB

Chain r:  85% 6% 10%

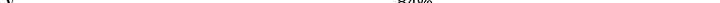


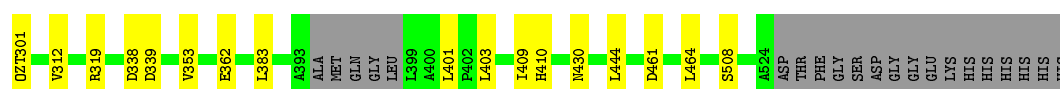
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain t:  83% 8% 10%

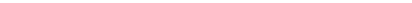


- Molecule 2: Proteasome (Beta subunit) PrCB

Chain v:  84% 7% 9%

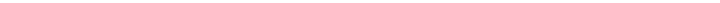


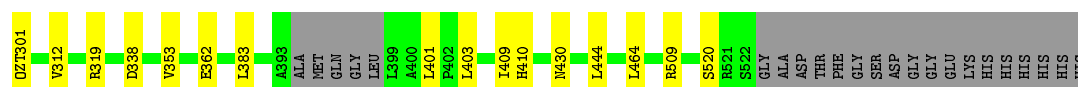
- Molecule 2: Proteasome (Beta subunit) PrCB

Chain x:  83% 7% 10%



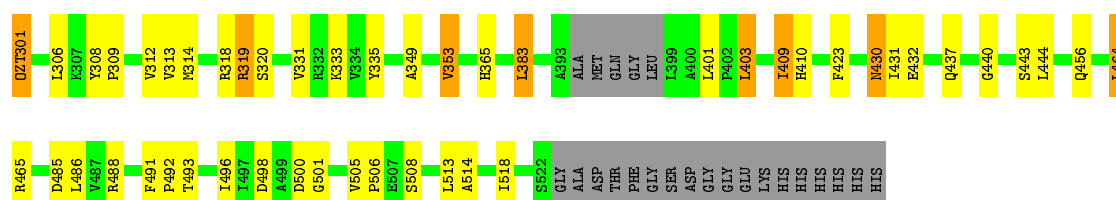
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain z:  84% 7% 10%



- Molecule 2: Proteasome (Beta subunit) PrCB

Chain 4:  70% 17% 10%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.58Å 209.62Å 284.93Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	25.12 – 2.88	Depositor
% Data completeness (in resolution range)	88.6 (25.12-2.88)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, $R_{free}$	0.217 , 0.267	Depositor
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.140	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Total number of atoms	90443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.50	0/1657	0.63	0/2238
1	3	0.52	0/1649	0.64	0/2227
1	A	0.55	0/1657	0.71	2/2238 (0.1%)
1	B	0.62	2/1657 (0.1%)	0.72	1/2238 (0.0%)
1	D	0.44	0/1649	0.63	0/2227
1	F	0.57	0/1514	0.71	0/2050
1	I	0.50	0/1664	0.65	0/2248
1	K	0.49	0/1657	0.68	0/2238
1	M	0.48	0/1613	0.65	0/2178
1	O	0.53	0/1657	0.67	1/2238 (0.0%)
1	Q	0.43	0/1657	0.62	0/2238
1	S	0.50	0/1657	0.65	0/2238
1	U	0.49	0/1657	0.62	0/2238
1	W	0.43	0/1511	0.60	0/2046
1	Y	0.48	0/1649	0.65	1/2227 (0.0%)
1	a	0.52	0/1657	0.65	0/2238
1	b	0.56	0/1657	0.67	0/2238
1	d	0.44	0/1657	0.61	0/2238
1	f	0.48	0/1657	0.60	0/2238
1	i	0.53	0/1657	0.64	0/2238
1	k	0.48	0/1657	0.64	0/2238
1	m	0.47	0/1636	0.62	0/2209
1	o	0.48	0/1657	0.62	0/2238
1	q	0.45	0/1657	0.61	0/2238
1	s	0.51	0/1657	0.65	1/2238 (0.0%)
1	u	0.48	0/1657	0.63	1/2238 (0.0%)
1	w	0.45	0/1657	0.60	0/2238
1	y	0.45	0/1657	0.62	0/2238
2	2	0.63	0/1620	0.70	0/2196
2	4	0.62	0/1620	0.69	0/2196
2	C	0.56	0/1620	0.68	0/2196
2	E	0.53	0/1620	0.66	0/2196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	G	0.64	0/1620	0.69	0/2196
2	H	0.62	0/1620	0.69	0/2196
2	J	0.55	0/1620	0.65	0/2196
2	L	0.63	0/1620	0.69	0/2196
2	N	0.70	0/1620	0.74	0/2196
2	P	0.73	0/1620	0.74	0/2196
2	R	0.52	0/1620	0.65	0/2196
2	T	0.61	0/1620	0.70	0/2196
2	V	0.69	0/1624	0.70	0/2201
2	X	0.65	0/1620	0.71	0/2196
2	Z	0.55	0/1620	0.67	0/2196
2	c	0.58	0/1610	0.68	0/2182
2	e	0.59	0/1620	0.70	0/2196
2	g	0.64	0/1620	0.69	0/2196
2	h	0.65	0/1602	0.71	1/2171 (0.0%)
2	j	0.57	0/1620	0.67	0/2196
2	l	0.63	0/1620	0.71	0/2196
2	n	0.67	0/1620	0.72	0/2196
2	p	0.71	0/1620	0.72	0/2196
2	r	0.56	0/1620	0.67	0/2196
2	t	0.58	0/1620	0.66	0/2196
2	v	0.67	0/1629	0.71	0/2208
2	x	0.60	0/1620	0.68	0/2196
2	z	0.52	0/1620	0.65	0/2196
All	All	0.56	2/91370 (0.0%)	0.67	8/123638 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	CYS	CB-SG	-5.97	1.72	1.81
1	B	205	VAL	CB-CG1	5.49	1.64	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	92	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	h	353	VAL	CB-CA-C	-5.33	101.28	111.40
1	O	213	LEU	N-CA-C	-5.20	96.95	111.00
1	u	513	LEU	N-CA-C	-5.20	96.96	111.00
1	Y	213	LEU	N-CA-C	-5.17	97.04	111.00
1	B	11	GLN	N-CA-C	-5.09	97.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	s	326	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	66	0
1	3	1625	0	1622	57	0
1	A	1633	0	1633	101	0
1	B	1633	0	1633	86	0
1	D	1625	0	1622	145	0
1	F	1490	0	1483	76	0
1	I	1640	0	1642	90	0
1	K	1633	0	1633	70	0
1	M	1589	0	1587	75	0
1	O	1633	0	1633	54	0
1	Q	1633	0	1633	85	0
1	S	1633	0	1633	98	0
1	U	1633	0	1633	54	0
1	W	1487	0	1477	64	0
1	Y	1625	0	1622	91	0
1	a	1633	0	1633	0	0
1	b	1633	0	1633	0	0
1	d	1633	0	1633	0	0
1	f	1633	0	1633	0	0
1	i	1633	0	1633	0	0
1	k	1633	0	1633	0	0
1	m	1612	0	1606	0	0
1	o	1633	0	1633	0	0
1	q	1633	0	1633	0	0
1	s	1633	0	1633	0	0
1	u	1633	0	1633	0	0
1	w	1633	0	1633	0	0
1	y	1633	0	1633	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1606	0	1593	46	0
2	4	1606	0	1593	35	0
2	C	1606	0	1593	46	0
2	E	1606	0	1593	69	0
2	G	1606	0	1593	46	0
2	H	1606	0	1593	58	0
2	J	1606	0	1593	49	0
2	L	1606	0	1593	55	0
2	N	1606	0	1593	44	0
2	P	1606	0	1593	40	0
2	R	1606	0	1593	69	0
2	T	1606	0	1593	43	0
2	V	1610	0	1596	64	0
2	X	1606	0	1593	57	0
2	Z	1606	0	1593	56	0
2	c	1596	0	1583	0	0
2	e	1606	0	1593	0	0
2	g	1606	0	1593	0	0
2	h	1588	0	1572	0	0
2	j	1606	0	1593	0	0
2	l	1606	0	1593	0	0
2	n	1606	0	1593	0	0
2	p	1606	0	1593	0	0
2	r	1606	0	1593	0	0
2	t	1606	0	1593	0	0
2	v	1615	0	1601	0	0
2	x	1606	0	1593	0	0
2	z	1606	0	1593	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0	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	0	0
3	f	1	0	0	0	0
3	g	3	0	0	0	0
3	h	3	0	0	0	0
3	i	1	0	0	0	0
3	j	3	0	0	0	0
3	k	2	0	0	0	0
3	l	3	0	0	0	0
3	n	2	0	0	0	0
3	o	1	0	0	0	0
3	p	2	0	0	0	0
3	q	1	0	0	0	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	0	0
3	v	4	0	0	0	0
3	w	4	0	0	0	0
3	x	1	0	0	0	0
3	y	2	0	0	0	0
3	z	4	0	0	0	0
All	All	90443	0	89905	1864	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 (1864) 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:35:TYR:CE2	1:D:40:LEU:HB2	1.65	1.32
1:M:35:TYR:CE1	1:M:37:GLY:HA3	1.68	1.26
1:S:230:LEU:C	1:S:230:LEU:HD23	1.51	1.21
1:B:19:LEU:HD23	1:B:19:LEU:C	1.61	1.18
1:1:229:ALA:O	1:1:233:LEU:HD13	1.41	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
1:S:35:TYR:CE1	1:S:37:GLY:HA3	1.83	1.14
1:K:178:THR:HB	1:K:233:LEU:HD22	1.24	1.13
1:I:11:GLN:HG2	1:I:14:ARG:NH2	1.63	1.12
1:D:13:MET:HE3	1:D:13:MET:N	1.65	1.11
1:1:231:GLN:HA	1:1:234:LEU:CD1	1.78	1.11
1:S:231:GLN:HE21	1:S:234:LEU:HD12	1.13	1.08
1:B:19:LEU:O	1:B:19:LEU:HD23	1.51	1.08
2:G:187:VAL:HA	2:V:222:SER:HB3	1.13	1.08
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.35	1.08
1:D:10:GLU:OE2	1:Q:19:LEU:HB2	1.51	1.08
1:S:227:GLY:CA	1:S:230:LEU:HB3	1.84	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
1:3:335:TYR:CE1	1:3:337:GLY:HA3	1.89	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:Q:35:TYR:CE1	1:Q:38:GLY:N	2.25	1.04
1:D:90:ASP:OD1	1:D:93:ASP:HB2	1.59	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: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
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
2:E:165:ARG:CG	2:E:213:LEU:HD22	1.90	0.99
1:U:112:THR:HG23	1:1:115:ALA:HB3	1.40	0.99
1:D:35:TYR:HE2	1:D:40:LEU:CB	1.74	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH1	1:A:223:ARG:HB2	1.75	0.99
1:B:19:LEU:CD2	1:B:19:LEU:C	2.30	0.99
2:E:144:LEU:HB2	3:E:242:HOH:O	1.61	0.98
2:G:187:VAL:CA	2:V:222:SER:HB3	1.93	0.98
1:W:115:ALA:HB3	1:Y:112:THR:HG23	1.45	0.98
1:M:152:HIS:HB3	1:M:171:TYR:CE2	1.99	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:I:231:GLN:CA	1:I: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:I:231:GLN:HA	1:I: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
1:3:335:TYR:CE1	1:3:337:GLY:CA	2.48	0.95
1:S:230:LEU:HD23	1:S:230:LEU:O	1.67	0.95
1:M:35:TYR:HE1	1:M:37:GLY:HA3	1.09	0.94
1:S:230:LEU:C	1:S:230:LEU:CD2	2.30	0.94
1:S:35:TYR:CE1	1:S:37:GLY:N	2.36	0.94
1:S:225:ILE:HG22	1:S:230:LEU:HB2	1.47	0.94
2:R:37:THR:HG21	2:R:59:TYR:HD2	1.28	0.94
1:A:217:ARG:HH11	1:A:223:ARG:HB2	1.26	0.93
1:D:13:MET:CE	1:D:13:MET:N	2.30	0.93
1:S:35:TYR:CD1	1:S:37:GLY:N	2.37	0.93
1:A:135:ARG:CB	1:A:135:ARG:HH11	1.82	0.93
1:I:11:GLN:CD	1:I:14:ARG:HH21	1.72	0.93
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: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
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: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:A:97:ARG:O	1:A:97:ARG:HD2	1.71	0.90
1:O:210:VAL:HB	1:O:230:LEU:HD21	1.52	0.90
1:D:112:THR:HG23	1:Q:115:ALA:HB3	1.53	0.90
1:D:20:ALA:O	1:D:24:ILE:HG13	1.71	0.90
1:K:51:GLN:HB3	1:K:209:GLU:OE1	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:115:ALA:HB3	1:K:112:THR:HG23	1.51	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: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
2:T:37:THR:CG2	2:T:43:THR:HG23	2.03	0.89
1:D:219:ARG:NH2	1:D:220:ARG:HD3	1.87	0.89
1:D:12:ALA:C	1:D:13:MET:HE3	1.91	0.89
1:U:112:THR:HG22	1:U:113:GLU:HG3	1.54	0.89
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:I:230:LEU:O	1:I:234:LEU:HG	1.73	0.88
1:S:69:ASN:HB2	1:1:105:GLN:HG2	1.55	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: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: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: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: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
2:N:198:ASP:OD1	2:N:200:ASP:HB2	1.74	0.86
1:S:230:LEU:HD23	1:S:231:GLN:N	1.90	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
2:Z:40:TYR:CD1	2:Z:109:ILE:HD13	2.12	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:K:35:TYR:CD2	1:K:38:GLY:O	2.30	0.85
2:V:209:ARG:O	2:V:212:GLU:HG2	1.75	0.85
2:4:301:OZT:H17	2:4:333:LYS:NZ	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:112:THR:HG22	1:S:113:GLU:HG3	1.55	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
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
2:G:187:VAL:HA	2:V:222:SER:CB	2.05	0.84
1:I:231:GLN:O	1:I:235:VAL:HG22	1.77	0.84
1:W:112:THR:HG22	1:W:113:GLU:HG3	1.57	0.84
1:3:311:GLN:O	1:3:311:GLN:HG2	1.75	0.84
1:D:35:TYR:CE2	1:D:38:GLY:O	2.30	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:Q:35:TYR:CE1	1:Q:37:GLY:CA	2.61	0.84
1:Q:35:TYR:HE1	1:Q:37:GLY:HA3	1.41	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: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
2:V:172:TYR:CE1	2:V:218:ILE:CD1	2.62	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:12:ALA:HB3	1:D:13:MET:HE3	1.61	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:HB2	1:A:135:ARG:HH11	1.45	0.82
1:D:181:LEU:CD2	1:D:233:LEU:HD22	2.10	0.82
1:U:11:GLN:HA	1:U:11:GLN:HE21	1.44	0.82
2:V:212:GLU:HG3	2:V:213:LEU:N	1.95	0.82
2:H:107:TYR:HB2	2:H:197:ILE:HG22	1.62	0.82
1:Q:35:TYR:CE1	1:Q:37:GLY:HA3	2.15	0.82
2:J:37:THR:HG21	2:J:43:THR:HG23	1.62	0.81
1:B:98:GLN:O	1:B:102:VAL:HG23	1.81	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
1:A:36:ALA:HA	1:A:174:ASN:HD22	1.45	0.81
1:A:135:ARG:NH1	1:A:135:ARG:CB	2.43	0.81
1:Q:35:TYR:HE1	1:Q:37:GLY:CA	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:41:PHE:HB3	1:B:53:ILE:HD13	1.63	0.80
1:K:182:ARG:HG2	3:K:250:HOH:O	1.81	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
2:J:37:THR:CG2	2:J:43:THR:HG23	2.11	0.79
1:M:176:SER:CB	1:M:179:ASP:OD1	2.30	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
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:D:12:ALA:CB	1:D:13:MET:HE3	2.13	0.79
2:2:1:OZT:H17	2:2:33:LYS:NZ	1.98	0.78
2:4:301:OZT:H17	2:4:333:LYS:HZ3	1.46	0.78
2:E:214:ALA:O	2:E:218:ILE:HG13	1.82	0.78
1:3:335:TYR:CD1	1:3:337:GLY:N	2.52	0.78
1:I:11:GLN:HG2	1:I:14:ARG:HH22	1.44	0.78
1:I:31:VAL:HG12	1:I:33:LEU:CD2	2.14	0.78
2:E:215:ARG:O	2:E:219:GLU:HG3	1.82	0.78
2:H:165:ARG:HG3	2:H:213:LEU:HD22	1.64	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
1:3:517:ARG:HD3	1:3:520:ARG:O	1.83	0.78
1:K:35:TYR:CE1	1:K:37:GLY:CA	2.67	0.78
2:H:107:TYR:CE2	2:H:199:ALA:HA	2.19	0.78
1:Q:35:TYR:CD2	1:Q:38:GLY:O	2.36	0.78
2:P:37:THR:HG21	2:P:43:THR:HG23	1.64	0.78
1:1:229:ALA:O	1:1:233:LEU:CD1	2.30	0.77
1:F:182:ARG:HD2	3:F:250:HOH:O	1.83	0.77
1:1:41:PHE:HB3	1:1:53:ILE:HD13	1.67	0.77
1:D:35:TYR:CD2	1:D:38:GLY:O	2.37	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:Y:227:GLY:HA2	1:Y:230:LEU:HD12	1.66	0.77
1:Q:35:TYR:CE1	1:Q:37:GLY:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:227:GLY:C	1:S:230:LEU:HB3	2.06	0.76
1:F:58:ASP:HB3	1:F:219:ARG:O	1.86	0.76
1:S:217:ARG:HH22	1:S:223:ARG:HG3	1.49	0.76
2:R:37:THR:CG2	2:R:59:TYR:HD2	1.99	0.76
1:Y:35:TYR:CE1	1:Y:37:GLY:C	2.59	0.76
2:Z:107:TYR:HB2	2:Z:197:ILE:CG2	2.16	0.76
1:S:48:ARG:HH21	1:I:137:GLU:HG2	1.45	0.76
1:D:12:ALA:HB3	1:D:13:MET:CE	2.16	0.76
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: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
1:Y:36:ALA:HB2	1:Y:174:ASN:HA	1.67	0.75
1:D:18:GLU:HA	1:D:18:GLU:OE1	1.86	0.75
1:S:10:GLU:O	1:S:14:ARG:HD2	1.86	0.75
1:3:335:TYR:HD1	1:3:337:GLY:H	1.33	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
2:T:192:PRO:O	2:T:210:ILE:HD13	1.87	0.75
1:Q:140:ARG:HE	1:Q:154:VAL:HG13	1.50	0.75
1:B:11:GLN:O	1:B:14:ARG:CB	2.35	0.75
2:E:165:ARG:CB	2:E:213:LEU:HD22	2.17	0.75
1:D:153:PHE:CD1	1:D:167:LEU:HD13	2.22	0.74
1:I:11:GLN:HE21	1:I:14:ARG:NE	1.84	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:A:182:ARG:HH12	1:A:234:LEU:C	1.90	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:E:107:TYR:HB2	2:E:197:ILE:CG2	2.17	0.74
1:B:155:VAL:HG12	1:B:160:THR:HG22	1.70	0.73
2:2:19:ARG:HG3	2:2:20:SER:N	2.04	0.73
1:K:178:THR:HB	1:K:233:LEU:CD2	2.12	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
1:Q:35:TYR:CE2	1:Q:38:GLY:O	2.41	0.73
2:E:19:ARG:HG3	2:E:20:SER:N	2.04	0.73
1:I:11:GLN:CG	1:I:14:ARG:HH21	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:28:LYS:HB3	1:S:44:GLU:HG3	1.70	0.73
1:D:35:TYR:OH	1:D:212:VAL:HB	1.88	0.73
2:L:37:THR:CG2	2:L:43:THR:HG23	2.18	0.73
2:2:115:GLN:HA	2:2:115:GLN:OE1	1.89	0.73
1:I:181:LEU:HD23	1:I:233:LEU:HB3	1.70	0.73
1:3:328:LYS:HB3	1:3:344:GLU:HG3	1.70	0.73
1:O:28:LYS:HB3	1:O:44:GLU:HG3	1.70	0.73
2:V:18:ARG:HD3	2:V:193:THR:HG23	1.71	0.73
1:A:113:GLU:O	1:A:113:GLU:HG2	1.88	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:O:10:GLU:O	1:O:14:ARG:HG3	1.89	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
2:J:18:ARG:HD3	2:J:193:THR:HG23	1.71	0.72
1:W:28:LYS:HB3	1:W:44:GLU:HG3	1.71	0.72
1:M:127:VAL:HG11	1:M:215:ALA:HB2	1.70	0.72
2:2:1:OZT:H17	2:2:33:LYS:HZ3	1.52	0.72
1:O:217:ARG:NH2	1:O:223:ARG:HG3	2.04	0.72
1:D:40:LEU:HD13	1:D:212:VAL:HG12	1.69	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
1:U:28:LYS:HB3	1:U:44:GLU:HG3	1.72	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
1:S:217:ARG:HH21	1:S:223:ARG:HG3	1.50	0.72
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.72	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
2:R:18:ARG:HD3	2:R:193:THR:HG23	1.69	0.72
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
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:O	1:Y:177:LEU:HD12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:3:478:THR:OG1	1:3:533:LEU:CD1	2.39	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
1:1:28:LYS:HB3	1:1:44:GLU:HG3	1.72	0.71
1:W:230:LEU:HD13	1:W:230:LEU:C	2.11	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:D:155:VAL:HG12	1:D:160:THR:HG22	1.73	0.70
1:F:36:ALA:HA	1:F:174:ASN:HD22	1.56	0.70
2:C:38:ASP:C	2:C:38:ASP:OD1	2.30	0.70
1:Y:176:SER:OG	1:Y:179:ASP:CG	2.30	0.70
1:D:97:ARG:HD2	1:D:97:ARG:C	2.12	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
2:T:38:ASP:OD1	2:T:38:ASP:C	2.30	0.70
2:Z:38:ASP:C	2:Z:38:ASP:OD1	2.30	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:11:GLN:CD	1:I:14:ARG:NH2	2.45	0.70
2:H:37:THR:HG21	2:H:59:TYR:HD2	1.55	0.70
1:I:130:TYR:CD1	1:I:216:ASN:O	2.44	0.70
2:G:19:ARG:HG3	2:G:20:SER:N	2.06	0.70
1:Q:28:LYS:HB3	1:Q:44:GLU:HG3	1.72	0.70
2:R:107:TYR:HB2	2:R:197:ILE:HG22	1.73	0.70
1:W:230:LEU:HD13	1:W:230:LEU:O	1.92	0.70
1:M:58:ASP:OD1	1:M:219:ARG:NH1	2.24	0.70
2:R:38:ASP:OD1	2:R:38:ASP:C	2.30	0.70
2:2:198:ASP:OD1	2:2:200:ASP:HB2	1.92	0.70
1:D:90:ASP:OD1	1:D:93:ASP:CB	2.39	0.70
1:K:230:LEU:HG	1:K:234:LEU:HD12	1.73	0.70
1:D:181:LEU:HD22	1:D:233:LEU:HD22	1.74	0.69
2:G:37:THR:HG21	2:G:43:THR:HG23	1.74	0.69
2:H:38:ASP:OD1	2:H:38:ASP:C	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:ASN:HB2	3:I:252:HOH:O	1.91	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
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
1:D:219:ARG:HH22	2:E:64:GLU:CD	1.95	0.69
2:R:129:TRP:HD1	3:R:243:HOH:O	1.74	0.69
1:F:217:ARG:HH11	1:F:217:ARG:HB3	1.58	0.69
2:G:18:ARG:HD3	2:G:193:THR:HG23	1.73	0.69
1:M:41:PHE:HB3	1:M:53:ILE:HD13	1.75	0.69
1:U:41:PHE:HB3	1:U:53:ILE:HD13	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:L:38:ASP:OD1	2:L:38:ASP:C	2.30	0.69
2:N:38:ASP:C	2:N:38:ASP:OD1	2.30	0.69
2:G:38:ASP:C	2:G:38:ASP:OD1	2.30	0.69
1:Q:10:GLU:CB	1:Y:15:GLU:OE2	2.40	0.69
2:4:301:OZT:C7	2:4:333:LYS:NZ	2.56	0.68
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:M:35:TYR:HD1	1:M:37:GLY:H	1.33	0.68
1:I:181:LEU:HD23	1:I:233:LEU:HB3	1.74	0.68
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.75	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:I:225:ILE:HG21	1:I:233:LEU:HD22	1.74	0.68
2:N:19:ARG:HG3	2:N:20:SER:N	2.08	0.68
1:Y:178:THR:CG2	1:Y:179:ASP:OD1	2.42	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:I:230:LEU:O	1:I:234:LEU:HG	1.94	0.68
2:4:319:ARG:HG3	2:4:320:SER:N	2.08	0.68
1:D:40:LEU:HD12	1:D:212:VAL:HG12	1.75	0.68
1:W:178:THR:O	1:W:182:ARG:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:38:ASP:OD1	2:2:38:ASP:C	2.30	0.67
2:P:38:ASP:OD1	2:P:38:ASP:C	2.30	0.67
1:Q:10:GLU:HB3	1:Y:15:GLU:OE2	1.93	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:W:225:ILE:HG22	1:W:230:LEU:HB2	1.75	0.67
1:A:152:HIS:HB3	1:A:171:TYR:CE2	2.29	0.67
1:U:137:GLU:HG2	1:1:48:ARG:NH2	2.10	0.67
1:S:227:GLY:O	1:S:230:LEU:HB3	1.95	0.67
2:C:19:ARG:HG3	2:C:20:SER:N	2.08	0.67
1:D:81:PHE:CE2	1:D:85:ARG:HG3	2.30	0.67
2:E:1:OZT:O	2:E:140:GLY:HA3	1.94	0.67
1:U:217:ARG:NH2	1:U:223:ARG:HG3	2.10	0.67
1:M:152:HIS:HB3	1:M:171:TYR:CZ	2.29	0.67
1:S:230:LEU:CD2	1:S:231:GLN:N	2.57	0.67
2:T:19:ARG:HG3	2:T:20:SER:N	2.10	0.67
1:A:229:ALA:O	1:A:233:LEU:HD13	1.95	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
1:3:355:GLU:HB2	1:3:522:PHE:CG	2.29	0.67
1:F:54:SER:CB	1:F:75:ARG:HD2	2.25	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
1:A:57:TYR:HB3	1:A:60:VAL:CG1	2.24	0.66
2:Z:18:ARG:HD3	2:Z:193:THR:HG23	1.75	0.66
1:B:79:ILE:HD13	2:C:68:LYS:HB3	1.75	0.66
1:S:10:GLU:HG3	1:S:11:GLN:N	2.10	0.66
1:A:127:VAL:CG2	1:A:213:LEU:HB3	2.25	0.66
1:D:35:TYR:CD1	1:D:38:GLY:O	2.48	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:F:115:ALA:CB	1:W:112:THR:HG23	2.25	0.66
1:B:113:GLU:O	1:B:113:GLU:HG2	1.95	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
2:T:38:ASP:OD1	2:T:40:TYR:N	2.28	0.66
2:E:90:ASN:HA	2:E:93:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:38:ASP:OD2	2:J:38:ASP:C	2.34	0.66
2:L:14:MET:CE	2:L:105:ALA:HB2	2.25	0.66
2:L:37:THR:HG21	2:L:43:THR:HG23	1.78	0.66
1:3:479:ASP:O	1:3:483:ILE:HG13	1.96	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
2:L:38:ASP:OD1	2:L:40:TYR:N	2.28	0.66
1:D:232:ALA:O	1:D:233:LEU:C	2.34	0.66
1:U:53:ILE:O	1:U:224:ARG:NH2	2.26	0.66
2:X:18:ARG:HD3	2:X:193:THR:HG23	1.76	0.66
1:S:214:ASP:OD2	1:S:216:ASN:N	2.30	0.65
1:F:114:GLN:HG2	1:F:115:ALA:H	1.60	0.65
2:N:165:ARG:HD3	3:N:245:HOH:O	1.96	0.65
1:I:15:GLU:OE2	1:S:10:GLU:CD	2.34	0.65
1:Q:182:ARG:NH1	1:Q:234:LEU:CD2	2.58	0.65
2:2:18:ARG:HD3	2:2:193:THR:HG23	1.79	0.65
1:B:115:ALA:HB3	1:I:112:THR:HG23	1.77	0.65
2:G:37:THR:CG2	2:G:43:THR:HG23	2.26	0.65
1:I:11:GLN:NE2	1:I:14:ARG:CZ	2.59	0.65
2:J:165:ARG:HA	2:J:213:LEU:HD13	1.79	0.65
1:K:35:TYR:CD1	1:K:37:GLY:N	2.64	0.65
2:N:38:ASP:OD1	2:N:40:TYR:N	2.30	0.65
1:Q:144:ASP:OD1	1:Q:146:SER:HB2	1.94	0.65
2:R:212:GLU:CD	2:R:215:ARG:HH21	2.00	0.65
2:R:169:GLU:CB	2:R:217:ILE:HD13	2.25	0.65
2:2:38:ASP:OD1	2:2:40:TYR:N	2.30	0.65
1:A:114:GLN:HG2	1:A:115:ALA:H	1.62	0.65
2:Z:38:ASP:OD1	2:Z:40:TYR: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
1:W:83:ASP:OD2	2:X:65:HIS:HD2	1.79	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
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
1:Q:182:ARG:HH12	1:Q:234:LEU:CA	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:38:ASP:OD1	2:C:40:TYR:N	2.30	0.65
1:K:51:GLN:N	1:K:51:GLN:OE1	2.30	0.65
1:D:181:LEU:HD22	1:D:233:LEU:CD2	2.26	0.64
1:D:35:TYR:CE2	1:D:39:VAL:C	2.70	0.64
2:L:8:TYR:CZ	2:L:11:GLY:HA3	2.32	0.64
1:O:225:ILE:HG23	1:O:229:ALA:HB1	1.79	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
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
1:D:214:ASP:OD1	1:D:216:ASN:N	2.30	0.64
1:D:32:ALA:HB3	1:D:154:VAL:HB	1.79	0.64
2:V:19:ARG:HG3	2:V:20:SER:N	2.11	0.64
2:Z:107:TYR:CE2	2:Z:199:ALA:HA	2.32	0.64
2:Z:19:ARG:HG3	2:Z:20:SER:N	2.12	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
2:G:38:ASP:OD1	2:G:40:TYR:N	2.30	0.64
1:K:83:ASP:OD2	2:L:65:HIS:HD2	1.81	0.64
1:Q:144:ASP:CG	1:Q:146:SER:HG	2.00	0.64
1:O:163:ILE:HG23	1:O:187:ALA:O	1.97	0.64
2:L:12:VAL:HG22	2:L:197:ILE:HB	1.80	0.64
1:S:178:THR:HA	1:S:233:LEU:HD22	1.80	0.64
1:K:182:ARG:CG	3:K:250:HOH:O	2.40	0.64
2:L:38:ASP:OD1	2:L:39:ASP:N	2.31	0.64
1:U:58:ASP:OD1	1:U:219:ARG:NH1	2.31	0.64
1:S:176:SER:HB2	1:S:179:ASP:CG	2.18	0.64
1:F:205:VAL:N	1:F:208:LEU:HG	2.13	0.64
1:A:127:VAL:CG1	1:A:215:ALA:HB2	2.28	0.63
2:H:19:ARG:HG3	2:H:20:SER:N	2.12	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
1:3:335:TYR:CE1	1:3:337:GLY:N	2.66	0.63
1:A:217:ARG:HH11	1:A:223:ARG:CB	2.07	0.63
2:P:18:ARG:HD3	2:P:193:THR:HG23	1.80	0.63
1:U:35:TYR:CE1	1:U:37:GLY:HA3	2.32	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
1:U:10:GLU:CA	1:1:15:GLU:OE2	2.35	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:169:GLU:HB2	2:R:217:ILE:CD1	2.29	0.63
1:A:97:ARG:HD2	1:A:97:ARG:C	2.18	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
2:N:161:ASP:OD2	2:N:209:ARG:NH1	2.32	0.63
2:H:18:ARG:HD3	2:H:193:THR:HG23	1.80	0.63
1:W:176:SER:OG	1:W:179:ASP:CG	2.37	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:I:35:TYR:CE1	1:I:37:GLY:N	2.66	0.62
1:M:129:HIS:HB2	1:M:132:GLU:CD	2.19	0.62
1:1:181:LEU:CD2	1:1:233:LEU:HB3	2.29	0.62
1:A:57:TYR:CB	1:A:60:VAL:CG1	2.77	0.62
2:V:217:ILE:CG2	2:V:221:ARG:NH1	2.59	0.62
1:1:83:ASP:OD2	2:2:65:HIS:HD2	1.82	0.62
1:3:526:THR:HG22	1:3:527:GLY:N	2.13	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:O:233:LEU:C	1:O:234:LEU:HD13	2.19	0.62
2:V:212:GLU:HG3	2:V:213:LEU:H	1.62	0.62
2:C:1:OZT:H17	2:C:17:ASP:OD1	1.99	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
1:1:18:GLU:OE1	1:1:21:ARG:NH2	2.30	0.62
1:Q:230:LEU:C	1:Q:230:LEU:HD23	2.20	0.62
1:Y:55:GLU:HG3	1:Y:222:PHE:HB2	1.82	0.62
1:3:383:ASP:OD2	2:4:365:HIS:HD2	1.83	0.62
1:A:35:TYR:CE1	1:A:37:GLY:HA3	2.34	0.62
2:H:107:TYR:HB2	2:H:197:ILE:CG2	2.27	0.62
1:I:128:ALA:HB2	1:I:134:LYS:CB	2.21	0.62
2:N:18:ARG:HD3	2:N:193:THR:HG23	1.81	0.62
1:S:35:TYR:CD2	1:S:38:GLY:O	2.52	0.62
2:V:172:TYR:CE1	2:V:218:ILE:HD12	2.33	0.62
1:Y:179:ASP:OD1	1:Y:179:ASP:N	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:V:130:ASN:HD22	2:V:131:ILE:N	1.97	0.62
1:1:173:GLU:O	1:1:174:ASN:HB2	1.98	0.61
2:4:486:LEU:HG	3:4:23:HOH:O	2.00	0.61
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:B:114:GLN:HG2	1:B:115:ALA:N	2.15	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
2:H:1:OZT:H17	2:H:33:LYS:NZ	2.15	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
2:R:164:LEU:CD1	2:R:213:LEU:HD11	2.30	0.61
1:S:177:LEU:HD12	1:S:177:LEU:O	2.00	0.61
2:X:107:TYR:HB2	2:X:197:ILE:HG22	1.82	0.61
2:R:14:MET:HE2	2:R:103:LEU:HD13	1.81	0.61
1:S:214:ASP:OD2	1:S:215:ALA:N	2.33	0.61
2:E:1:OZT:H17	2:E:17:ASP:OD1	2.00	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: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:D:56:LEU:HB2	1:D:60:VAL:HG22	1.82	0.61
2:T:130:ASN:HD22	2:T:131:ILE:N	1.99	0.61
2:Z:40:TYR:CE1	2:Z:109:ILE:CD1	2.81	0.61
2:Z:37:THR:HG21	2:Z:43:THR:HG23	1.81	0.61
1:1:35:TYR:CE1	1:1:37:GLY:HA3	2.36	0.61
1:Q:173:GLU:O	1:Q:174:ASN:HB2	2.01	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: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
1:1:112:THR:HG22	1:1:113:GLU:CG	2.30	0.60
2:2:1:OZT:C7	2:2:33:LYS:NZ	2.64	0.60
1:Q:182:ARG:HH12	1:Q:234:LEU:HA	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:40:LEU:HD13	1:W:212:VAL:HG12	1.82	0.60
2:E:165:ARG:HB2	2:E:213:LEU:CD2	2.31	0.60
1:F:229:ALA:O	1:F:233:LEU:HD12	2.01	0.60
2:R:218:ILE:O	2:R:218:ILE:HG22	2.01	0.60
1:W:181:LEU:O	1:W:185:VAL:HG23	2.01	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:Q:35:TYR:HE1	1:Q:37:GLY:C	2.00	0.60
1:Y:176:SER:HG	1:Y:179:ASP:CG	2.04	0.60
1:B:54:SER:CB	1:B:75:ARG:HD2	2.32	0.60
2:L:14:MET:HE3	2:L:105:ALA:HB2	1.82	0.60
2:P:164:LEU:HD13	2:P:213:LEU:HD12	1.83	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
2:V:215:ARG:O	2:V:219:GLU:HG3	2.01	0.60
1:I:56:LEU:HD13	1:I:99:LEU:HD13	1.84	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
2:R:107:TYR:HB2	2:R:197:ILE:CG2	2.30	0.60
1:A:205:VAL:N	1:A:208:LEU:HG	2.16	0.60
2:H:1:OZT:C7	2:H:33:LYS:NZ	2.65	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:K:178:THR:CB	1:K:233:LEU:HD22	2.16	0.59
2:H:38:ASP:OD1	2:H:41:THR:N	2.35	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
1:3:463:ILE:HG23	1:3:487:ALA:O	2.02	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
2:V:37:THR:HG21	2:V:59:TYR:HD2	1.66	0.59
2:E:37:THR:HG21	2:E:43:THR:HG23	1.84	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
2:J:37:THR:HG21	2:J:43:THR:CG2	2.31	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:I:13:MET:HE2	1:I:16:ARG:HD3	1.84	0.59
1:U:178:THR:O	1:U:182:ARG:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:3:412:THR:HG22	1:3:413:GLU:CG	2.30	0.59
1:D:227:GLY:O	1:D:230:LEU:HB3	2.01	0.59
2:N:165:ARG:HA	2:N:213:LEU:HD13	1.83	0.59
1:S:181:LEU:HD23	1:S:233:LEU:HB3	1.83	0.59
2:X:14:MET:HE2	2:X:103:LEU:HB3	1.85	0.59
1:1:35:TYR:HE1	1:1:37:GLY:HA3	1.68	0.59
1:B:59:ARG:NH2	1:B:128:ALA:O	2.31	0.59
2:R:192:PRO:O	2:R:210:ILE:HD13	2.02	0.59
1:S:231:GLN:HA	1:S:234:LEU:CD1	2.32	0.59
2:V:37:THR:CG2	2:V:43:THR:HG23	2.33	0.59
1:Y:112:THR:HG22	1:Y:113:GLU:CG	2.32	0.59
1:1:163:ILE:HG23	1:1:187:ALA:O	2.02	0.59
1:A:28:LYS:HB3	1:A:44:GLU:HG3	1.85	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:A:205:VAL:CG2	1:A:206:ALA:N	2.66	0.58
1:D:181:LEU:HD23	1:D:233:LEU:HD23	1.83	0.58
2:L:12:VAL:CG1	2:L:118:GLY:CA	2.80	0.58
1:M:179:ASP:O	1:M:183:ILE:HG13	2.03	0.58
2:V:37:THR:HG21	2:V:43:THR:HG23	1.85	0.58
1:3:328:LYS:HG2	3:3:129:HOH:O	2.03	0.58
1:B:152:HIS:HB3	1:B:171:TYR:CE2	2.37	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
1:S:214:ASP:OD2	1:S:214:ASP:C	2.40	0.58
1:F:112:THR:HG22	1:F:113:GLU:N	2.18	0.58
2:E:165:ARG:CB	2:E:213:LEU:CD2	2.82	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:L:37:THR:HG21	2:L:59:TYR:HD2	1.67	0.58
2:E:165:ARG:HB2	2:E:213:LEU:HD21	1.85	0.58
1:I:83:ASP:OD2	2:J:65:HIS:HD2	1.86	0.58
1:A:97:ARG:HG3	1:O:49:SER:HB2	1.85	0.58
1:W:217:ARG:NH1	1:W:220:ARG:O	2.37	0.58
1:B:16:ARG:NH2	1:B:111:PHE:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:N:37:THR:HG21	2:N:43:THR:HG23	1.86	0.58
1:W:112:THR:HG22	1:W:113:GLU:CG	2.31	0.58
1:B:16:ARG:HH21	1:B:111:PHE:C	2.05	0.58
2:L:12:VAL:HG12	2:L:118:GLY:HA3	1.85	0.58
2:C:161:ASP:CG	2:C:209:ARG:HH21	2.08	0.58
1:M:225:ILE:HG22	1:M:230:LEU:HB2	1.86	0.58
1:I:130:TYR:CE1	1:I:216:ASN:O	2.57	0.57
2:J:165:ARG:HG3	2:J:213:LEU:HD22	1.86	0.57
1:U:112:THR:HG22	1:U:113:GLU:CG	2.29	0.57
1:D:114:GLN:HG2	1:D:115:ALA:N	2.19	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
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:S:149:ASP:CG	1:S:149:ASP:O	2.42	0.57
1:3:476:SER:HB3	1:3:479:ASP:OD1	2.04	0.57
1:D:12:ALA:CA	1:D:13:MET:HE3	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:U:56:LEU:HD11	1:U:62:PHE:HB2	1.86	0.57
2:G:37:THR:HG21	2:G:59:TYR:HD2	1.69	0.57
1:U:163:ILE:HG23	1:U:187:ALA:O	2.04	0.57
2:X:165:ARG:HG3	2:X:213:LEU:HD22	1.87	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
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: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:A:205:VAL:HG22	1:A:206:ALA:H	1.68	0.57
2:E:198:ASP:OD1	2:E:200:ASP:HB2	2.04	0.57
2:X:19:ARG:HG3	2:X:20:SER:N	2.18	0.57
1:Y:141:ILE:N	1:Y:141:ILE:HD12	2.20	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:229:ALA:O	1:Y:233:LEU:N	2.38	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
2:H:37:THR:CG2	2:H:43:THR:HG23	2.34	0.57
1:B:48:ARG:HH22	1:I:135:ARG:HH11	1.51	0.57
2:J:161:ASP:CG	2:J:209:ARG:HH21	2.08	0.57
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.40	0.57
2:T:18:ARG:HD3	2:T:193:THR:HG23	1.87	0.57
2:J:130:ASN:HD22	2:J:131:ILE:N	2.03	0.57
2:V:14:MET:HE2	2:V:103:LEU:HD13	1.85	0.57
1:3:481:LEU:HD23	1:3:533:LEU:HB3	1.85	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
1:D:233:LEU:O	1:D:233:LEU:HG	2.05	0.56
2:R:13:VAL:HG21	2:R:164:LEU:HD23	1.87	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
1:1:12:ALA:O	1:1:16:ARG:HG3	2.05	0.56
1:D:40:LEU:HD13	1:D:212:VAL:CG1	2.35	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
1:Y:55:GLU:HB2	1:Y:222:PHE:CB	2.35	0.56
1:S:49:SER:HB2	1:1:97:ARG:HG3	1.87	0.56
1:A:59:ARG:NH1	1:A:128:ALA:O	2.34	0.56
1:F:114:GLN:HG2	1:F:115:ALA:N	2.20	0.56
1:F:90:ASP:HB2	1:F:93:ASP:H	1.70	0.56
2:L:14:MET:HE3	2:L:105:ALA:CB	2.35	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:B:10:GLU:C	1:B:12:ALA:N	2.52	0.56
1:Q:112:THR:HG22	1:Q:113:GLU:CG	2.32	0.56
1:I:112:THR:HG22	1:I:113:GLU:CG	2.33	0.56
2:J:214:ALA:O	2:J:218:ILE:HG13	2.05	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:F:51:GLN:HA	1:F:209:GLU:OE2	2.05	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
2:Z:37:THR:HG21	2:Z:59:TYR:CD2	2.39	0.56
1:A:214:ASP:OD2	1:A:223:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ALA:CA	1:D:174:ASN:HD22	2.19	0.56
1:D:36:ALA:HA	1:D:174:ASN:HD22	1.70	0.56
1:D:56:LEU:CD1	1:D:62:PHE:HB2	2.36	0.55
2:H:107:TYR:CE2	2:H:199:ALA:CA	2.89	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
1:1:35:TYR:CD2	1:1:38:GLY:O	2.59	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:D:152:HIS:HB3	1:D:171:TYR:CE2	2.41	0.55
1:A:114:GLN:HG2	1:A:115:ALA:N	2.21	0.55
2:H:76:PHE:CE2	2:H:80:ILE:HD11	2.42	0.55
2:J:38:ASP:OD2	2:J:41:THR:N	2.38	0.55
2:T:14:MET:HE2	2:T:103:LEU:HB3	1.88	0.55
2:4:318:ARG:HD3	2:4:493:THR:HG23	1.89	0.55
2:X:1:OZT:C7	2:X:33:LYS:NZ	2.69	0.55
1:A:161:GLU:HB2	1:A:162:PRO:HD3	1.89	0.55
1:D:152:HIS:HB3	1:D:171:TYR:CZ	2.42	0.55
1:D:35:TYR:OH	1:D:212:VAL:CB	2.55	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
1:F:35:TYR:CE2	1:F:40:LEU:HB2	2.42	0.55
2:G:130:ASN:HD22	2:G:131:ILE:N	2.05	0.55
2:H:186:LEU:HD11	2:H:218:ILE:CD1	2.36	0.55
2:H:37:THR:HG21	2:H:43:THR:HG23	1.89	0.55
2:N:130:ASN:HD22	2:N:131:ILE:N	2.05	0.55
2:N:45:ILE:CD1	3:N:243:HOH:O	2.55	0.55
1:B:62:PHE:C	1:B:62:PHE:CD1	2.80	0.55
1:S:112:THR:HG22	1:S:113:GLU:CG	2.34	0.55
2:X:1:OZT:H27	2:X:33:LYS:NZ	2.21	0.55
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.71	0.55
1:B:83:ASP:OD2	2:C:65:HIS:HD2	1.89	0.55
1:D:62:PHE:C	1:D:62:PHE:CD1	2.79	0.55
2:R:130:ASN:HD22	2:R:131:ILE:N	2.05	0.55
2:G:185:ASP:OD1	2:G:188:ARG:HB2	2.07	0.55
1:M:92:ARG:HH12	1:M:132:GLU:CD	2.10	0.55
1:1:41:PHE:CB	1:1:53:ILE:HD13	2.36	0.55
1:B:35:TYR:CE1	1:B:37:GLY:CA	2.90	0.55
1:W:41:PHE:CB	1:W:53:ILE:HD13	2.36	0.55
1:B:69:ASN:HB2	1:I:105:GLN:HG2	1.89	0.54
2:J:169:GLU:HA	2:J:217:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.42	0.54
2:V:172:TYR:CE1	2:V:218:ILE:HD11	2.42	0.54
1:W:214:ASP:OD1	1:W:214:ASP:C	2.45	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
1:I:13:MET:HA	1:I:13:MET:HE2	1.90	0.54
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.90	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
2:H:132:GLU:HG3	2:H:137:GLN:HB2	1.90	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
2:C:198:ASP:OD1	2:C:200:ASP:N	2.30	0.54
2:H:1:OZT:H27	2:H:33:LYS:HE2	1.89	0.54
2:L:37:THR:HG23	2:L:43:THR:HG23	1.88	0.54
2:4:514:ALA:O	2:4:518:ILE:HG13	2.08	0.54
1:A:62:PHE:CD1	1:A:62:PHE:C	2.81	0.54
1:W:54:SER:CB	1:W:75:ARG:HD2	2.38	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
2:4:301:OZT:C7	2:4:333:LYS:HZ1	2.19	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: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
2:R:212:GLU:CD	2:R:215:ARG:NH2	2.61	0.54
1:D:12:ALA:CB	1:D:13:MET:CE	2.81	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
2:2:1:OZT:H27	2:2:33:LYS:HE2	1.89	0.53
1:D:33:LEU:HD23	1:D:33:LEU:N	2.23	0.53
2:N:14:MET:HE2	2:N:103:LEU:HD13	1.89	0.53
1:S:41:PHE:CB	1:S:53:ILE:HD13	2.38	0.53
2:Z:130:ASN:HD22	2:Z:131:ILE:N	2.06	0.53
2:C:83:LEU:HD13	2:C:123:PHE:CZ	2.43	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
2:Z:83:LEU:HD13	2:Z:123:PHE:CE1	2.42	0.53
1:M:163:ILE:HG23	1:M:187:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:145:PHE:CE1	2:Z:144:LEU:HD13	2.43	0.53
1:1:128:ALA:HB2	1:1:134:LYS:HB3	1.88	0.53
2:2:35:TYR:CZ	2:2:53:VAL:HG13	2.44	0.53
1:3:333:LEU:HD23	1:3:333:LEU:N	2.24	0.53
1:D:11:GLN:CA	1:D:11:GLN:OE1	2.52	0.53
1:D:127:VAL:HG21	1:D:213:LEU:HB3	1.90	0.53
2:X:31:VAL:HG11	2:X:33:LYS:HE3	1.91	0.53
1:1:10:GLU:O	1:1:14:ARG:HG3	2.08	0.53
2:X:164:LEU:HD13	2:X:213:LEU:CD1	2.39	0.53
1:D:13:MET:CA	1:D:13:MET:CE	2.86	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
2:C:83:LEU:HD13	2:C:123:PHE:CE1	2.43	0.53
2:N:45:ILE:N	2:N:45:ILE:HD12	2.24	0.53
2:X:6:LEU:HD12	2:X:6:LEU:C	2.29	0.53
1:1:54:SER:CB	1:1:75:ARG:HD2	2.39	0.53
2:E:130:ASN:HD22	2:E:131:ILE:N	2.06	0.53
1:S:48:ARG:HH21	1:1:137:GLU:CG	2.18	0.53
1:3:476:SER:HB3	1:3:479:ASP:CG	2.29	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
2:R:169:GLU:HB2	2:R:217:ILE:HD13	1.90	0.53
1:Y:83:ASP:OD2	2:Z:65:HIS:HD2	1.92	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
2:G:161:ASP:CG	2:G:209:ARG:HH21	2.12	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
1:S:176:SER:HB2	1:S:179:ASP:OD2	2.08	0.53
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
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
1:1:152:HIS:HB3	1:1:171:TYR:CE2	2.44	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
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:P:1:OZT:H17	2:P:33:LYS:NZ	2.23	0.52
2:R:169:GLU:HB2	2:R:217:ILE:HD11	1.90	0.52
1:U:226:THR:CG2	1:U:227:GLY:N	2.72	0.52
1:U:56:LEU:CD1	1:U:62:PHE:HB2	2.40	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:D:35:TYR:OH	1:D:212:VAL:CG1	2.57	0.52
1:F:205:VAL:HG22	1:F:206:ALA:H	1.73	0.52
1:F:205:VAL:HG23	1:F:206:ALA:N	2.24	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: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
2:T:164:LEU:HD13	2:T:213:LEU:CD1	2.39	0.52
2:2:107:TYR:CE1	2:2:117:ALA:HB3	2.45	0.52
1:D:153:PHE:CD1	1:D:167:LEU:CD1	2.93	0.52
2:E:83:LEU:HD13	2:E:123:PHE:CE1	2.44	0.52
1:K:69:ASN:HB3	1:M:104:ALA:HB1	1.91	0.52
1:I:15:GLU:OE2	1:S:10:GLU:OE2	2.27	0.52
1:S:178:THR:HB	1:S:233:LEU:CD2	2.39	0.52
2:V:164:LEU:HD13	2:V:213:LEU:HD11	1.91	0.52
2:V:65:HIS:CE1	2:V:69:LEU:HD11	2.43	0.52
1:Y:35:TYR:CZ	1:Y:38:GLY:N	2.77	0.52
2:E:1:OZT:H27	2:E:33:LYS:NZ	2.24	0.52
2:H:1:OZT:H17	2:H:33:LYS:HZ3	1.74	0.52
2:R:169:GLU:CA	2:R:217:ILE:HD13	2.39	0.52
2:R:83:LEU:HD13	2:R:123:PHE:CE1	2.45	0.52
2:T:83:LEU:HD13	2:T:123:PHE:CZ	2.44	0.52
1:W:55:GLU:OE2	1:W:220:ARG:HD2	2.10	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
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
1:U:22:LYS:O	1:U:26:ARG:HG3	2.10	0.52
1:U:112:THR:CG2	1:1:115:ALA:HB3	2.28	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
2:J:198:ASP:OD2	2:J:200:ASP:HB2	2.10	0.52
1:M:68:PHE:HA	1:M:71:PHE:CE2	2.45	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:G:14:MET:HE2	2:G:103:LEU:HD13	1.92	0.52
2:H:58:LEU:HD12	2:H:58:LEU:O	2.10	0.52
1:B:48:ARG:HH22	1:I:135:ARG:NH1	2.07	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:B:227:GLY:O	1:B:228:SER:C	2.46	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
1:F:56:LEU:HD13	1:F:99:LEU:HD13	1.92	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
1:D:182:ARG:HG2	1:D:182:ARG:HH11	1.76	0.51
1:D:97:ARG:O	1:D:97:ARG:HD2	2.10	0.51
2:J:13:VAL:HG21	2:J:164:LEU:HD23	1.93	0.51
1:O:56:LEU:HD13	1:O:99:LEU:HD13	1.92	0.51
2:P:38:ASP:OD1	2:P:39:ASP:N	2.42	0.51
1:W:230:LEU:C	1:W:230:LEU:CD1	2.79	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
1:D:149:ASP:N	1:D:149:ASP:OD1	2.43	0.51
1:D:15:GLU:OE1	1:K:10:GLU:CG	2.54	0.51
1:D:83:ASP:OD2	2:E:65:HIS:HD2	1.93	0.51
2:L:14:MET:HE2	2:L:105:ALA:HB2	1.91	0.51
1:A:139:TYR:HH	1:O:49:SER:HG	1.58	0.51
2:P:45:ILE:HD12	2:P:45:ILE:N	2.25	0.51
1:W:179:ASP:OD1	1:W:179:ASP:N	2.44	0.51
2:C:31:VAL:HG11	2:C:33:LYS:HE3	1.92	0.51
1:I:13:MET:CE	1:I:13:MET:HA	2.40	0.51
1:I:41:PHE:CB	1:I:53:ILE:HD13	2.39	0.51
2:P:130:ASN:HD22	2:P:131:ILE:N	2.09	0.51
2:E:49:ALA:O	2:E:53:VAL:HG23	2.11	0.51
1:W:40:LEU:HD12	1:W:212:VAL:HG12	1.93	0.51
2:Z:107:TYR:CB	2:Z:197:ILE:HG22	2.35	0.51
2:4:335:TYR:CZ	2:4:353:VAL:HG13	2.46	0.50
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
2:N:140:GLY:O	2:N:143:SER:HB3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLN:O	1:B:14:ARG:N	2.43	0.50
2:N:35:TYR:CZ	2:N:53:VAL:HG13	2.46	0.50
1:S:231:GLN:O	1:S:234:LEU:HB2	2.11	0.50
2:4:301:OZT:H27	2:4:333:LYS:HE2	1.92	0.50
1:D:13:MET:HE3	1:D:13:MET:H	1.66	0.50
2:E:6:LEU:C	2:E:6:LEU:HD12	2.30	0.50
2:J:49:ALA:O	2:J:53:VAL:HG23	2.11	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
2:V:172:TYR:HE1	2:V:218:ILE:CD1	2.14	0.50
1:1:35:TYR:CE1	1:1:37:GLY:CA	2.94	0.50
2:2:14:MET:HE2	2:2:103:LEU:HD13	1.94	0.50
2:C:130:ASN:HD22	2:C:131:ILE:N	2.10	0.50
1:I:178:THR:HA	1:I:233:LEU:HD13	1.94	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
2:R:37:THR:HG21	2:R:43:THR:HG23	1.91	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
2:4:383:LEU:HD13	2:4:423:PHE:CE1	2.46	0.50
1:A:205:VAL:HG23	1:A:206:ALA:N	2.27	0.50
1:A:90:ASP:HB2	1:A:93:ASP:N	2.26	0.50
2:G:14:MET:CE	2:G:103:LEU:HD13	2.42	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
1:3:530:LEU:CD2	1:3:530:LEU:O	2.57	0.50
1:A:225:ILE:HG22	1:A:230:LEU:HB2	1.92	0.50
1:1:83:ASP:OD2	2:2:65:HIS:CD2	2.64	0.50
2:G:13:VAL:HG21	2:G:164:LEU:HD23	1.94	0.50
2:H:144:LEU:HD13	2:E:145:PHE:CE1	2.47	0.50
2:H:1:OZT:O	2:H:140:GLY:HA3	2.12	0.50
1:I:230:LEU:O	1:I:234:LEU:N	2.44	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
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.93	0.50
2:C:1:OZT:O	2:C:140:GLY:HA3	2.12	0.50
2:H:14:MET:HE2	2:H:103:LEU:HD13	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:144:ASP:OD1	1:Q:146:SER:OG	2.30	0.50
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.42	0.50
2:R:208:SER:O	2:R:212:GLU:OE2	2.30	0.50
2:4:430:ASN:HD22	2:4:431:ILE:N	2.10	0.50
2:C:156:GLN:OE1	2:C:165:ARG:NH2	2.45	0.50
1:F:182:ARG:HH11	1:F:182:ARG:HG2	1.77	0.50
1:B:115:ALA:HB3	1:I:112:THR:CG2	2.41	0.50
1:U:55:GLU:HB2	1:U:222:PHE:CG	2.46	0.50
2:V:218:ILE:O	2:V:222:SER:OG	2.30	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
2:E:49:ALA:O	2:E:53:VAL:CG2	2.59	0.49
1:A:83:ASP:OD2	2:H:65:HIS:HD2	1.95	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
1:3:311:GLN:CG	1:3:311:GLN:O	2.56	0.49
1:3:530:LEU:CD2	1:3:530:LEU:C	2.81	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:129:HIS:CB	1:M:132:GLU:OE2	2.54	0.49
1:M:127:VAL:HG21	1:M:213:LEU:O	2.12	0.49
2:X:1:OZT:H17	2:X:17:ASP:OD1	2.13	0.49
1:F:62:PHE:C	1:F:62:PHE:CD1	2.85	0.49
2:G:164:LEU:HD13	2:G:213:LEU:CD1	2.42	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:S:149:ASP:OD1	1:S:149:ASP:O	2.30	0.49
2:G:187:VAL:N	2:V:222:SER:HB3	2.26	0.49
2:4:486:LEU:HD11	2:4:518:ILE:HD12	1.94	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
2:P:185:ASP:OD1	2:P:188:ARG:HB2	2.11	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
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:Y:178:THR:HA	1:Y:233:LEU:CD2	2.43	0.49
2:2:83:LEU:HD13	2:2:123:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:37:THR:HG21	2:C:43:THR:CG2	2.38	0.49
1:F:182:ARG:HH12	1:F:234:LEU:C	2.16	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:V:209:ARG:C	2:V:212:GLU:HG2	2.33	0.49
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.93	0.49
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.77	0.49
1:A:40:LEU:CD1	1:A:212:VAL:HG12	2.42	0.49
1:W:30:VAL:HG22	1:W:43:ALA:HB1	1.94	0.49
2:2:132:GLU:HG3	2:2:137:GLN:HB2	1.95	0.49
1:F:217:ARG:NH1	1:F:217:ARG:HB3	2.26	0.49
1:U:41:PHE:CB	1:U:53:ILE:HD13	2.42	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
1:F:54:SER:OG	1:F:75:ARG:HD2	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
1:K:176:SER:O	1:K:177:LEU:C	2.51	0.49
1:K:47:SER:CB	1:M:149:ASP:OD2	2.58	0.49
2:V:45:ILE:N	2:V:45:ILE:HD12	2.28	0.49
2:G:37:THR:HG21	2:G:43:THR:CG2	2.43	0.49
1:I:11:GLN:NE2	1:I:11:GLN:HA	2.28	0.49
1:I:141:ILE:N	1:I:141:ILE:HD12	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
2:E:156:GLN:OE1	2:E:165:ARG:NH2	2.46	0.48
1:F:141:ILE:HD12	1:F:141:ILE:H	1.77	0.48
1:F:153:PHE:CD1	1:F:167:LEU:HD13	2.49	0.48
2:G:49:ALA:O	2:G:53:VAL:HG23	2.13	0.48
2:H:130:ASN:HD22	2:H:131:ILE:N	2.10	0.48
2:P:83:LEU:HD13	2:P:123:PHE:CZ	2.47	0.48
1:Q:107:LEU:HD12	1:Q:141:ILE:HG22	1.95	0.48
2:V:213:LEU:O	2:V:217:ILE:HG13	2.12	0.48
1:Y:41:PHE:CB	1:Y:53:ILE:HD13	2.42	0.48
1:B:115:ALA:CB	1:I:112:THR:HG23	2.43	0.48
2:J:1:OZT:O	2:J:140:GLY:HA3	2.13	0.48
2:R:198:ASP:OD2	2:R:201:GLY:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:79:ILE:HD12	2:Z:69:LEU:HD23	1.94	0.48
1:1:68:PHE:HA	1:1:71:PHE:CE2	2.47	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
1:3:479:ASP:OD1	1:3:479:ASP:N	2.47	0.48
1:B:205:VAL:HG23	1:B:206:ALA:N	2.29	0.48
2:E:83:LEU:HD13	2:E:123:PHE:CZ	2.48	0.48
2:G:45:ILE:N	2:G:45:ILE:HD12	2.28	0.48
1:I:44:GLU:HA	1:I:208:LEU:HD23	1.95	0.48
2:L:130:ASN:HD22	2:L:131:ILE:N	2.11	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
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
1:D:150:GLU:OE2	1:D:153:PHE:O	2.30	0.48
2:L:109:ILE:HG12	2:L:109:ILE:H	1.44	0.48
2:L:211:ALA:HB1	2:L:215:ARG:HH21	1.78	0.48
1:M:92:ARG:NH1	1:M:132:GLU:OE2	2.42	0.48
2:T:101:LEU:HA	2:T:102:PRO:HD3	1.66	0.48
1:1:226:THR:HG22	1:1:227:GLY:N	2.27	0.48
1:3:355:GLU:HB2	1:3:522:PHE:CB	2.43	0.48
1:B:153:PHE:CD1	1:B:167:LEU:HD13	2.49	0.48
2:C:198:ASP:OD1	2:C:199:ALA:N	2.46	0.48
1:F:59:ARG:NH2	1:F:128:ALA:O	2.34	0.48
1:F:141:ILE:N	1:F:141:ILE:HD12	2.28	0.48
2:H:83:LEU:HD13	2:H:123:PHE:CE1	2.48	0.48
1:I:44:GLU:O	1:I:44:GLU:HG3	2.13	0.48
2:L:12:VAL:CG1	2:L:118:GLY:HA3	2.43	0.48
1:O:54:SER:CB	1:O:75:ARG:HD2	2.44	0.48
1:Q:142:THR:OG1	1:Q:146:SER:HB2	2.13	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
1:A:54:SER:OG	1:A:75:ARG:HD2	2.13	0.48
2:H:191:PHE:HB3	2:H:192:PRO:HD2	1.95	0.48
2:L:45:ILE:N	2:L:45:ILE:HD12	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
1:F:127:VAL:HG21	1:F:213:LEU:HB3	1.95	0.48
1:M:176:SER:OG	1:M:179:ASP:OD1	2.30	0.48
2:P:14:MET:HE2	2:P:103:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:83:LEU:HD13	2:Z:123:PHE:CZ	2.49	0.48
1:3:368:PHE:HA	1:3:371:PHE:CE2	2.49	0.48
2:E:45:ILE:HD12	2:E:45:ILE:N	2.29	0.48
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.95	0.48
1:Q:35:TYR:HE2	1:Q:40:LEU:HB2	1.79	0.48
1:W:178:THR:HG23	1:W:179:ASP:N	2.29	0.48
1:W:83:ASP:OD2	2:X:65:HIS:CD2	2.62	0.48
2:2:83:LEU:HD13	2:2:123:PHE:CZ	2.48	0.48
2:2:38:ASP:OD1	2:2:41:THR:N	2.46	0.48
1:F:161:GLU:HB2	1:F:162:PRO:HD3	1.95	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:E:14:MET:HE2	2:E:103:LEU:HB3	1.94	0.47
2:H:31:VAL:HG11	2:H:33:LYS:HE3	1.96	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:Z:14:MET:HE2	2:Z:103:LEU:HB3	1.96	0.47
2:4:331:VAL:HG11	2:4:333:LYS:HE3	1.96	0.47
1:A:90:ASP:HB2	1:A:93:ASP:H	1.77	0.47
1:B:231:GLN:HB2	1:B:231:GLN:HE21	1.52	0.47
1:F:163:ILE:HG23	1:F:187:ALA:O	2.14	0.47
2:H:109:ILE:H	2:H:109:ILE:HG12	1.40	0.47
1:W:173:GLU:O	1:W:174:ASN:CB	2.61	0.47
2:X:196:ILE:HG13	2:X:205:VAL:HG22	1.94	0.47
2:X:37:THR:CG2	2:X:59:TYR:HD2	2.27	0.47
1:D:86:GLY:O	1:D:89:TYR:O	2.32	0.47
2:L:1:OZT:H27	2:L:33:LYS:HZ1	1.79	0.47
1:M:176:SER:OG	1:M:178:THR:HG22	2.14	0.47
2:C:144:LEU:HD13	2:R:145:PHE:CE1	2.49	0.47
1:Y:54:SER:CB	1:Y:75:ARG:HD2	2.43	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
2:L:37:THR:OG1	2:L:41:THR:OG1	2.30	0.47
1:S:227:GLY:HA2	1:S:230:LEU:CD1	2.43	0.47
1:S:56:LEU:HD23	1:S:56:LEU:HA	1.72	0.47
2:X:213:LEU:O	2:X:217:ILE:HG13	2.13	0.47
1:Y:30:VAL:HG22	1:Y:43:ALA:HB1	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:TYR:CD2	1:K:171:TYR:C	2.88	0.47
2:L:31:VAL:HG12	2:L:33:LYS:HG3	1.97	0.47
1:M:30:VAL:HG22	1:M:43:ALA:HB1	1.96	0.47
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
1:Y:229:ALA:HA	1:Y:232:ALA:HB3	1.96	0.47
1:Y:55:GLU:CG	1:Y:222:PHE:HB2	2.45	0.47
1:1:141:ILE:HD12	1:1:141:ILE:N	2.29	0.47
2:4:314:MET:HE2	2:4:403:LEU:HB3	1.96	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
2:H:156:GLN:OE1	2:H:165:ARG:NH2	2.47	0.47
1:U:30:VAL:HG22	1:U:43:ALA:HB1	1.96	0.47
2:V:185:ASP:OD1	2:V:188:ARG:HB2	2.14	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:61:GLY:N	1:B:213:LEU:HD21	2.30	0.47
1:D:57:TYR:HB3	1:D:60:VAL:HG13	1.96	0.47
1:F:74:LEU:HD13	1:F:122:LEU:HD21	1.95	0.47
2:N:215:ARG:O	2:N:219:GLU:HG3	2.14	0.47
2:P:14:MET:HE2	2:P:103:LEU:HB3	1.96	0.47
1:Q:182:ARG:HH12	1:Q:234:LEU:CB	2.27	0.47
2:4:498:ASP:OD1	2:4:501:GLY:O	2.33	0.47
1:B:205:VAL:HG23	1:B:206:ALA:H	1.77	0.47
1:B:35:TYR:CE1	1:B:37:GLY:N	2.83	0.47
1:D:167:LEU:O	1:D:168:LYS:C	2.53	0.47
2:E:165:ARG:HA	2:E:213:LEU:HD13	1.96	0.47
2:H:1:OZT:C7	2:H:33:LYS:HZ1	2.27	0.47
1:I:54:SER:CB	1:I:75:ARG:HD2	2.45	0.47
2:J:31:VAL:HG11	2:J:33:LYS:HE3	1.96	0.47
1:I:15:GLU:OE2	1:S:10:GLU:HA	2.15	0.47
2:T:38:ASP:OD1	2:T:39:ASP:N	2.47	0.47
1:U:152:HIS:HB3	1:U:171:TYR:CE2	2.50	0.47
2:J:144:LEU:HD13	2:Z:145:PHE:CE1	2.50	0.47
1:A:179:ASP:O	1:A:183:ILE:HG13	2.15	0.47
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.60	0.47
2:N:132:GLU:HG3	2:N:137:GLN:HB2	1.95	0.47
1:U:11:GLN:HA	1:U:11:GLN:NE2	2.21	0.47
1:1:35:TYR:HD1	1:1:37:GLY:H	1.61	0.47
1:3:529:ALA:O	1:3:533:LEU:HD23	2.15	0.47
2:4:349:ALA:O	2:4:353:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Q:137:GLU:OE1	1:Q:139:TYR:OH	2.29	0.47
2:Z:132:GLU:HA	2:Z:132:GLU:OE1	2.14	0.47
1:B:167:LEU:O	1:B:168:LYS:C	2.54	0.47
1:D:57:TYR:HB3	1:D:60:VAL:CG1	2.45	0.47
1:K:28:LYS:HB3	1:K:44:GLU:HG3	1.97	0.47
1:I:69:ASN:HB3	1:S:104:ALA:HB1	1.96	0.47
1:U:181:LEU:HD23	1:U:233:LEU:CB	2.45	0.47
2:4:306:LEU:HD12	2:4:306:LEU:C	2.36	0.46
1:D:219:ARG:NH2	2:E:64:GLU:CD	2.66	0.46
2:E:65:HIS:CE1	2:E:69:LEU:HD11	2.50	0.46
1:I:182:ARG:HH12	1:I:234:LEU:C	2.17	0.46
1:I:31:VAL:CG1	1:I:33:LEU:HD22	2.45	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
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
2:T:35:TYR:CZ	2:T:53:VAL:HG13	2.50	0.46
1:U:141:ILE:N	1:U:141:ILE:HD12	2.30	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
2:2:198:ASP:OD1	2:2:200:ASP:CB	2.63	0.46
1:3:383:ASP:OD2	2:4:365:HIS:CD2	2.65	0.46
1:B:75:ARG:O	1:B:79:ILE:HG13	2.15	0.46
2:C:196:ILE:HG13	2:C:205:VAL:CG2	2.45	0.46
2:H:83:LEU:HD13	2:H:123:PHE:CZ	2.50	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
1:S:173:GLU:CD	1:S:174:ASN:OD1	2.53	0.46
1:S:227:GLY:O	1:S:230:LEU:CB	2.62	0.46
1:S:79:ILE:HD12	2:T:69:LEU:HD23	1.97	0.46
2:V:31:VAL:HG11	2:V:33:LYS:HE3	1.97	0.46
1:D:35:TYR:HH	1:D:212:VAL:HB	1.80	0.46
2:L:37:THR:HG21	2:L:43:THR:CG2	2.44	0.46
2:V:38:ASP:C	2:V:38:ASP:OD1	2.54	0.46
1:W:128:ALA:HB2	1:W:134:LYS:HB3	1.98	0.46
2:X:65:HIS:CE1	2:X:69:LEU:HD11	2.50	0.46
1:Y:152:HIS:HB3	1:Y:171:TYR:CE2	2.50	0.46
1:3:481:LEU:CD2	1:3:533:LEU:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:GLN:HE22	1:I:14:ARG:HE	1.60	0.46
2:J:109:ILE:H	2:J:109:ILE:HG12	1.46	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
2:X:1:OZT:C7	2:X:33:LYS:HZ3	2.28	0.46
1:Y:177:LEU:C	1:Y:177:LEU:HD12	2.35	0.46
2:Z:132:GLU:HG3	2:Z:137:GLN:HB2	1.96	0.46
2:Z:107:TYR:OH	2:Z:199:ALA:HB2	2.14	0.46
2:4:314:MET:HE2	2:4:403:LEU:HD13	1.96	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
2:E:59:TYR:CE2	2:E:63:LEU:HD11	2.51	0.46
2:H:54:GLU:OE1	2:H:54:GLU:HA	2.15	0.46
2:J:45:ILE:HD12	2:J:45:ILE:N	2.30	0.46
1:K:141:ILE:HD12	1:K:141:ILE:N	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
1:U:62:PHE:C	1:U:62:PHE:CD1	2.89	0.46
1:B:54:SER:OG	1:B:75:ARG:HD2	2.16	0.46
2:C:31:VAL:CG1	2:C:33:LYS:HE3	2.45	0.46
2:G:164:LEU:HD13	2:G:213:LEU:HD12	1.96	0.46
2:G:8:TYR:HB2	2:G:9:PRO:CD	2.45	0.46
2:J:48:THR:OG1	2:J:51:VAL:HG23	2.16	0.46
2:R:169:GLU:HA	2:R:217:ILE:CD1	2.45	0.46
2:R:48:THR:OG1	2:R:51:VAL:HG23	2.16	0.46
1:D:57:TYR:CB	1:D:60:VAL:HG13	2.46	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
1:1:217:ARG:HH21	1:1:223:ARG:HG3	1.81	0.46
1:A:178:THR:HG23	1:A:179:ASP:N	2.30	0.46
1:A:24:ILE:HG22	1:A:157:GLY:HA2	1.97	0.46
2:C:14:MET:HE2	2:C:103:LEU:HD13	1.98	0.46
1:Q:10:GLU:HB2	1:Y:15:GLU:HG2	1.98	0.46
2:T:198:ASP:N	2:T:198:ASP:OD1	2.49	0.46
2:T:31:VAL:HG12	2:T:33:LYS:HG3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:57:TYR:OH	1:1:86:GLY:HA3	2.16	0.46
1:3:341:PHE:CB	1:3:353:ILE:HD13	2.43	0.46
2:4:496:ILE:HG13	2:4:505:VAL:CG2	2.46	0.46
1:F:111:PHE:CG	1:F:111:PHE:O	2.68	0.46
1:Q:30:VAL:HG22	1:Q:43:ALA:HB1	1.98	0.46
2:2:191:PHE:HB3	2:2:192:PRO:HD2	1.98	0.45
1:3:333:LEU:H	1:3:333:LEU:HD23	1.79	0.45
1:F:57:TYR:CB	1:F:60:VAL:HG13	2.47	0.45
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.98	0.45
2:Z:38:ASP:OD1	2:Z:41:THR:N	2.48	0.45
2:4:485:ASP:OD1	2:4:488:ARG:HB2	2.16	0.45
1:A:217:ARG:NH1	1:A:223:ARG:HG3	2.31	0.45
1:A:74:LEU:HA	1:A:74:LEU:HD23	1.64	0.45
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
2:J:164:LEU:HD13	2:J:213:LEU:HD12	1.98	0.45
1:K:70:GLU:HB3	1:K:118:TYR:CD2	2.51	0.45
2:N:83:LEU:HD13	2:N:123:PHE:CE1	2.51	0.45
2:N:38:ASP:OD1	2:N:41:THR:N	2.48	0.45
2:P:156:GLN:OE1	2:P:165:ARG:NH2	2.50	0.45
2:P:37:THR:OG1	2:P:41:THR:OG1	2.32	0.45
1:Y:178:THR:CA	1:Y:233:LEU:HG	2.47	0.45
1:3:509:GLU:OE1	1:3:524:ARG:NH2	2.50	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
2:L:83:LEU:HD13	2:L:123:PHE:CZ	2.51	0.45
2:P:6:LEU:C	2:P:6:LEU:HD12	2.36	0.45
1:Y:33:LEU:HD11	1:Y:180:ALA:HB1	1.98	0.45
1:1:18:GLU:OE1	1:1:18:GLU:HA	2.17	0.45
2:2:14:MET:HE2	2:2:103:LEU:HB3	1.97	0.45
2:4:313:VAL:HG21	2:4:464:LEU:HD23	1.98	0.45
2:C:213:LEU:O	2:C:217:ILE:HG13	2.17	0.45
1:D:217:ARG:HA	1:D:218:PRO:HD3	1.85	0.45
1:D:93:ASP:OD1	2:R:66:TYR:OH	2.24	0.45
1:F:217:ARG:HA	1:F:218:PRO:HD3	1.84	0.45
2:G:218:ILE:HG22	2:G:219:GLU:N	2.31	0.45
1:K:35:TYR:CE1	1:K:37:GLY:N	2.84	0.45
1:M:35:TYR:CD2	1:M:38:GLY:O	2.69	0.45
1:Q:35:TYR:CE2	1:Q:40:LEU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:191:PHE:HB3	2:X:192:PRO:HD2	1.98	0.45
2:2:1:OZT:H17	2:2:33:LYS:HZ1	1.81	0.45
1:F:74:LEU:HA	1:F:74:LEU:HD23	1.46	0.45
2:G:6:LEU:C	2:G:6:LEU:HD12	2.37	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:181:LEU:CD2	1:U:233:LEU:CB	2.95	0.45
1:U:35:TYR:CE2	1:U:38:GLY:O	2.70	0.45
2:Z:198:ASP:N	2:Z:198:ASP:OD1	2.50	0.45
1:1:35:TYR:CD1	1:1:37:GLY:N	2.85	0.45
2:2:156:GLN:OE1	2:2:165:ARG:NH2	2.50	0.45
2:E:191:PHE:HB3	2:E:192:PRO:HD2	1.99	0.45
2:H:1:OZT:H27	2:H:33:LYS:CE	2.47	0.45
2:L:211:ALA:HB1	2:L:215:ARG:NH2	2.32	0.45
2:N:103:LEU:HA	2:N:103:LEU:HD23	1.84	0.45
1:Q:10:GLU:C	1:Q:12:ALA:N	2.66	0.45
2:R:101:LEU:HA	2:R:102:PRO:HD3	1.69	0.45
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.51	0.45
2:V:6:LEU:HD12	2:V:6:LEU:C	2.36	0.45
2:4:464:LEU:HD13	2:4:513:LEU:CD1	2.46	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
2:H:45:ILE:HD12	2:H:45:ILE:N	2.32	0.45
2:H:49:ALA:O	2:H:53:VAL:CG2	2.65	0.45
1:K:20:ALA:O	1:K:24:ILE:HG13	2.17	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
1:O:83:ASP:OD2	2:P:65:HIS:HD2	1.99	0.45
2:X:109:ILE:HG12	2:X:109:ILE:H	1.52	0.45
2:Z:169:GLU:HA	2:Z:217:ILE:CD1	2.46	0.45
2:2:216:ALA:O	2:2:220:SER:HB3	2.16	0.45
2:G:101:LEU:HA	2:G:102:PRO:HD3	1.71	0.45
2:G:49:ALA:O	2:G:53:VAL:CG2	2.65	0.45
2:H:185:ASP:OD1	2:H:188:ARG:HB2	2.17	0.45
1:M:127:VAL:HG12	1:M:128:ALA:N	2.31	0.45
1:M:41:PHE:CB	1:M:53:ILE:HD13	2.45	0.45
1:Q:56:LEU:HA	1:Q:56:LEU:HD23	1.79	0.45
1:U:217:ARG:HH21	1:U:223:ARG:HG3	1.80	0.45
2:Z:54:GLU:OE1	2:Z:54:GLU:HA	2.16	0.45
2:4:349:ALA:O	2:4:353:VAL:CG2	2.65	0.45
1:D:56:LEU:HA	1:D:56:LEU:HD23	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:225:ILE:CG2	1:O:229:ALA:HB1	2.47	0.45
1:Q:141:ILE:N	1:Q:141:ILE:HD12	2.32	0.45
2:R:103:LEU:HD23	2:R:103:LEU:HA	1.85	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
1:1:30:VAL:HG22	1:1:43:ALA:HB1	1.99	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
2:N:171:LEU:HA	2:N:171:LEU:HD23	1.77	0.45
2:R:31:VAL:HG11	2:R:33:LYS:HE3	1.98	0.45
1:S:233:LEU:HD23	1:S:233:LEU:HA	1.70	0.45
1:W:123:CYS:HA	1:W:139:TYR:O	2.17	0.45
1:W:69:ASN:HB3	1:Y:104:ALA:HB1	1.97	0.45
2:X:1:OZT:H17	2:X:33:LYS:HZ3	1.82	0.45
2:X:37:THR:HG23	2:X:43:THR:HG23	1.99	0.45
1:1:226:THR:CG2	1:1:227:GLY:N	2.80	0.44
2:C:49:ALA:O	2:C:53:VAL:HG23	2.17	0.44
1:K:62:PHE:CD1	1:K:62:PHE:C	2.90	0.44
1:Q:57:TYR:OH	1:Q:86:GLY:HA3	2.17	0.44
2:T:31:VAL:CG1	2:T:33:LYS:HE3	2.47	0.44
2:V:83:LEU:HD13	2:V:123:PHE:CE1	2.52	0.44
2:V:48:THR:OG1	2:V:51:VAL:HG23	2.17	0.44
2:X:156:GLN:OE1	2:X:165:ARG:NH2	2.51	0.44
2:X:83:LEU:HD13	2:X:123:PHE:CE1	2.52	0.44
2:2:31:VAL:HG11	2:2:33:LYS:HE3	2.00	0.44
2:4:491:PHE:HB3	2:4:492:PRO:HD2	1.99	0.44
1:I:161:GLU:N	1:I:162:PRO:CD	2.80	0.44
1:O:167:LEU:O	1:O:168:LYS:C	2.55	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
1:S:230:LEU:HD23	1:S:231:GLN:CA	2.46	0.44
2:T:156:GLN:OE1	2:T:165:ARG:NH2	2.50	0.44
2:Z:156:GLN:OE1	2:Z:165:ARG:NH2	2.51	0.44
2:H:145:PHE:CE1	2:E:144:LEU:HD13	2.52	0.44
2:H:101:LEU:HA	2:H:102:PRO:HD3	1.63	0.44
2:J:14:MET:HE2	2:J:103:LEU:HD13	1.99	0.44
2:L:49:ALA:O	2:L:53:VAL:CG2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:168:VAL:HG12	2:N:217:ILE:CD1	2.47	0.44
2:N:1:OZT:H27	2:N:33:LYS:NZ	2.31	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
1:3:451:PRO:HB3	3:3:110:HOH:O	2.17	0.44
2:4:432:GLU:HG3	2:4:437:GLN:HB2	1.99	0.44
1:A:59:ARG:NH2	1:A:221:ALA:HB2	2.32	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
1:I:129:HIS:HB2	1:I:132:GLU:HG2	1.99	0.44
1:D:116:LYS:HB2	1:K:13:MET:HE2	2.00	0.44
1:K:30:VAL:HG22	1:K:43:ALA:HB1	1.98	0.44
2:N:58:LEU:O	2:N:58:LEU:HD12	2.17	0.44
1:O:225:ILE:CG2	1:O:229:ALA:CB	2.95	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
1:3:526:THR:CG2	1:3:527:GLY:N	2.78	0.44
1:F:212:VAL:O	1:F:212:VAL:HG23	2.17	0.44
1:F:230:LEU:O	1:F:231:GLN:C	2.55	0.44
2:L:185:ASP:OD1	2:L:188:ARG:HB2	2.17	0.44
2:L:31:VAL:CG1	2:L:33:LYS:HE3	2.48	0.44
2:R:45:ILE:HD12	2:R:45:ILE:N	2.32	0.44
1:S:49:SER:HB2	1:1:97:ARG:CG	2.46	0.44
2:V:109:ILE:HG12	2:V:109:ILE:H	1.47	0.44
1:3:362:PHE:CD1	1:3:362:PHE:C	2.91	0.44
2:4:505:VAL:HA	2:4:506:PRO:HD3	1.83	0.44
1:B:10:GLU:C	1:B:12:ALA:H	2.15	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
2:L:213:LEU:O	2:L:217:ILE:HG13	2.17	0.44
1:Q:31:VAL:CG1	1:Q:33:LEU:CD2	2.94	0.44
1:1:79:ILE:HD12	2:2:69:LEU:HD23	2.00	0.44
2:E:31:VAL:CG1	2:E:33:LYS:HE3	2.48	0.44
1:F:207:SER:O	1:F:208:LEU:HD23	2.18	0.44
2:H:48:THR:OG1	2:H:51:VAL:HG23	2.16	0.44
1:I:62:PHE:CD1	1:I:62:PHE:C	2.90	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
2:X:103:LEU:HA	2:X:103:LEU:HD23	1.85	0.44
2:X:49:ALA:O	2:X:53:VAL:HG23	2.17	0.44
2:Z:194:ALA:HB3	2:Z:210:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:330:VAL:HG13	1:3:343:ALA:HB2	1.99	0.44
2:4:440:GLY:O	2:4:443:SER:HB3	2.18	0.44
2:E:107:TYR:CB	2:E:197:ILE:HG22	2.38	0.44
2:H:13:VAL:HG21	2:H:164:LEU:HD23	1.99	0.44
2:L:1:OZT:H17	2:L:17:ASP:CG	2.38	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
2:T:19:ARG:HH11	2:T:26:ILE:CD1	2.31	0.44
1:W:30:VAL:HG13	1:W:43:ALA:HB2	2.00	0.44
1:Y:138:LEU:N	1:Y:138:LEU:HD12	2.33	0.44
1:1:56:LEU:HD23	1:1:56:LEU:HA	1.84	0.44
2:E:61:VAL:HG12	2:E:61:VAL:O	2.17	0.44
1:F:48:ARG:HH22	1:W:135:ARG:NH1	2.16	0.44
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.53	0.44
1:K:167:LEU:O	1:K:168:LYS:C	2.57	0.44
1:K:97:ARG:NH1	3:K:249:HOH:O	2.50	0.44
2:N:6:LEU:HD12	2:N:6:LEU:C	2.38	0.44
2:T:109:ILE:HG12	2:T:109:ILE:H	1.43	0.44
2:T:132:GLU:HG3	2:T:137:GLN:HB2	2.00	0.44
1:U:178:THR:HB	1:U:233:LEU:CD2	2.48	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:181:LEU:HA	1:F:181:LEU:HD12	1.76	0.43
1:F:35:TYR:CD2	1:F:40:LEU:HB2	2.53	0.43
2:P:65:HIS:CE1	2:P:69:LEU:HD11	2.53	0.43
1:S:163:ILE:HG23	1:S:187:ALA:O	2.18	0.43
1:1:114:GLN:HB3	1:1:114:GLN:HE21	1.60	0.43
1:B:130:TYR:HE1	1:B:216:ASN:O	2.00	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
2:E:132:GLU:HA	2:E:132:GLU:OE1	2.18	0.43
2:H:8:TYR:C	2:H:8:TYR:CD1	2.91	0.43
1:I:208:LEU:HA	1:I:208:LEU:HD23	1.69	0.43
1:S:62:PHE:C	1:S:62:PHE:CD1	2.91	0.43
2:T:37:THR:HG23	2:T:43:THR:HG23	1.97	0.43
2:V:54:GLU:HA	2:V:54:GLU:OE1	2.18	0.43
1:W:62:PHE:CD1	1:W:62:PHE:C	2.91	0.43
1:Y:163:ILE:HG23	1:Y:187:ALA:HB1	2.00	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
2:E:198:ASP:C	2:E:198:ASP:OD1	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:198:ASP:N	2:J:198:ASP:OD1	2.51	0.43
2:N:191:PHE:HB3	2:N:192:PRO:HD2	2.00	0.43
2:N:65:HIS:CE1	2:N:69:LEU:HD11	2.53	0.43
1:U:210:VAL:HG12	1:U:225:ILE:HD12	2.00	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: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:B:205:VAL:HG22	1:B:207:SER:OG	2.18	0.43
2:C:31:VAL:HG12	2:C:33:LYS:HG3	2.00	0.43
1:D:94:VAL:HA	1:D:98:GLN:NE2	2.33	0.43
1:M:129:HIS:HB2	1:M:132:GLU:CG	2.48	0.43
2:N:113:ASP:HA	2:N:114:PRO:HD3	1.86	0.43
2:E:50:ALA:HB2	2:R:129:TRP:O	2.18	0.43
1:U:123:CYS:HA	1:U:139:TYR:O	2.18	0.43
1:A:56:LEU:HD11	1:A:62:PHE:HB2	1.98	0.43
2:E:76:PHE:CE2	2:E:80:ILE:HD11	2.53	0.43
2:G:14:MET:HE2	2:G:103:LEU:HB3	2.00	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
1:3:335:TYR:CE1	1:3:338:GLY:N	2.87	0.43
1:A:151:PRO:HD2	3:A:249:HOH:O	2.19	0.43
1:B:156:MET:HE2	1:B:156:MET:HB2	1.87	0.43
1:B:181:LEU:HA	1:B:181:LEU:HD12	1.80	0.43
2:E:1:OZT:H27	2:E:33:LYS:HZ1	1.83	0.43
1:I:83:ASP:OD2	2:J:65:HIS:CD2	2.69	0.43
1:M:212:VAL:HG23	1:M:223:ARG:HB3	2.01	0.43
2:N:31:VAL:HG12	2:N:33:LYS:HG3	2.01	0.43
1:S:141:ILE:N	1:S:141:ILE:HD12	2.34	0.43
2:T:45:ILE:N	2:T:45:ILE:HD12	2.34	0.43
1:W:209:GLU:OE1	1:W:224:ARG:NH2	2.52	0.43
1:Y:208:LEU:HA	1:Y:208:LEU:HD23	1.75	0.43
1:Y:58:ASP:OD1	1:Y:219:ARG:NH1	2.51	0.43
1:1:18:GLU:O	1:1:22:LYS:HG3	2.18	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
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
1:Q:62:PHE:C	1:Q:62:PHE:CD1	2.92	0.43
1:S:90:ASP:OD2	1:S:93:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:144:LEU:HA	2:T:144:LEU:HD22	1.88	0.43
2:X:134:GLU:OE2	2:Z:29:ARG:NH1	2.51	0.43
2:X:35:TYR:CZ	2:X:53:VAL:HG13	2.53	0.43
2:Z:37:THR:HG21	2:Z:43:THR:CG2	2.47	0.43
2:2:8:TYR:HB2	2:2:9:PRO:CD	2.49	0.43
2:4:308:TYR:HB2	2:4:309:PRO:CD	2.49	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
2:E:19:ARG:HG3	2:E:20:SER:H	1.83	0.43
1:K:49:SER:O	1:K:51:GLN:OE1	2.36	0.43
2:N:156:GLN:OE1	2:N:165:ARG:NH2	2.52	0.43
2:N:54:GLU:OE1	2:N:54:GLU:HA	2.18	0.43
2:T:164:LEU:HD13	2:T:213:LEU:HD11	2.00	0.43
1:U:178:THR:HB	1:U:233:LEU:HD22	2.00	0.43
2:Z:31:VAL:HG11	2:Z:33:LYS:HE3	1.99	0.43
2:4:456:GLN:OE1	2:4:465:ARG:NH2	2.51	0.43
2:C:3:ILE:HG22	2:C:4:VAL:N	2.34	0.43
2:G:38:ASP:OD1	2:G:41:THR:N	2.52	0.43
2:H:76:PHE:HE2	2:H:80:ILE:HD11	1.82	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
2:E:29:ARG:NH1	2:R:134:GLU:OE2	2.52	0.43
2:R:37:THR:HG21	2:R:43:THR:CG2	2.49	0.43
1:S:210:VAL:HG12	1:S:225:ILE:HD12	2.01	0.43
2:T:107:TYR:HB2	2:T:197:ILE:HG22	2.00	0.43
2:V:144:LEU:HA	2:V:144:LEU:HD22	1.81	0.43
2:V:191:PHE:N	2:V:191:PHE:CD1	2.86	0.43
2:X:37:THR:HG21	2:X:59:TYR:CD2	2.47	0.43
1:1:57:TYR:O	1:1:58:ASP:C	2.56	0.42
1:3:330:VAL:HG22	1:3:343:ALA:HB1	2.01	0.42
1:D:219:ARG:NH2	1:D:220:ARG:CD	2.69	0.42
2:G:164:LEU:HA	2:G:164:LEU:HD23	1.91	0.42
2:J:6:LEU:C	2:J:6:LEU:HD12	2.40	0.42
2:L:101:LEU:HA	2:L:102:PRO:HD3	1.72	0.42
1:M:90:ASP:OD2	1:M:93:ASP:N	2.52	0.42
2:N:107:TYR:HB2	2:N:197:ILE:HG22	2.00	0.42
1:Q:90:ASP:OD2	1:Q:93:ASP:N	2.52	0.42
2:V:14:MET:CE	2:V:103:LEU:HD13	2.49	0.42
2:Z:109:ILE:HG12	2:Z:109:ILE:H	1.51	0.42
2:2:49:ALA:O	2:2:53:VAL:CG2	2.67	0.42
1:3:311:GLN:HG3	1:3:314:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:CZ	1:A:135:ARG:HB3	2.48	0.42
1:A:130:TYR:HE1	1:A:216:ASN:O	2.00	0.42
2:C:6:LEU:C	2:C:6:LEU:HD12	2.39	0.42
2:J:14:MET:HE2	2:J:103:LEU:HB3	2.01	0.42
2:J:144:LEU:HD22	2:J:144:LEU:HA	1.88	0.42
1:O:208:LEU:HD23	1:O:208:LEU:HA	1.66	0.42
1:Q:208:LEU:HD23	1:Q:208:LEU:HA	1.71	0.42
2:R:156:GLN:OE1	2:R:165:ARG:NH2	2.52	0.42
2:C:151:LYS:HE2	2:R:221:ARG:HH12	1.83	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:A:33:LEU:HD23	1:A:40:LEU:HB3	2.01	0.42
2:E:101:LEU:HA	2:E:102:PRO:HD3	1.70	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
2:R:6:LEU:HD12	2:R:6:LEU:C	2.39	0.42
2:T:185:ASP:OD1	2:T:188:ARG:HB2	2.19	0.42
1:Y:167:LEU:O	1:Y:168:LYS:C	2.57	0.42
1:1:90:ASP:HA	3:1:6:HOH:O	2.19	0.42
1:3:430:TYR:CE1	1:3:516:ASN:O	2.72	0.42
1:A:205:VAL:HG23	1:A:206:ALA:H	1.79	0.42
2:C:109:ILE:H	2:C:109:ILE:HG12	1.58	0.42
1:D:45:ASN:HD22	1:D:209:GLU:HG3	1.84	0.42
1:F:156:MET:HE2	1:F:156:MET:HB2	1.71	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:123:CYS:HA	1:Y:139:TYR:O	2.19	0.42
2:2:65:HIS:CE1	2:2:69:LEU:HD11	2.55	0.42
1:3:427:VAL:HG13	1:3:428:ALA:N	2.33	0.42
1:A:35:TYR:CE2	1:A:38:GLY:C	2.93	0.42
1:D:71:PHE:CD1	1:D:71:PHE:C	2.92	0.42
2:E:13:VAL:HG21	2:E:164:LEU:HD23	2.01	0.42
2:G:58:LEU:O	2:G:58:LEU:HD12	2.20	0.42
2:H:144:LEU:HA	2:H:144:LEU:HD22	1.86	0.42
1:K:90:ASP:OD2	1:K:93:ASP:N	2.52	0.42
1:M:35:TYR:CZ	1:M:37:GLY:HA3	2.40	0.42
2:R:31:VAL:CG1	2:R:33:LYS:HE3	2.50	0.42
2:R:66:TYR:C	2:R:66:TYR:CD2	2.93	0.42
1:I:48:ARG:NH2	1:S:137:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:ASP:OD2	1:I:93:ASP:N	2.52	0.42
1:A:56:LEU:HA	1:A:56:LEU:HD23	1.92	0.42
1:A:79:ILE:HD12	2:H:69:LEU:HD23	2.01	0.42
2:C:37:THR:HG23	2:C:43:THR:HG23	2.01	0.42
1:D:74:LEU:HD13	1:D:122:LEU:HD21	2.02	0.42
2:E:37:THR:CG2	2:E:43:THR:HG23	2.48	0.42
1:I:130:TYR:C	1:I:130:TYR:CD2	2.93	0.42
2:L:164:LEU:HD13	2:L:213:LEU:HD12	2.02	0.42
1:M:163:ILE:HD13	1:M:188:LEU:HD23	2.01	0.42
1:S:57:TYR:O	1:S:58:ASP:C	2.58	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:HD2	2:V:82:ARG:HA	1.84	0.42
1:Y:36:ALA:HB2	1:Y:174:ASN:CA	2.42	0.42
2:Z:6:LEU:HD12	2:Z:6:LEU:C	2.40	0.42
2:2:31:VAL:HG12	2:2:33:LYS:HG3	2.01	0.42
2:C:214:ALA:O	2:C:218:ILE:HG13	2.20	0.42
1:D:141:ILE:N	1:D:141:ILE:HD12	2.34	0.42
1:K:35:TYR:CE2	1:K:38:GLY:O	2.72	0.42
2:L:54:GLU:HA	2:L:54:GLU:OE1	2.20	0.42
2:V:14:MET:HE2	2:V:103:LEU:HB3	2.01	0.42
2:X:45:ILE:HD12	2:X:45:ILE:N	2.34	0.42
2:Z:80:ILE:CD1	2:Z:121:VAL:HG21	2.49	0.42
2:X:178:ASP:OD1	2:2:24:ASN:HB3	2.19	0.42
1:3:428:ALA:HB2	1:3:434:LYS:HB3	2.01	0.42
1:A:56:LEU:HG	1:A:62:PHE:HB2	2.01	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
2:E:103:LEU:HA	2:E:103:LEU:HD23	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
1:F:80:GLN:HE21	1:F:80:GLN:HB3	1.62	0.42
2:H:37:THR:HG23	2:H:43:THR:HG23	2.02	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:O:163:ILE:HG23	1:O:187:ALA:C	2.39	0.42
2:P:1:OZT:O	2:P:140:GLY:HA3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:20:SER:HB3	2:T:31:VAL:HG21	2.01	0.42
1:1:56:LEU:HB2	1:1:60:VAL:HG22	2.02	0.42
1:3:390:ASP:OD2	1:3:393:ASP:N	2.53	0.42
1:B:217:ARG:HB3	1:B:217:ARG:NH1	2.29	0.42
2:C:13:VAL:HG21	2:C:164:LEU:HD23	2.01	0.42
1:D:214:ASP:OD1	1:D:214:ASP:C	2.58	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
1:I:16:ARG:HH21	1:I:111:PHE:C	2.21	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
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
2:2:168:VAL:HG12	2:2:217:ILE:HD12	2.02	0.42
1:B:16:ARG:NH2	1:B:111:PHE:C	2.72	0.42
1:D:56:LEU:HD11	1:D:62:PHE:HB2	2.01	0.42
1:F:130:TYR:CE1	1:F:216:ASN:O	2.73	0.42
2:H:205:VAL:HA	2:H:206:PRO:HD3	1.81	0.42
2:H:31:VAL:CG1	2:H:33:LYS:HE3	2.50	0.42
1:O:107:LEU:HA	1:O:107:LEU:HD23	1.86	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
1:Y:30:VAL:HG22	1:Y:43:ALA:CB	2.50	0.42
1:D:35:TYR:OH	1:D:212:VAL:HG12	2.19	0.41
2:E:213:LEU:O	2:E:217:ILE:HG13	2.20	0.41
1:K:30:VAL:HG12	1:K:31:VAL:N	2.35	0.41
2:R:65:HIS:CE1	2:R:69:LEU:HD11	2.54	0.41
1:Y:213:LEU:HA	1:Y:213:LEU:HD12	1.95	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
2:2:185:ASP:OD1	2:2:188:ARG:HB2	2.20	0.41
2:2:6:LEU:C	2:2:6:LEU:HD12	2.40	0.41
2:C:45:ILE:N	2:C:45:ILE:HD12	2.35	0.41
1:M:127:VAL:HG11	1:M:215:ALA:CB	2.45	0.41
2:R:218:ILE:O	2:R:218:ILE:CG2	2.68	0.41
1:S:178:THR:HB	1:S:233:LEU:HD22	2.00	0.41
2:V:219:GLU:O	2:V:223:GLY:C	2.59	0.41
2:X:49:ALA:O	2:X:53:VAL:CG2	2.69	0.41
1:3:330:VAL:HG12	1:3:331:VAL:N	2.35	0.41
1:A:23:GLY:HA3	1:A:119:GLU:OE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ALA:HB2	1:A:134:LYS:HB3	2.01	0.41
1:A:35:TYR:CE2	1:A:38:GLY:O	2.72	0.41
2:G:37:THR:HG23	2:G:43:THR:HG23	2.01	0.41
1:I:47:SER:HB2	1:S:149:ASP:OD1	2.20	0.41
2:L:76:PHE:CE2	2:L:80:ILE:HD11	2.55	0.41
1:O:126:GLU:HG2	1:O:127:VAL:N	2.35	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
2:Z:49:ALA:O	2:Z:53:VAL:HG23	2.20	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
2:H:165:ARG:CG	2:H:213:LEU:HD22	2.43	0.41
2:H:1:OZT:H27	2:H:33:LYS:NZ	2.33	0.41
2:J:185:ASP:OD1	2:J:188:ARG:HB2	2.21	0.41
2:J:31:VAL:CG1	2:J:33:LYS:HE3	2.49	0.41
1:M:35:TYR:CE2	1:M:177:LEU:HD13	2.55	0.41
2:N:205:VAL:HA	2:N:206:PRO:HD3	1.84	0.41
1:Q:10:GLU:CD	1:Y:15:GLU:HG2	2.40	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
2:2:45:ILE:HD12	2:2:45:ILE:N	2.34	0.41
1:D:207:SER:O	1:D:208:LEU:HD23	2.21	0.41
1:F:167:LEU:O	1:F:168:LYS:C	2.57	0.41
2:G:33:LYS:O	2:G:44:GLY:HA2	2.20	0.41
2:G:54:GLU:HA	2:G:54:GLU:OE1	2.20	0.41
1:I:230:LEU:HA	1:I:230:LEU:HD23	1.80	0.41
1:A:10:GLU:N	1:O:15:GLU:OE2	2.53	0.41
1:O:56:LEU:HB2	1:O:60:VAL:HG22	2.03	0.41
1:Q:167:LEU:O	1:Q:168:LYS:C	2.59	0.41
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	2.03	0.41
1:Y:229:ALA:O	1:Y:232:ALA:HB3	2.20	0.41
1:Y:35:TYR:CE2	1:Y:38:GLY:O	2.73	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:H:191:PHE:HB3	2:H:192:PRO:CD	2.51	0.41
1:I:48:ARG:HH21	1:S:137:GLU:HG2	1.80	0.41
2:J:107:TYR:HB2	2:J:197:ILE:HG22	2.01	0.41
1:O:62:PHE:CD1	1:O:62:PHE:C	2.93	0.41
2:P:76:PHE:CE2	2:P:80:ILE:HD11	2.56	0.41
2:P:8:TYR:HB2	2:P:9:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:49:ALA:O	2:T:53:VAL:CG2	2.69	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
2:X:25:MET:HG2	2:2:145:PHE:HZ	1.85	0.41
1:3:430:TYR:HE1	1:3:516:ASN:O	2.03	0.41
1:D:13:MET:HE2	1:D:13:MET:HA	2.03	0.41
1:D:53:ILE:HG22	1:D:54:SER:N	2.34	0.41
2:E:61:VAL:O	2:E:61:VAL:CG1	2.68	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:N	1:O:141:ILE:HD12	2.35	0.41
1:A:10:GLU:HA	1:O:15:GLU:OE2	2.20	0.41
1:S:35:TYR:HD1	1:S:36:ALA:N	2.19	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
2:2:1:OZT:C7	2:2:33:LYS:HZ1	2.34	0.41
2:E:31:VAL:HG12	2:E:33:LYS:HG3	2.03	0.41
2:H:45:ILE:CD1	3:H:241:HOH:O	2.69	0.41
1:K:58:ASP:HB3	1:K:219:ARG:O	2.21	0.41
2:L:83:LEU:HD13	2:L:123:PHE:CE1	2.55	0.41
1:M:167:LEU:O	1:M:168:LYS:C	2.58	0.41
1:M:127:VAL:HG13	1:M:215:ALA:HB2	1.96	0.41
2:P:171:LEU:HD23	2:P:171:LEU:HA	1.87	0.41
1:W:114:GLN:HB3	1:W:114:GLN:HE21	1.59	0.41
2:Z:45:ILE:HG21	2:Z:100:ALA:HB1	2.03	0.41
2:2:54:GLU:OE1	2:2:54:GLU:HA	2.21	0.41
1:D:12:ALA:HB3	1:D:13:MET:HE1	2.01	0.41
1:D:123:CYS:HA	1:D:139:TYR:O	2.20	0.41
1:K:147:ILE:HG21	1:K:147:ILE:HD13	1.84	0.41
1:K:56:LEU:HB2	1:K:60:VAL:HG22	2.02	0.41
1:O:30:VAL:HG22	1:O:43:ALA:HB1	2.03	0.41
1:Q:17:SER:HA	1:Q:143:TYR:HE2	1.85	0.41
1:D:10:GLU:HG2	1:Q:19:LEU:HD13	2.03	0.41
2:R:191:PHE:CD2	2:R:211:ALA:HA	2.55	0.41
1:S:227:GLY:CA	1:S:230:LEU:CB	2.77	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
1:Y:173:GLU:HG3	1:Y:174:ASN:CG	2.38	0.41
2:2:38:ASP:OD1	2:2:39:ASP:N	2.54	0.41
1:3:354:SER:CB	1:3:375:ARG:HD2	2.51	0.41
2:4:409:ILE:H	2:4:409:ILE:HG12	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:164:LEU:HD13	2:C:213:LEU:HD12	2.02	0.41
1:F:176:SER:OG	1:F:178:THR:HG23	2.21	0.41
2:G:187:VAL:HG13	2:V:221:ARG:HB3	2.01	0.41
1:M:19:LEU:HD21	1:M:116:LYS:HG3	2.03	0.41
1:O:128:ALA:HB2	1:O:134:LYS:HB3	2.03	0.41
1:O:123:CYS:HA	1:O:139:TYR:O	2.21	0.41
1:O:161:GLU:N	1:O:162:PRO:CD	2.84	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
2:P:31:VAL:HG11	2:P:33:LYS:HE3	2.03	0.41
1:S:121:GLU:HG2	1:S:156:MET:HG2	2.03	0.41
2:T:218:ILE:HG22	2:T:219:GLU:N	2.36	0.41
1:U:181:LEU:HD23	1:U:233:LEU:C	2.40	0.41
1:U:79:ILE:HD13	2:V:68:LYS:HB3	2.01	0.41
2:V:130:ASN:C	2:V:130:ASN:HD22	2.23	0.41
2:V:64:GLU:O	2:V:65:HIS:C	2.59	0.41
2:Z:205:VAL:HA	2:Z:206:PRO:HD3	1.81	0.41
1:A:207:SER:O	1:A:208:LEU:HD23	2.21	0.41
1:B:161:GLU:N	1:B:162:PRO:CD	2.83	0.41
1:B:33:LEU:HD23	1:B:33:LEU:O	2.20	0.41
2:C:37:THR:HG21	2:C:59:TYR:HD2	1.86	0.41
1:D:181:LEU:CD2	1:D:233:LEU:HD21	2.46	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
1:O:59:ARG:HA	1:O:59:ARG:HD2	1.98	0.41
2:T:6:LEU:HD12	2:T:6:LEU:C	2.40	0.41
1:K:123:CYS:HA	1:K:139:TYR:O	2.21	0.40
1:K:182:ARG:HH12	1:K:234:LEU:C	2.25	0.40
1:M:62:PHE:C	1:M:62:PHE:CD1	2.94	0.40
2:R:40:TYR:CE1	2:R:109:ILE:HD13	2.56	0.40
1:S:30:VAL:HG12	1:S:31:VAL:N	2.36	0.40
2:T:144:LEU:HD13	2:X:145:PHE:CE1	2.55	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
2:X:54:GLU:HA	2:X:54:GLU:OE1	2.21	0.40
1:A:130:TYR:CD1	1:A:216:ASN:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:VAL:HA	2:C:206:PRO:HD3	1.86	0.40
2:C:49:ALA:O	2:C:53:VAL:CG2	2.69	0.40
1:D:167:LEU:HA	1:D:167:LEU:HD23	1.86	0.40
2:G:35:TYR:CZ	2:G:53:VAL:HG13	2.56	0.40
2:H:65:HIS:CE1	2:H:69:LEU:HD11	2.56	0.40
2:N:101:LEU:HA	2:N:102:PRO:HD3	1.69	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
2:V:103:LEU:HA	2:V:103:LEU:HD23	1.83	0.40
2:V:37:THR:HG23	2:V:43:THR:HG23	2.04	0.40
1:W:161:GLU:N	1:W:162:PRO:CD	2.85	0.40
1:W:56:LEU:HA	1:W:56:LEU:HD23	1.81	0.40
1:1:152:HIS:CD2	1:1:171:TYR:HE2	2.39	0.40
2:2:164:LEU:HD13	2:2:213:LEU:HD12	2.02	0.40
2:4:403:LEU:HA	2:4:403:LEU:HD23	1.80	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:P:54:GLU:HA	2:P:54:GLU:OE1	2.21	0.40
1:Q:56:LEU:HD13	1:Q:99:LEU:HD13	2.02	0.40
1:U:175:ALA:C	1:U:176:SER:O	2.60	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
1:1:231:GLN:HG3	1:1:234:LEU:HD12	2.03	0.40
2:2:164:LEU:HA	2:2:164:LEU:HD23	1.92	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
1:B:31:VAL:HG22	1:B:155:VAL:HG22	2.03	0.40
2:C:191:PHE:HB3	2:C:192:PRO:HD2	2.03	0.40
1:D:12:ALA:C	1:D:13:MET:CE	2.74	0.40
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
2:E:8:TYR:HB2	2:E:9:PRO:CD	2.52	0.40
1:F:161:GLU:H	1:F:161:GLU:CD	2.25	0.40
1:K:151:PRO:HD2	1:K:152:HIS:H	1.85	0.40
2:N:73:PRO:HA	3:N:241:HOH:O	2.21	0.40
1:O:23:GLY:HA2	1:O:26:ARG:HD3	2.04	0.40
2:R:164:LEU:HA	2:R:164:LEU:HD23	1.95	0.40
2:R:49:ALA:O	2:R:53:VAL:HG23	2.20	0.40
1:S:225:ILE:CG2	1:S:230:LEU:HB2	2.34	0.40
2:X:58:LEU:HD12	2:X:58:LEU:O	2.21	0.40
1:Y:116:LYS:HA	1:Y:117:PRO:HD2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:3:340:LEU:HD13	1:3:512:VAL:HG12	2.02	0.40
1:A:233:LEU:HD12	1:A:233:LEU:N	2.37	0.40
2:C:113:ASP:HA	2:C:114:PRO:HD3	1.82	0.40
2:H:191:PHE:N	2:H:191:PHE:CD1	2.89	0.40
2:J:103:LEU:HD23	2:J:103:LEU:HA	1.86	0.40
2:J:31:VAL:HG12	2:J:33:LYS:HG3	2.03	0.40
1:M:152:HIS:CG	1:M:171:TYR:CE2	3.09	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
2:N:45:ILE:HD13	3:N:243:HOH:O	2.19	0.40
1:Q:230:LEU:C	1:Q:230:LEU:CD2	2.87	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
2:Z:80:ILE:HD11	2:Z:121:VAL:HG21	2.04	0.40
2:Z:76:PHE:CE2	2:Z:80:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	29	59
1	3	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	29	59
1	A	207/240 (86%)	189 (91%)	18 (9%)	0	100	100
1	B	207/240 (86%)	187 (90%)	19 (9%)	1 (0%)	29	59
1	D	206/240 (86%)	185 (90%)	21 (10%)	0	100	100
1	F	189/240 (79%)	170 (90%)	18 (10%)	1 (0%)	29	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	208/240 (87%)	199 (96%)	8 (4%)	1 (0%)	29	59
1	K	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	29	59
1	M	201/240 (84%)	190 (94%)	11 (6%)	0	100	100
1	O	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
1	Q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	S	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	U	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	W	189/240 (79%)	175 (93%)	13 (7%)	1 (0%)	29	59
1	Y	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	29	59
1	a	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
1	b	207/240 (86%)	193 (93%)	13 (6%)	1 (0%)	29	59
1	d	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	29	59
1	f	207/240 (86%)	190 (92%)	16 (8%)	1 (0%)	29	59
1	i	207/240 (86%)	195 (94%)	11 (5%)	1 (0%)	29	59
1	k	207/240 (86%)	199 (96%)	7 (3%)	1 (0%)	29	59
1	m	204/240 (85%)	190 (93%)	13 (6%)	1 (0%)	29	59
1	o	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	29	59
1	s	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	29	59
1	u	207/240 (86%)	198 (96%)	8 (4%)	1 (0%)	29	59
1	w	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
1	y	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	29	59
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	59
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%)	47	76

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
1	O	151	PRO
1	Q	151	PRO
1	S	151	PRO
1	U	151	PRO
1	Y	151	PRO

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Mol	Chain	Res	Type
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	l	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	3	161/184 (88%)	150 (93%)	11 (7%)	16	40
1	A	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	B	162/184 (88%)	141 (87%)	21 (13%)	4	11
1	D	161/184 (88%)	143 (89%)	18 (11%)	6	16
1	F	149/184 (81%)	132 (89%)	17 (11%)	5	16
1	I	163/184 (89%)	150 (92%)	13 (8%)	12	32
1	K	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	M	158/184 (86%)	151 (96%)	7 (4%)	28	59
1	O	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	Q	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	S	162/184 (88%)	150 (93%)	12 (7%)	13	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	W	148/184 (80%)	139 (94%)	9 (6%)	18	45
1	Y	161/184 (88%)	149 (92%)	12 (8%)	13	35
1	a	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	b	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	d	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	f	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	i	162/184 (88%)	150 (93%)	12 (7%)	13	36
1	k	162/184 (88%)	152 (94%)	10 (6%)	18	45
1	m	160/184 (87%)	151 (94%)	9 (6%)	21	49
1	o	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	q	162/184 (88%)	149 (92%)	13 (8%)	12	32
1	s	162/184 (88%)	153 (94%)	9 (6%)	21	49
1	u	162/184 (88%)	154 (95%)	8 (5%)	25	55
1	w	162/184 (88%)	151 (93%)	11 (7%)	16	40
1	y	162/184 (88%)	147 (91%)	15 (9%)	9	25
2	2	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	4	161/177 (91%)	148 (92%)	13 (8%)	11	31
2	C	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	E	161/177 (91%)	149 (92%)	12 (8%)	13	35
2	G	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	H	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	J	161/177 (91%)	149 (92%)	12 (8%)	13	35
2	L	161/177 (91%)	143 (89%)	18 (11%)	6	16
2	N	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	P	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	R	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	T	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	V	161/177 (91%)	143 (89%)	18 (11%)	6	16
2	X	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	Z	161/177 (91%)	147 (91%)	14 (9%)	10	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	e	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	g	161/177 (91%)	147 (91%)	14 (9%)	10	28
2	h	160/177 (90%)	145 (91%)	15 (9%)	8	24
2	j	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	l	161/177 (91%)	146 (91%)	15 (9%)	9	25
2	n	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	p	161/177 (91%)	148 (92%)	13 (8%)	11	31
2	r	161/177 (91%)	148 (92%)	13 (8%)	11	31
2	t	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	v	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	x	161/177 (91%)	145 (90%)	16 (10%)	8	22
2	z	161/177 (91%)	146 (91%)	15 (9%)	9	25
All	All	9008/10108 (89%)	8251 (92%)	757 (8%)	11	30

All (757) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	19	LEU
1	A	33	LEU
1	A	49	SER
1	A	58	ASP
1	A	59	ARG
1	A	62	PHE
1	A	92	ARG
1	A	112	THR
1	A	122	LEU
1	A	159	THR
1	A	205	VAL
1	A	207	SER
1	B	10	GLU
1	B	13	MET
1	B	19	LEU
1	B	33	LEU
1	B	49	SER
1	B	60	VAL

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Mol	Chain	Res	Type
1	B	62	PHE
1	B	112	THR
1	B	122	LEU
1	B	140	ARG
1	B	147	ILE
1	B	159	THR
1	B	174	ASN
1	B	178	THR
1	B	179	ASP
1	B	205	VAL
1	B	207	SER
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	92	ARG
1	D	112	THR
1	D	140	ARG
1	D	147	ILE
1	D	159	THR
1	D	178	THR
1	D	205	VAL
1	D	207	SER
1	D	213	LEU
1	D	225	ILE
1	D	230	LEU
1	F	49	SER
1	F	60	VAL
1	F	62	PHE
1	F	80	GLN
1	F	112	THR
1	F	140	ARG
1	F	147	ILE
1	F	160	THR
1	F	174	ASN

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Mol	Chain	Res	Type
1	F	178	THR
1	F	179	ASP
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	57	TYR
1	I	58	ASP
1	I	60	VAL
1	I	62	PHE
1	I	147	ILE
1	I	149	ASP
1	I	205	VAL
1	I	233	LEU
1	K	33	LEU
1	K	57	TYR
1	K	60	VAL
1	K	62	PHE
1	K	127	VAL
1	K	133	THR
1	K	135	ARG
1	K	147	ILE
1	K	149	ASP
1	K	205	VAL
1	K	216	ASN
1	K	228	SER
1	K	234	LEU
1	M	13	MET
1	M	33	LEU
1	M	60	VAL
1	M	62	PHE
1	M	176	SER
1	M	216	ASN
1	M	228	SER
1	O	13	MET

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Mol	Chain	Res	Type
1	O	33	LEU
1	O	60	VAL
1	O	62	PHE
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	127	VAL
1	Q	133	THR
1	Q	144	ASP
1	Q	149	ASP
1	Q	205	VAL
1	Q	216	ASN
1	Q	230	LEU
1	S	13	MET
1	S	33	LEU
1	S	48	ARG
1	S	60	VAL
1	S	62	PHE
1	S	127	VAL
1	S	147	ILE
1	S	149	ASP
1	S	173	GLU
1	S	178	THR
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	127	VAL
1	U	133	THR
1	U	135	ARG

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Mol	Chain	Res	Type
1	U	147	ILE
1	U	149	ASP
1	U	216	ASN
1	W	33	LEU
1	W	60	VAL
1	W	62	PHE
1	W	127	VAL
1	W	133	THR
1	W	135	ARG
1	W	147	ILE
1	W	149	ASP
1	W	179	ASP
1	Y	11	GLN
1	Y	13	MET
1	Y	33	LEU
1	Y	60	VAL
1	Y	62	PHE
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	1	10	GLU
1	1	33	LEU
1	1	60	VAL
1	1	62	PHE
1	1	127	VAL
1	1	133	THR
1	1	135	ARG
1	1	147	ILE
1	1	149	ASP
1	1	205	VAL
1	1	216	ASN
1	a	313	MET
1	a	333	LEU
1	a	349	SER
1	a	360	VAL
1	a	362	PHE
1	a	427	VAL
1	a	433	THR

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Mol	Chain	Res	Type
1	a	435	ARG
1	a	447	ILE
1	a	449	ASP
1	a	505	VAL
1	a	533	LEU
1	a	534	LEU
1	b	313	MET
1	b	357	TYR
1	b	360	VAL
1	b	362	PHE
1	b	427	VAL
1	b	447	ILE
1	b	449	ASP
1	b	476	SER
1	b	505	VAL
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	335	TYR
1	d	360	VAL
1	d	362	PHE
1	d	427	VAL
1	d	433	THR
1	d	435	ARG
1	d	447	ILE
1	d	449	ASP
1	f	310	GLU
1	f	313	MET
1	f	333	LEU
1	f	360	VAL
1	f	362	PHE
1	f	427	VAL
1	f	435	ARG
1	f	447	ILE
1	f	449	ASP
1	f	516	ASN
1	f	528	SER
1	i	313	MET

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Mol	Chain	Res	Type
1	i	333	LEU
1	i	360	VAL
1	i	362	PHE
1	i	427	VAL
1	i	433	THR
1	i	435	ARG
1	i	444	ASP
1	i	447	ILE
1	i	449	ASP
1	i	505	VAL
1	i	516	ASN
1	k	311	GLN
1	k	313	MET
1	k	333	LEU
1	k	358	ASP
1	k	360	VAL
1	k	362	PHE
1	k	447	ILE
1	k	449	ASP
1	k	505	VAL
1	k	530	LEU
1	m	313	MET
1	m	360	VAL
1	m	362	PHE
1	m	427	VAL
1	m	433	THR
1	m	447	ILE
1	m	449	ASP
1	m	516	ASN
1	m	531	GLN
1	o	313	MET
1	o	333	LEU
1	o	360	VAL
1	o	362	PHE
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	310	GLU

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Mol	Chain	Res	Type
1	q	313	MET
1	q	333	LEU
1	q	335	TYR
1	q	359	ARG
1	q	360	VAL
1	q	362	PHE
1	q	427	VAL
1	q	433	THR
1	q	447	ILE
1	q	449	ASP
1	q	516	ASN
1	q	530	LEU
1	s	313	MET
1	s	333	LEU
1	s	360	VAL
1	s	362	PHE
1	s	427	VAL
1	s	447	ILE
1	s	449	ASP
1	s	514	ASP
1	s	516	ASN
1	u	313	MET
1	u	360	VAL
1	u	362	PHE
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	333	LEU
1	w	335	TYR
1	w	360	VAL
1	w	362	PHE
1	w	427	VAL
1	w	447	ILE
1	w	449	ASP
1	w	474	ASN
1	w	533	LEU
1	w	534	LEU
1	y	311	GLN
1	y	313	MET

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Mol	Chain	Res	Type
1	y	333	LEU
1	y	357	TYR
1	y	362	PHE
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	311	GLN
1	3	313	MET
1	3	357	TYR
1	3	360	VAL
1	3	362	PHE
1	3	427	VAL
1	3	447	ILE
1	3	449	ASP
1	3	479	ASP
1	3	505	VAL
1	3	530	LEU
2	H	19	ARG
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	110	HIS
2	H	130	ASN
2	H	144	LEU
2	H	164	LEU
2	H	200	ASP
2	H	209	ARG
2	H	212	GLU
2	H	220	SER
2	H	222	SER
2	C	19	ARG

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Mol	Chain	Res	Type
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	110	HIS
2	C	130	ASN
2	C	144	LEU
2	C	164	LEU
2	C	198	ASP
2	C	200	ASP
2	C	208	SER
2	E	19	ARG
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	110	HIS
2	E	130	ASN
2	E	144	LEU
2	E	164	LEU
2	E	208	SER
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	110	HIS
2	G	130	ASN
2	G	144	LEU
2	G	164	LEU
2	G	200	ASP
2	G	208	SER
2	J	19	ARG

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Mol	Chain	Res	Type
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	110	HIS
2	J	130	ASN
2	J	144	LEU
2	J	164	LEU
2	J	208	SER
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	110	HIS
2	L	130	ASN
2	L	144	LEU
2	L	161	ASP
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	19	ARG
2	N	38	ASP
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	110	HIS
2	N	130	ASN
2	N	144	LEU
2	N	164	LEU
2	N	200	ASP

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Mol	Chain	Res	Type
2	N	207	GLU
2	N	208	SER
2	N	209	ARG
2	N	220	SER
2	P	12	VAL
2	P	19	ARG
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	110	HIS
2	P	130	ASN
2	P	144	LEU
2	P	164	LEU
2	P	208	SER
2	P	220	SER
2	R	19	ARG
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	110	HIS
2	R	130	ASN
2	R	144	LEU
2	R	161	ASP
2	R	164	LEU
2	R	212	GLU
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

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Mol	Chain	Res	Type
2	T	110	HIS
2	T	130	ASN
2	T	144	LEU
2	T	164	LEU
2	T	196	ILE
2	T	208	SER
2	T	220	SER
2	V	4	VAL
2	V	12	VAL
2	V	19	ARG
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	110	HIS
2	V	130	ASN
2	V	144	LEU
2	V	161	ASP
2	V	164	LEU
2	V	208	SER
2	V	221	ARG
2	V	222	SER
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	110	HIS
2	X	130	ASN
2	X	144	LEU
2	X	161	ASP
2	X	164	LEU
2	X	208	SER
2	X	220	SER
2	Z	12	VAL
2	Z	19	ARG
2	Z	53	VAL

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Mol	Chain	Res	Type
2	Z	62	GLU
2	Z	83	LEU
2	Z	101	LEU
2	Z	103	LEU
2	Z	109	ILE
2	Z	110	HIS
2	Z	130	ASN
2	Z	144	LEU
2	Z	161	ASP
2	Z	164	LEU
2	Z	209	ARG
2	2	12	VAL
2	2	19	ARG
2	2	38	ASP
2	2	53	VAL
2	2	83	LEU
2	2	101	LEU
2	2	103	LEU
2	2	130	ASN
2	2	144	LEU
2	2	161	ASP
2	2	164	LEU
2	2	208	SER
2	2	209	ARG
2	2	220	SER
2	h	312	VAL
2	h	319	ARG
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	410	HIS
2	h	430	ASN
2	h	444	LEU
2	h	464	LEU
2	h	508	SER
2	h	509	ARG
2	h	520	SER
2	c	312	VAL
2	c	319	ARG

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Mol	Chain	Res	Type
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	410	HIS
2	c	430	ASN
2	c	444	LEU
2	c	461	ASP
2	c	464	LEU
2	c	509	ARG
2	c	520	SER
2	e	319	ARG
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	410	HIS
2	e	430	ASN
2	e	444	LEU
2	e	464	LEU
2	e	500	ASP
2	e	508	SER
2	e	520	SER
2	g	304	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	410	HIS
2	g	430	ASN
2	g	444	LEU
2	g	464	LEU
2	g	508	SER
2	g	509	ARG

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Mol	Chain	Res	Type
2	j	304	VAL
2	j	312	VAL
2	j	319	ARG
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	410	HIS
2	j	430	ASN
2	j	444	LEU
2	j	461	ASP
2	j	464	LEU
2	j	496	ILE
2	j	520	SER
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	410	HIS
2	l	430	ASN
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	312	VAL
2	n	319	ARG
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	430	ASN
2	n	444	LEU
2	n	461	ASP

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Mol	Chain	Res	Type
2	n	464	LEU
2	n	496	ILE
2	n	508	SER
2	n	520	SER
2	n	522	SER
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	410	HIS
2	p	430	ASN
2	p	444	LEU
2	p	464	LEU
2	p	496	ILE
2	p	500	ASP
2	p	508	SER
2	r	319	ARG
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	410	HIS
2	r	430	ASN
2	r	444	LEU
2	r	464	LEU
2	r	496	ILE
2	r	520	SER
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	410	HIS
2	t	430	ASN

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Mol	Chain	Res	Type
2	t	444	LEU
2	t	464	LEU
2	t	496	ILE
2	t	500	ASP
2	t	508	SER
2	t	520	SER
2	v	312	VAL
2	v	319	ARG
2	v	338	ASP
2	v	339	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	410	HIS
2	v	430	ASN
2	v	444	LEU
2	v	461	ASP
2	v	464	LEU
2	v	508	SER
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	410	HIS
2	x	430	ASN
2	x	444	LEU
2	x	461	ASP
2	x	464	LEU
2	x	508	SER
2	x	509	ARG
2	z	312	VAL
2	z	319	ARG
2	z	338	ASP
2	z	353	VAL

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Mol	Chain	Res	Type
2	z	362	GLU
2	z	383	LEU
2	z	401	LEU
2	z	403	LEU
2	z	409	ILE
2	z	410	HIS
2	z	430	ASN
2	z	444	LEU
2	z	464	LEU
2	z	509	ARG
2	z	520	SER
2	4	312	VAL
2	4	319	ARG
2	4	353	VAL
2	4	383	LEU
2	4	401	LEU
2	4	403	LEU
2	4	409	ILE
2	4	410	HIS
2	4	430	ASN
2	4	444	LEU
2	4	464	LEU
2	4	500	ASP
2	4	508	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	B	174	ASN
1	B	231	GLN
1	D	98	GLN
1	D	174	ASN
1	F	80	GLN
1	F	174	ASN
1	I	11	GLN
1	I	98	GLN
1	I	114	GLN
1	I	152	HIS
1	K	98	GLN
1	K	114	GLN
1	M	98	GLN

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Mol	Chain	Res	Type
1	M	114	GLN
1	O	98	GLN
1	O	114	GLN
1	O	152	HIS
1	Q	98	GLN
1	Q	114	GLN
1	Q	152	HIS
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	152	HIS
1	W	98	GLN
1	W	114	GLN
1	Y	11	GLN
1	Y	98	GLN
1	Y	114	GLN
1	Y	152	HIS
1	Y	174	ASN
1	l	98	GLN
1	l	114	GLN
1	a	398	GLN
1	a	414	GLN
1	a	452	HIS
1	b	398	GLN
1	b	414	GLN
1	b	452	HIS
1	d	414	GLN
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

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Mol	Chain	Res	Type
1	k	414	GLN
1	k	452	HIS
1	m	414	GLN
1	m	452	HIS
1	o	398	GLN
1	o	414	GLN
1	q	311	GLN
1	q	414	GLN
1	q	452	HIS
1	s	398	GLN
1	s	414	GLN
1	s	516	ASN
1	u	414	GLN
1	u	452	HIS
1	w	398	GLN
1	w	414	GLN
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	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

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Mol	Chain	Res	Type
2	T	65	HIS
2	T	130	ASN
2	V	65	HIS
2	V	130	ASN
2	X	65	HIS
2	X	130	ASN
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	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	J	1	2	7,9,10	2.92	2 (28%)	9,12,14	2.60	3 (33%)
2	OZT	2	1	2	7,9,10	2.65	2 (28%)	9,12,14	2.58	6 (66%)
2	OZT	4	301	2	7,9,10	3.07	2 (28%)	9,12,14	3.13	4 (44%)
2	OZT	Z	1	2	7,9,10	2.78	3 (42%)	9,12,14	2.60	3 (33%)
2	OZT	n	301	2	7,9,10	3.04	2 (28%)	9,12,14	2.34	4 (44%)
2	OZT	l	301	2	7,9,10	2.58	2 (28%)	9,12,14	2.46	4 (44%)
2	OZT	z	301	2	7,9,10	3.14	2 (28%)	9,12,14	3.22	4 (44%)
2	OZT	H	1	2	7,9,10	3.02	2 (28%)	9,12,14	2.38	4 (44%)
2	OZT	v	301	2	7,9,10	3.09	3 (42%)	9,12,14	3.30	4 (44%)
2	OZT	r	301	2	7,9,10	2.84	2 (28%)	9,12,14	3.09	4 (44%)
2	OZT	c	301	2	7,9,10	2.83	2 (28%)	9,12,14	2.70	6 (66%)
2	OZT	G	1	2	7,9,10	2.81	3 (42%)	9,12,14	2.74	3 (33%)
2	OZT	e	301	2	7,9,10	2.87	2 (28%)	9,12,14	2.22	5 (55%)
2	OZT	g	301	2	7,9,10	2.67	2 (28%)	9,12,14	2.53	5 (55%)
2	OZT	j	301	2	7,9,10	2.77	2 (28%)	9,12,14	2.12	5 (55%)
2	OZT	V	1	2	7,9,10	2.89	2 (28%)	9,12,14	2.19	4 (44%)
2	OZT	x	301	2	7,9,10	3.15	2 (28%)	9,12,14	2.75	5 (55%)
2	OZT	T	1	2	7,9,10	2.58	2 (28%)	9,12,14	2.75	3 (33%)
2	OZT	p	301	2	7,9,10	2.98	2 (28%)	9,12,14	3.29	4 (44%)
2	OZT	t	301	2	7,9,10	2.64	2 (28%)	9,12,14	2.06	4 (44%)
2	OZT	h	301	2	7,9,10	2.85	2 (28%)	9,12,14	2.41	4 (44%)
2	OZT	L	1	2	7,9,10	2.59	2 (28%)	9,12,14	3.02	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OZT	N	1	2	7,9,10	2.68	2 (28%)	9,12,14	2.23	5 (55%)
2	OZT	C	1	2	7,9,10	2.97	2 (28%)	9,12,14	2.48	4 (44%)
2	OZT	P	1	2	7,9,10	2.60	2 (28%)	9,12,14	2.50	5 (55%)
2	OZT	R	1	2	7,9,10	3.08	2 (28%)	9,12,14	3.26	4 (44%)
2	OZT	X	1	2	7,9,10	2.82	2 (28%)	9,12,14	2.51	5 (55%)
2	OZT	E	1	2	7,9,10	3.02	2 (28%)	9,12,14	2.93	6 (66%)

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	J	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	4	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	n	301	2	-	1/1/14/16	0/1/1/1
2	OZT	l	301	2	-	0/1/14/16	0/1/1/1
2	OZT	z	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	v	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	301	2	-	0/1/14/16	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	g	301	2	-	0/1/14/16	0/1/1/1
2	OZT	j	301	2	-	0/1/14/16	0/1/1/1
2	OZT	V	1	2	-	0/1/14/16	0/1/1/1
2	OZT	x	301	2	-	0/1/14/16	0/1/1/1
2	OZT	T	1	2	-	0/1/14/16	0/1/1/1
2	OZT	p	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	h	301	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	C	1	2	-	0/1/14/16	0/1/1/1
2	OZT	P	1	2	-	0/1/14/16	0/1/1/1
2	OZT	R	1	2	-	1/1/14/16	0/1/1/1
2	OZT	X	1	2	-	1/1/14/16	0/1/1/1
2	OZT	E	1	2	-	0/1/14/16	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	x	301	OZT	O1-C5	7.55	1.46	1.36
2	z	301	OZT	O1-C5	7.53	1.46	1.36
2	n	301	OZT	O1-C5	7.49	1.46	1.36
2	E	1	OZT	O1-C5	7.34	1.46	1.36
2	4	301	OZT	O1-C5	7.33	1.46	1.36
2	H	1	OZT	O1-C5	7.27	1.46	1.36
2	v	301	OZT	O1-C5	7.09	1.46	1.36
2	p	301	OZT	O1-C5	7.01	1.45	1.36
2	C	1	OZT	O1-C5	6.98	1.45	1.36
2	V	1	OZT	O1-C5	6.95	1.45	1.36
2	c	301	OZT	O1-C5	6.92	1.45	1.36
2	e	301	OZT	O1-C5	6.90	1.45	1.36
2	J	1	OZT	O1-C5	6.87	1.45	1.36
2	R	1	OZT	O1-C5	6.84	1.45	1.36
2	X	1	OZT	O1-C5	6.66	1.45	1.36
2	h	301	OZT	O1-C5	6.66	1.45	1.36
2	j	301	OZT	O1-C5	6.63	1.45	1.36
2	G	1	OZT	O1-C5	6.54	1.45	1.36
2	r	301	OZT	O1-C5	6.50	1.45	1.36
2	Z	1	OZT	O1-C5	6.44	1.45	1.36
2	N	1	OZT	O1-C5	6.29	1.44	1.36
2	T	1	OZT	O1-C5	6.22	1.44	1.36
2	l	301	OZT	O1-C5	6.20	1.44	1.36
2	2	1	OZT	O1-C5	6.17	1.44	1.36
2	L	1	OZT	O1-C5	6.15	1.44	1.36
2	t	301	OZT	O1-C5	6.14	1.44	1.36
2	P	1	OZT	O1-C5	5.92	1.44	1.36
2	g	301	OZT	O1-C5	5.91	1.44	1.36
2	R	1	OZT	O1-C2	-3.82	1.41	1.46
2	p	301	OZT	O1-C2	-3.24	1.41	1.46
2	v	301	OZT	O1-C2	-3.16	1.42	1.46
2	h	301	OZT	O1-C2	-3.15	1.42	1.46
2	g	301	OZT	O1-C2	-3.10	1.42	1.46
2	J	1	OZT	O1-C2	-3.10	1.42	1.46
2	H	1	OZT	O1-C2	-2.99	1.42	1.46
2	r	301	OZT	O1-C2	-2.97	1.42	1.46
2	N	1	OZT	O1-C2	-2.88	1.42	1.46
2	4	301	OZT	O1-C2	-2.84	1.42	1.46
2	P	1	OZT	O1-C2	-2.83	1.42	1.46
2	E	1	OZT	O1-C2	-2.81	1.42	1.46
2	t	301	OZT	O1-C2	-2.80	1.42	1.46
2	2	1	OZT	O1-C2	-2.75	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	301	OZT	O1-C2	-2.73	1.42	1.46
2	x	301	OZT	O1-C2	-2.71	1.42	1.46
2	G	1	OZT	O1-C2	-2.68	1.42	1.46
2	C	1	OZT	O1-C2	-2.63	1.42	1.46
2	e	301	OZT	O1-C2	-2.63	1.42	1.46
2	z	301	OZT	O1-C2	-2.60	1.42	1.46
2	n	301	OZT	O1-C2	-2.60	1.42	1.46
2	Z	1	OZT	O1-C2	-2.60	1.42	1.46
2	V	1	OZT	O1-C2	-2.56	1.43	1.46
2	l	301	OZT	O1-C2	-2.46	1.43	1.46
2	L	1	OZT	O1-C2	-2.26	1.43	1.46
2	v	301	OZT	C2-CA	-2.20	1.50	1.54
2	c	301	OZT	O1-C2	-2.16	1.43	1.46
2	T	1	OZT	O1-C2	-2.15	1.43	1.46
2	X	1	OZT	O1-C2	-2.14	1.43	1.46
2	Z	1	OZT	C2-CA	-2.03	1.50	1.54
2	G	1	OZT	C2-CA	-2.02	1.50	1.54

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	z	301	OZT	C7-C2-CA	-7.57	104.16	114.80
2	p	301	OZT	C7-C2-CA	-6.88	105.13	114.80
2	T	1	OZT	C7-C2-CA	-6.64	105.46	114.80
2	v	301	OZT	C7-C2-CA	-6.57	105.56	114.80
2	Z	1	OZT	C7-C2-CA	-6.32	105.92	114.80
2	G	1	OZT	C7-C2-CA	-6.12	106.20	114.80
2	L	1	OZT	C7-C2-CA	-6.10	106.22	114.80
2	r	301	OZT	C2-CA-C	-5.81	106.08	114.16
2	R	1	OZT	C7-C2-CA	-5.66	106.84	114.80
2	x	301	OZT	C7-C2-CA	-5.64	106.86	114.80
2	J	1	OZT	O1-C2-C7	-5.46	101.34	108.70
2	r	301	OZT	C7-C2-CA	-5.40	107.20	114.80
2	4	301	OZT	C2-O1-C5	-5.40	101.57	110.41
2	c	301	OZT	C7-C2-CA	-5.26	107.41	114.80
2	4	301	OZT	C7-C2-CA	-5.18	107.52	114.80
2	v	301	OZT	C2-CA-C	-5.17	106.98	114.16
2	C	1	OZT	C7-C2-CA	-4.98	107.80	114.80
2	R	1	OZT	O1-C2-C7	-4.90	102.09	108.70
2	g	301	OZT	C2-CA-C	-4.75	107.55	114.16
2	E	1	OZT	O1-C2-CA	4.74	108.15	103.58
2	L	1	OZT	C2-CA-C	-4.66	107.68	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	OZT	C7-C2-CA	-4.64	108.28	114.80
2	R	1	OZT	C2-CA-C	-4.39	108.06	114.16
2	p	301	OZT	O1-C2-C7	-4.34	102.84	108.70
2	l	301	OZT	O1-C2-C7	-4.32	102.88	108.70
2	J	1	OZT	C7-C2-CA	-4.20	108.90	114.80
2	2	1	OZT	C7-C2-CA	-4.12	109.00	114.80
2	E	1	OZT	C7-C2-CA	-4.09	109.04	114.80
2	4	301	OZT	O1-C5-O6	4.02	125.33	121.24
2	j	301	OZT	C7-C2-CA	-3.99	109.18	114.80
2	p	301	OZT	C2-O1-C5	-3.99	103.89	110.41
2	v	301	OZT	C2-O1-C5	-3.90	104.03	110.41
2	V	1	OZT	C7-C2-CA	-3.86	109.37	114.80
2	n	301	OZT	C7-C2-CA	-3.86	109.38	114.80
2	t	301	OZT	C2-CA-C	-3.83	108.83	114.16
2	R	1	OZT	C2-O1-C5	-3.79	104.20	110.41
2	G	1	OZT	C2-CA-C	-3.79	108.89	114.16
2	H	1	OZT	C2-O1-C5	-3.71	104.35	110.41
2	T	1	OZT	C2-O1-C5	-3.69	104.37	110.41
2	h	301	OZT	C2-O1-C5	-3.68	104.38	110.41
2	c	301	OZT	C2-CA-C	-3.66	109.07	114.16
2	2	1	OZT	C2-CA-C	-3.61	109.14	114.16
2	l	301	OZT	O1-C2-CA	3.58	107.03	103.58
2	r	301	OZT	C2-O1-C5	-3.51	104.67	110.41
2	h	301	OZT	O1-C2-C7	-3.50	103.98	108.70
2	P	1	OZT	C2-O1-C5	-3.49	104.70	110.41
2	E	1	OZT	C2-O1-C5	-3.47	104.73	110.41
2	N	1	OZT	C2-O1-C5	-3.43	104.79	110.41
2	l	301	OZT	C2-O1-C5	-3.43	104.80	110.41
2	h	301	OZT	C7-C2-CA	-3.42	109.99	114.80
2	X	1	OZT	C2-O1-C5	-3.40	104.84	110.41
2	N	1	OZT	O1-C2-CA	3.37	106.83	103.58
2	P	1	OZT	O1-C5-N	-3.36	107.04	109.86
2	z	301	OZT	C2-O1-C5	-3.35	104.93	110.41
2	n	301	OZT	C2-CA-C	-3.32	109.55	114.16
2	X	1	OZT	O1-C5-O6	3.26	124.56	121.24
2	X	1	OZT	C2-CA-C	-3.25	109.64	114.16
2	z	301	OZT	O1-C5-O6	3.23	124.52	121.24
2	X	1	OZT	C7-C2-CA	-3.20	110.30	114.80
2	P	1	OZT	C2-CA-C	-3.17	109.74	114.16
2	E	1	OZT	C2-CA-C	-3.17	109.75	114.16
2	C	1	OZT	O1-C5-O6	3.15	124.44	121.24
2	g	301	OZT	C2-O1-C5	-3.15	105.26	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	x	301	OZT	C2-CA-C	-3.04	109.93	114.16
2	x	301	OZT	O1-C5-O6	3.02	124.32	121.24
2	l	301	OZT	C7-C2-CA	-3.01	110.56	114.80
2	P	1	OZT	O1-C5-O6	2.94	124.23	121.24
2	L	1	OZT	C2-O1-C5	-2.92	105.63	110.41
2	2	1	OZT	C2-O1-C5	-2.90	105.66	110.41
2	t	301	OZT	C2-O1-C5	-2.90	105.67	110.41
2	e	301	OZT	O1-C2-CA	2.88	106.35	103.58
2	e	301	OZT	O6-C5-N	-2.87	125.88	129.22
2	g	301	OZT	C7-C2-CA	-2.86	110.78	114.80
2	n	301	OZT	C2-O1-C5	-2.86	105.73	110.41
2	V	1	OZT	O1-C2-C7	-2.86	104.85	108.70
2	g	301	OZT	O1-C5-O6	2.85	124.14	121.24
2	x	301	OZT	C2-O1-C5	-2.85	105.75	110.41
2	P	1	OZT	C7-C2-CA	-2.84	110.81	114.80
2	C	1	OZT	O1-C5-N	-2.80	107.51	109.86
2	H	1	OZT	C2-CA-C	-2.78	110.29	114.16
2	L	1	OZT	O1-C2-CA	2.73	106.21	103.58
2	4	301	OZT	O6-C5-N	-2.73	126.03	129.22
2	2	1	OZT	O1-C2-CA	2.67	106.15	103.58
2	x	301	OZT	O6-C5-N	-2.66	126.11	129.22
2	e	301	OZT	O1-C5-O6	2.63	123.92	121.24
2	e	301	OZT	C2-O1-C5	-2.61	106.14	110.41
2	j	301	OZT	C2-CA-C	-2.59	110.55	114.16
2	J	1	OZT	C2-O1-C5	-2.57	106.21	110.41
2	z	301	OZT	O6-C5-N	-2.55	126.24	129.22
2	G	1	OZT	C2-O1-C5	-2.51	106.31	110.41
2	g	301	OZT	O1-C5-N	-2.49	107.77	109.86
2	c	301	OZT	C2-O1-C5	-2.49	106.33	110.41
2	L	1	OZT	O-C-CA	-2.45	117.99	124.83
2	Z	1	OZT	C2-O1-C5	-2.45	106.41	110.41
2	2	1	OZT	O1-C5-O6	2.42	123.70	121.24
2	E	1	OZT	O-C-CA	-2.40	118.14	124.83
2	c	301	OZT	O1-C2-C7	2.40	111.93	108.70
2	t	301	OZT	C7-C2-CA	-2.37	111.46	114.80
2	p	301	OZT	O1-C2-CA	2.36	105.85	103.58
2	T	1	OZT	C2-CA-C	-2.34	110.90	114.16
2	j	301	OZT	O1-C2-CA	2.33	105.82	103.58
2	V	1	OZT	C2-O1-C5	-2.30	106.66	110.41
2	X	1	OZT	O1-C5-N	-2.29	107.94	109.86
2	r	301	OZT	O1-C2-CA	2.28	105.77	103.58
2	H	1	OZT	O1-C2-C7	-2.27	105.64	108.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	301	OZT	C2-O1-C5	-2.25	106.73	110.41
2	c	301	OZT	O-C-CA	-2.24	118.58	124.83
2	C	1	OZT	O-C-CA	-2.23	118.62	124.83
2	E	1	OZT	O6-C5-N	-2.19	126.66	129.22
2	t	301	OZT	O1-C2-C7	-2.17	105.77	108.70
2	e	301	OZT	C2-CA-C	-2.17	111.14	114.16
2	N	1	OZT	O1-C5-N	-2.16	108.05	109.86
2	j	301	OZT	O-C-CA	-2.12	118.92	124.83
2	V	1	OZT	O1-C5-O6	2.10	123.38	121.24
2	N	1	OZT	O1-C5-O6	2.09	123.37	121.24
2	c	301	OZT	O1-C2-CA	2.08	105.58	103.58
2	Z	1	OZT	C2-CA-C	-2.07	111.28	114.16
2	h	301	OZT	O1-C5-N	2.06	111.59	109.86
2	n	301	OZT	O1-C2-CA	2.04	105.54	103.58
2	N	1	OZT	C7-C2-CA	-2.03	111.94	114.80
2	2	1	OZT	O6-C5-N	-2.02	126.87	129.22
2	v	301	OZT	O6-C5-N	-2.01	126.87	129.22

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	OZT	1	0
2	2	1	OZT	6	0
2	4	301	OZT	5	0
2	Z	1	OZT	1	0
2	H	1	OZT	8	0
2	V	1	OZT	2	0
2	L	1	OZT	4	0
2	N	1	OZT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	OZT	2	0
2	P	1	OZT	2	0
2	X	1	OZT	6	0
2	E	1	OZT	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.