



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:03 AM GMT

PDB ID : 1Z7Q  
Title : Crystal structure of the 20s proteasome from yeast in complex with the proteasome activator PA26 from Trypanosome brucei at 3.2 angstroms resolution  
Authors : Forster, A.; Whitby, F.G.; Hill, C.P.  
Deposited on : 2005-03-26  
Resolution : 3.22 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

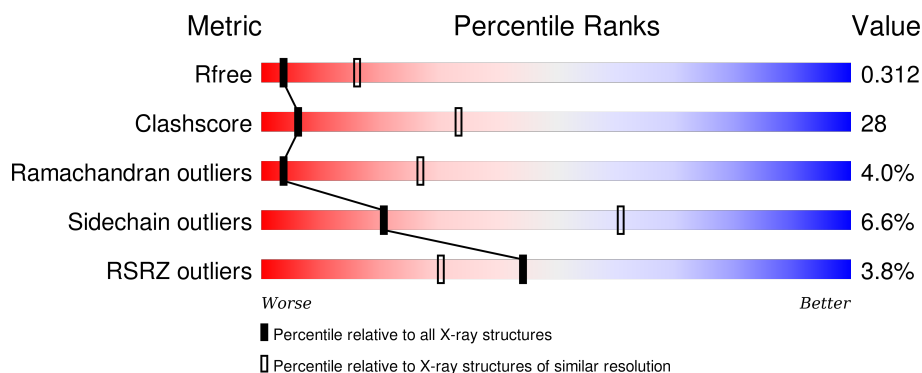
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	<div> <div>4%</div> <div>28% 58% 10% . .</div> </div>
1	O	252	<div> <div>5%</div> <div>29% 58% 9% . .</div> </div>
2	B	250	<div> <div>3%</div> <div>44% 46% 9% .</div> </div>
2	P	250	<div> <div>4%</div> <div>44% 46% 9% .</div> </div>
3	C	258	<div> <div>2%</div> <div>42% 41% 10% . 6%</div> </div>


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Mol	Chain	Length	Quality of chain
3	Q	258	
4	D	254	
4	R	254	
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	288	
7	U	288	
8	H	196	
8	V	196	
9	I	222	
9	W	222	
10	J	205	
10	X	205	
11	K	198	
11	Y	198	
12	L	212	
12	Z	212	
13	M	222	
13	a	222	
14	N	233	
14	b	233	
15	c	231	
15	d	231	

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Mol	Chain	Length	Quality of chain
15	e	231	
15	f	231	
15	g	231	
15	h	231	
15	i	231	
15	j	231	
15	k	231	
15	l	231	
15	m	231	
15	n	231	
15	o	231	
15	p	231	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 74222 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 component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	O	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 2 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
2	P	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 3 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	243	Total	C	N	O	S	0	0	0
			1900	1199	320	378	3			
3	Q	243	Total	C	N	O	S	0	0	0
			1900	1199	320	378	3			

- Molecule 4 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
4	R	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 5 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1888	1179	317	385	7			
5	S	245	Total	C	N	O	S	0	0	0
			1888	1179	317	385	7			

- Molecule 6 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			
6	T	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			

- Molecule 7 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
7	U	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 8 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
8	V	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 9 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	W	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 10 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 11 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	Y	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 12 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	CONFLICT	UNP P30656
Z	33	ARG	LYS	CONFLICT	UNP P30656

- Molecule 13 is a protein called Potential proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	a	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	b	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is a protein called proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	c	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	d	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	e	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	f	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	g	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	h	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	i	230	Total 1760	C 1101	N 310	O 343	S 6	249	0	0
15	j	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	k	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	l	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	m	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	n	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	o	230	Total 1760	C 1101	N 310	O 343	S 6	219	0	0
15	p	230	Total 1760	C 1101	N 310	O 343	S 6	249	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	1049	VAL	THR	CONFLICT	UNP Q9U8G2
c	?	-	SER	DELETION	UNP Q9U8G2
c	1171	GLY	-	INSERTION	UNP Q9U8G2
d	1049	VAL	THR	CONFLICT	UNP Q9U8G2
d	?	-	SER	DELETION	UNP Q9U8G2
d	1171	GLY	-	INSERTION	UNP Q9U8G2
e	1049	VAL	THR	CONFLICT	UNP Q9U8G2
e	?	-	SER	DELETION	UNP Q9U8G2
e	1171	GLY	-	INSERTION	UNP Q9U8G2
f	1049	VAL	THR	CONFLICT	UNP Q9U8G2
f	?	-	SER	DELETION	UNP Q9U8G2
f	1171	GLY	-	INSERTION	UNP Q9U8G2

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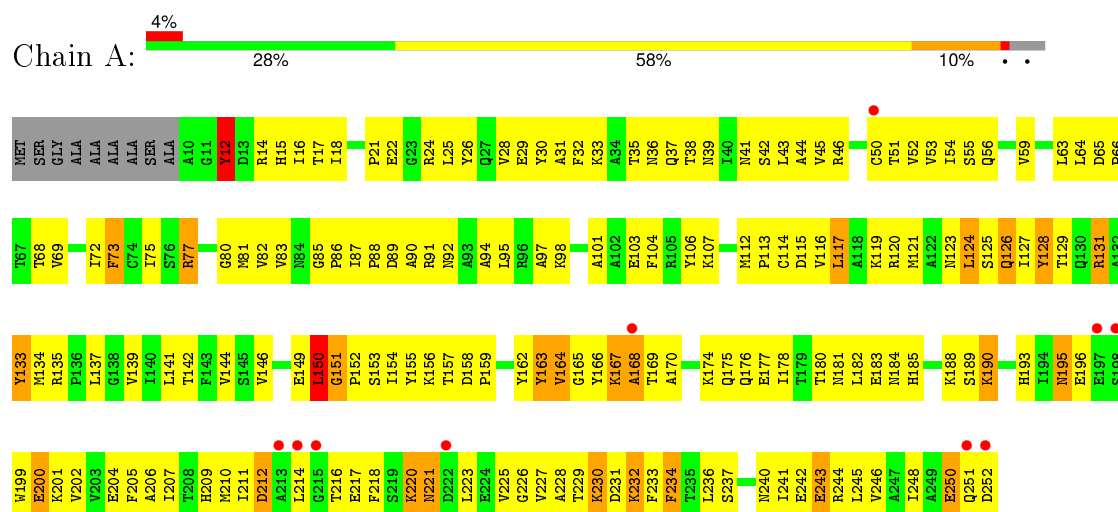
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Chain	Residue	Modelled	Actual	Comment	Reference
g	1049	VAL	THR	CONFLICT	UNP Q9U8G2
g	?	-	SER	DELETION	UNP Q9U8G2
g	1171	GLY	-	INSERTION	UNP Q9U8G2
h	1049	VAL	THR	CONFLICT	UNP Q9U8G2
h	?	-	SER	DELETION	UNP Q9U8G2
h	1171	GLY	-	INSERTION	UNP Q9U8G2
i	1049	VAL	THR	CONFLICT	UNP Q9U8G2
i	?	-	SER	DELETION	UNP Q9U8G2
i	1171	GLY	-	INSERTION	UNP Q9U8G2
j	1049	VAL	THR	CONFLICT	UNP Q9U8G2
j	?	-	SER	DELETION	UNP Q9U8G2
j	1171	GLY	-	INSERTION	UNP Q9U8G2
k	1049	VAL	THR	CONFLICT	UNP Q9U8G2
k	?	-	SER	DELETION	UNP Q9U8G2
k	1171	GLY	-	INSERTION	UNP Q9U8G2
l	1049	VAL	THR	CONFLICT	UNP Q9U8G2
l	?	-	SER	DELETION	UNP Q9U8G2
l	1171	GLY	-	INSERTION	UNP Q9U8G2
m	1049	VAL	THR	CONFLICT	UNP Q9U8G2
m	?	-	SER	DELETION	UNP Q9U8G2
m	1171	GLY	-	INSERTION	UNP Q9U8G2
n	1049	VAL	THR	CONFLICT	UNP Q9U8G2
n	?	-	SER	DELETION	UNP Q9U8G2
n	1171	GLY	-	INSERTION	UNP Q9U8G2
o	1049	VAL	THR	CONFLICT	UNP Q9U8G2
o	?	-	SER	DELETION	UNP Q9U8G2
o	1171	GLY	-	INSERTION	UNP Q9U8G2
p	1049	VAL	THR	CONFLICT	UNP Q9U8G2
p	?	-	SER	DELETION	UNP Q9U8G2
p	1171	GLY	-	INSERTION	UNP Q9U8G2

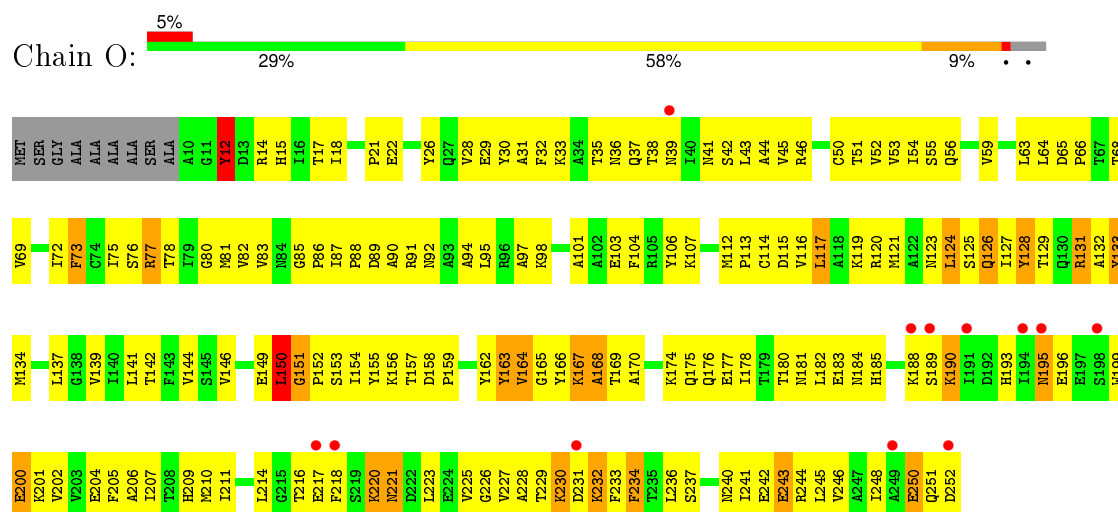
### 3 Residue-property plots

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

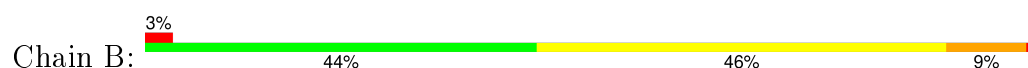
#### • Molecule 1: Proteasome component C7-alpha

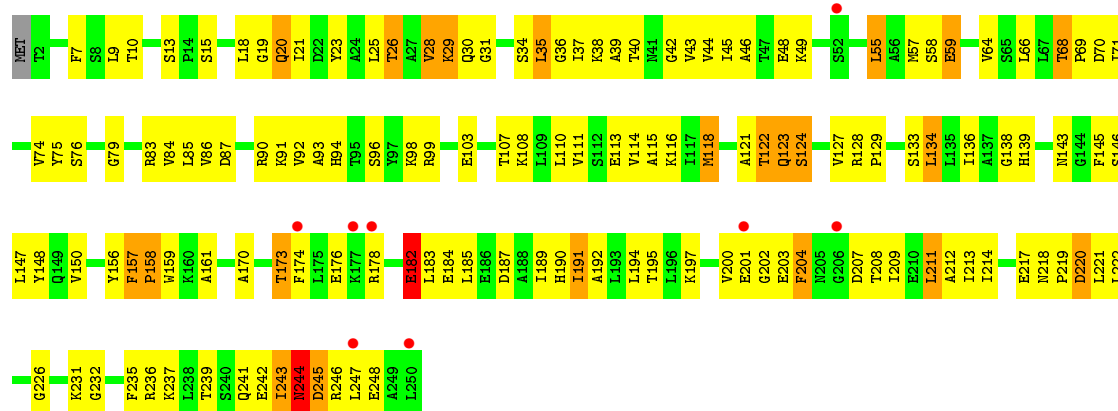


#### • Molecule 1: Proteasome component C7-alpha

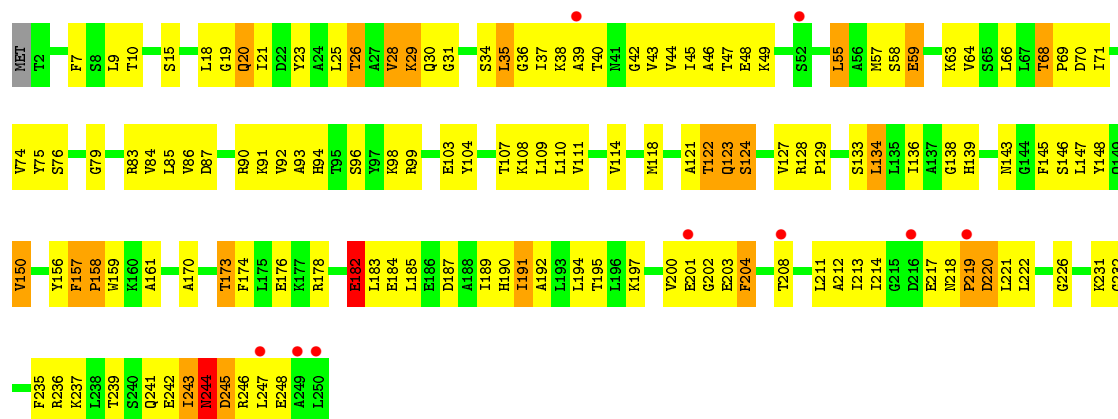
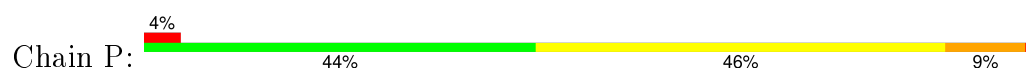


#### • Molecule 2: Proteasome component Y7

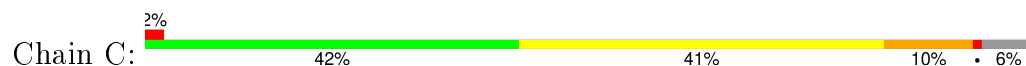




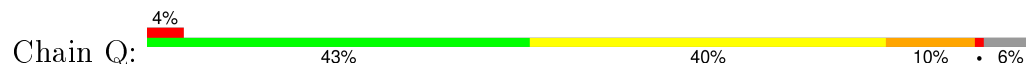
• Molecule 2: Proteasome component Y7

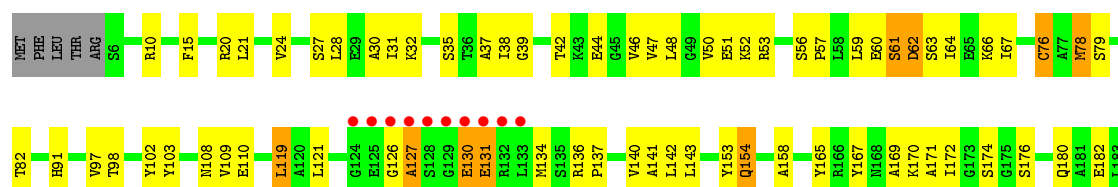


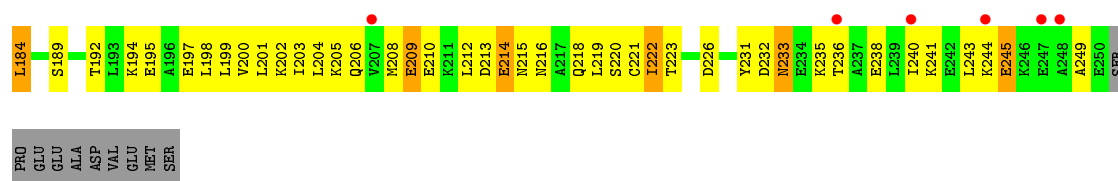
• Molecule 3: Proteasome component Y13



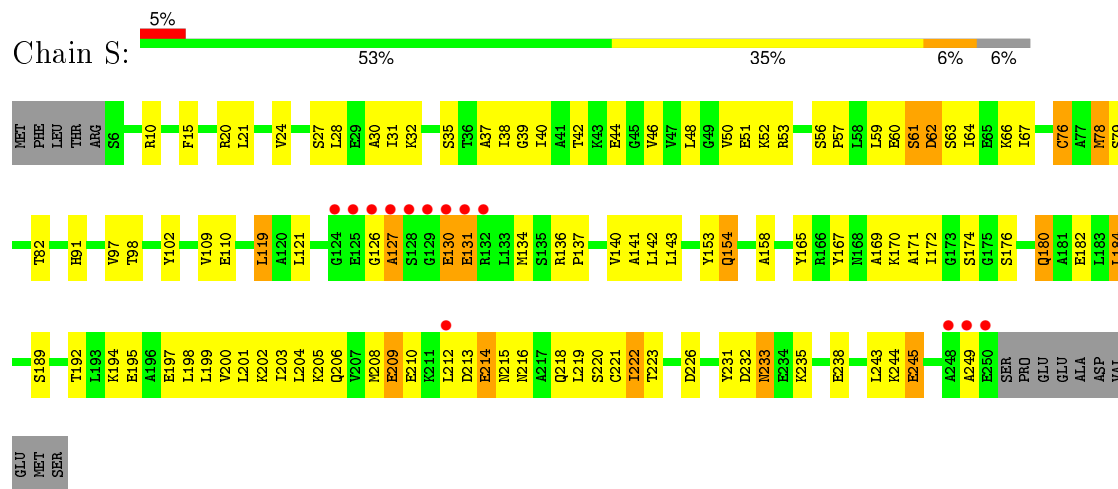
• Molecule 3: Proteasome component Y13



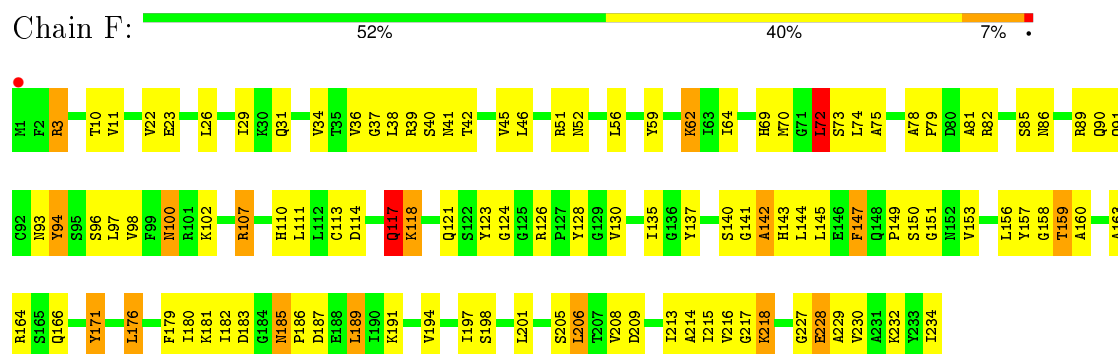




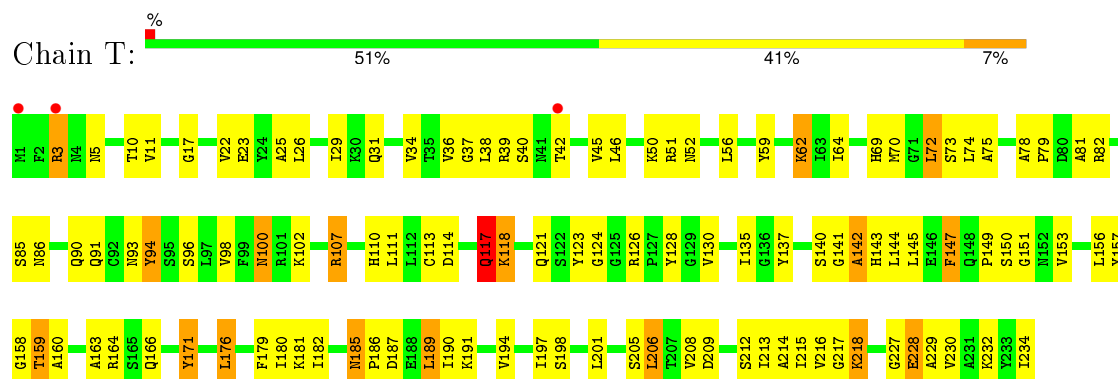
• Molecule 5: Proteasome component PUP2



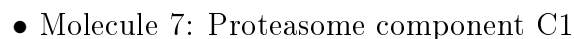
• Molecule 6: Proteasome component PRE5

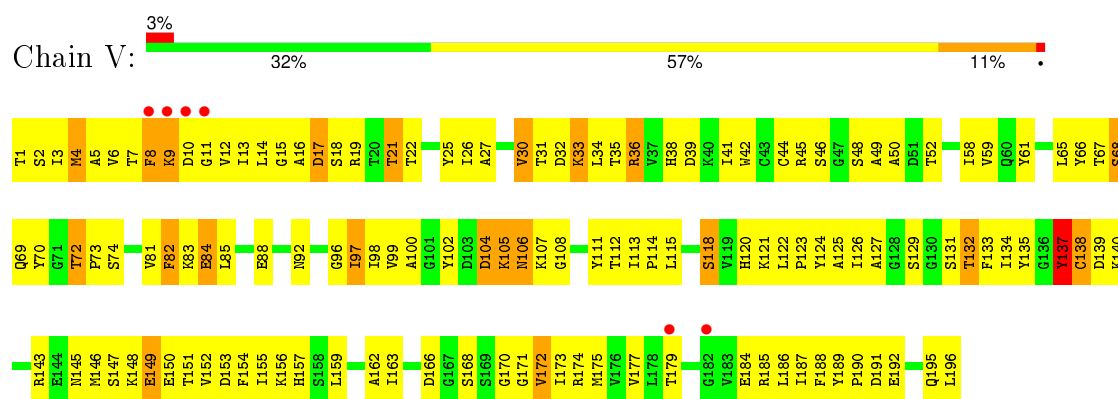


• Molecule 6: Proteasome component PRE5

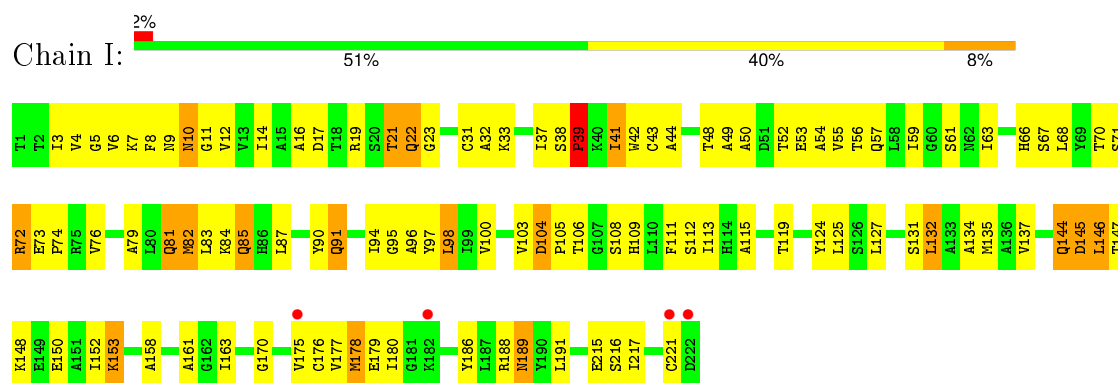


• Molecule 7: Proteasome component C1

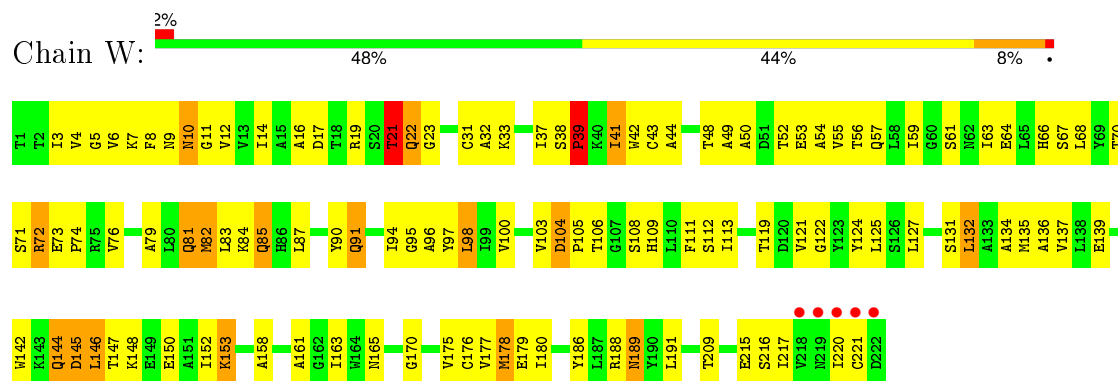




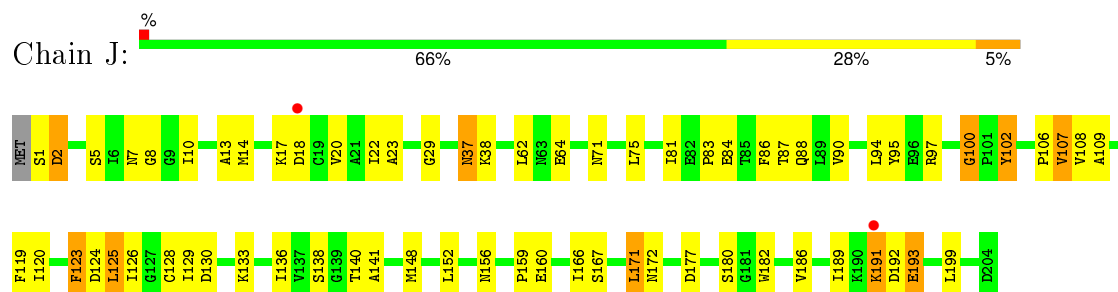
• Molecule 9: Proteasome component PUP1



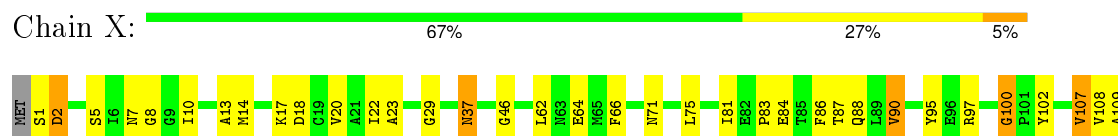
• Molecule 9: Proteasome component PUP1



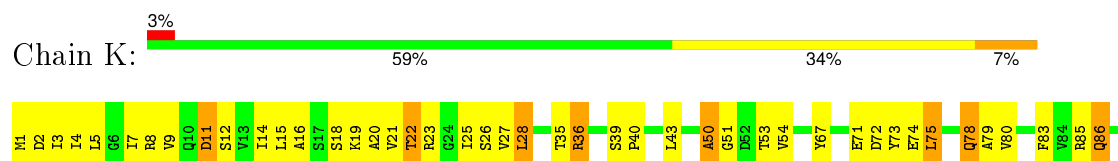
• Molecule 10: Proteasome component PUP3



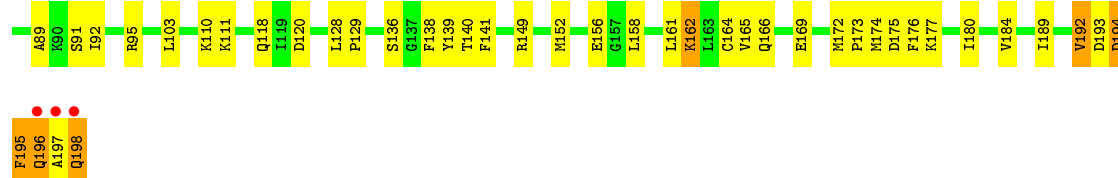
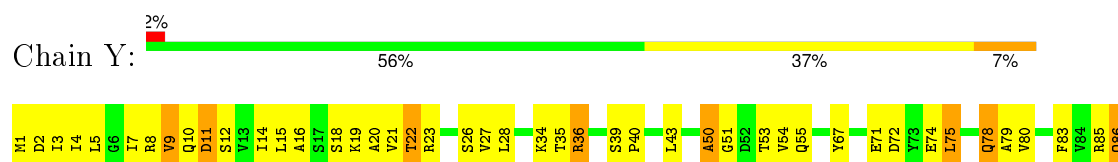
• Molecule 10: Proteasome component PUP3



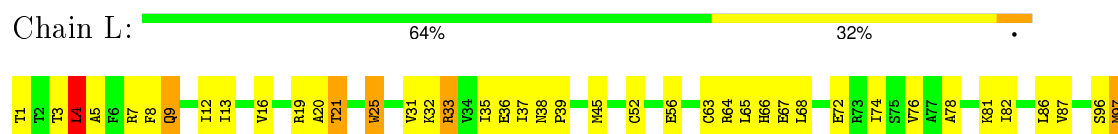
• Molecule 11: Proteasome component C11



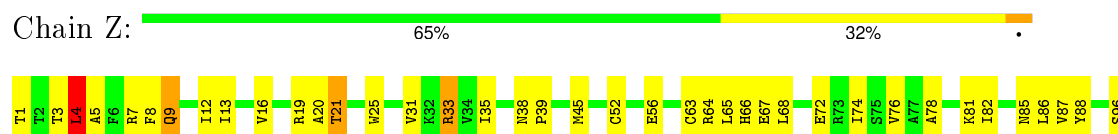
• Molecule 11: Proteasome component C11



• Molecule 12: Proteasome component PRE2

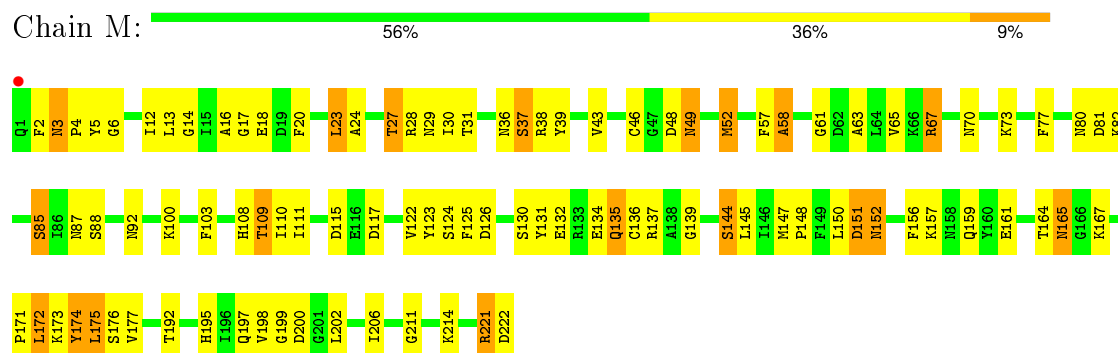


• Molecule 12: Proteasome component PRE2

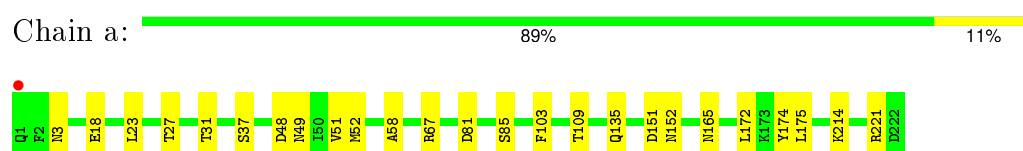




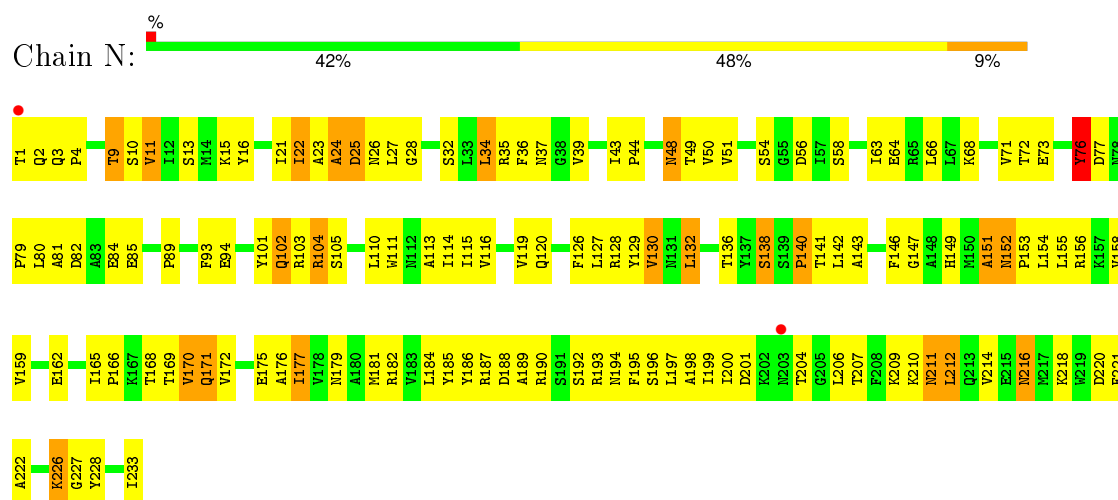
- Molecule 13: Potential proteasome component C5



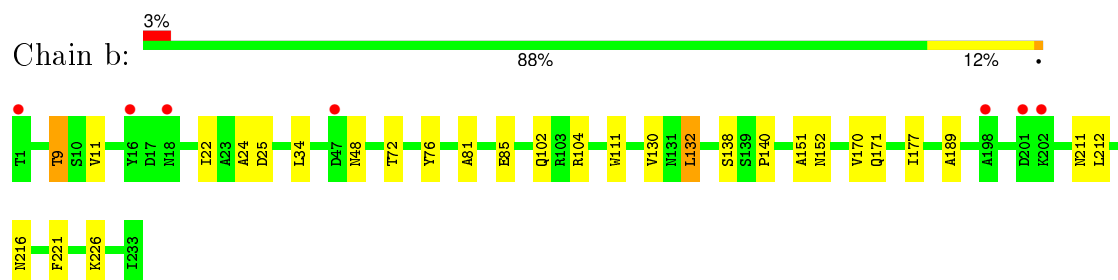
- Molecule 13: Potential proteasome component C5



- Molecule 14: Proteasome component PRE4

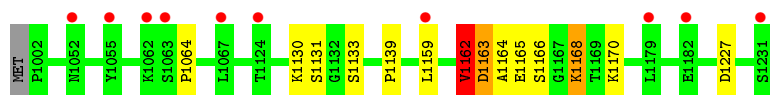


- Molecule 14: Proteasome component PRE4

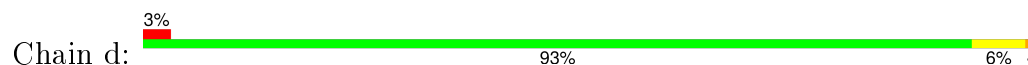


- Molecule 15: proteasome activator protein PA26

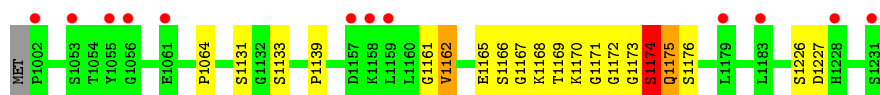




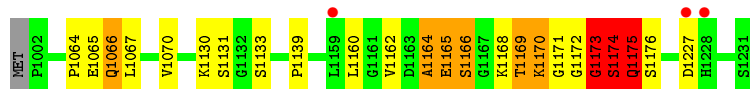
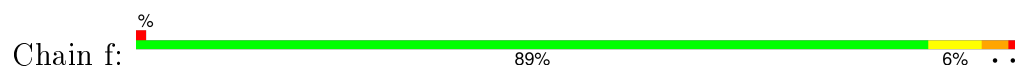
- Molecule 15: proteasome activator protein PA26



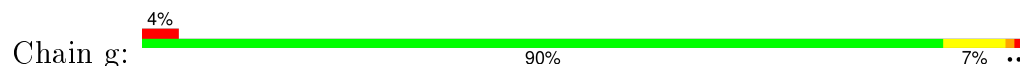
- Molecule 15: proteasome activator protein PA26



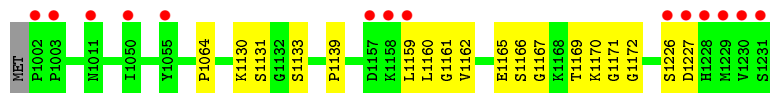
- Molecule 15: proteasome activator protein PA26



- Molecule 15: proteasome activator protein PA26



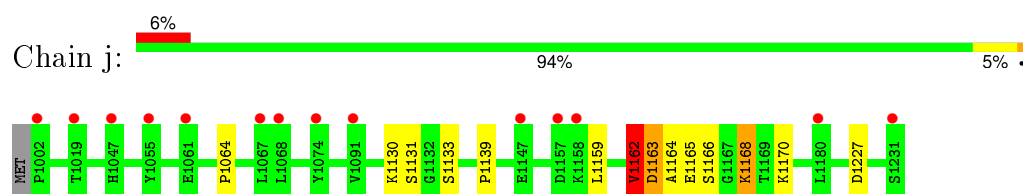
- Molecule 15: proteasome activator protein PA26



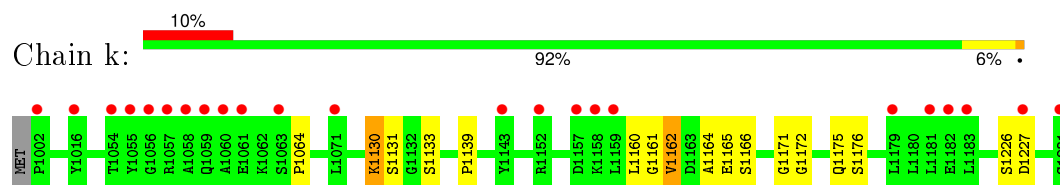
- Molecule 15: proteasome activator protein PA26



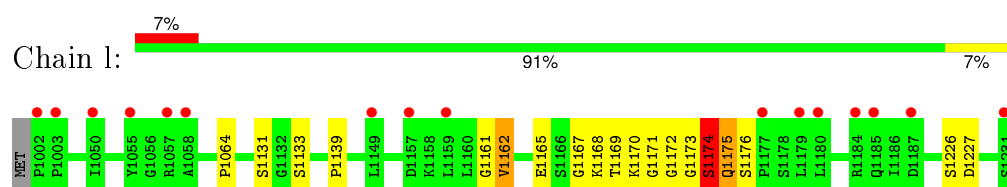
- Molecule 15: proteasome activator protein PA26



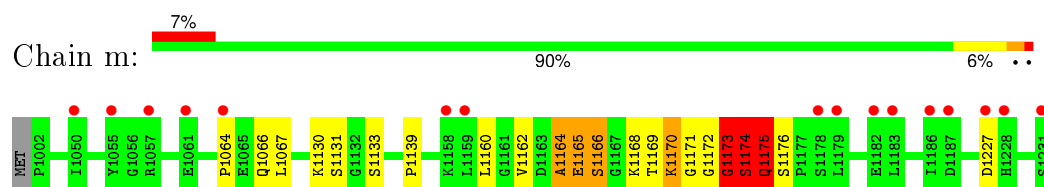
- Molecule 15: proteasome activator protein PA26



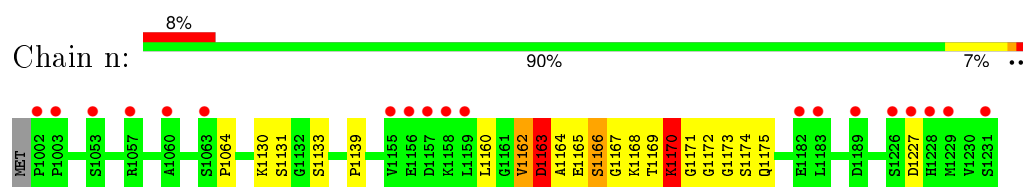
- Molecule 15: proteasome activator protein PA26



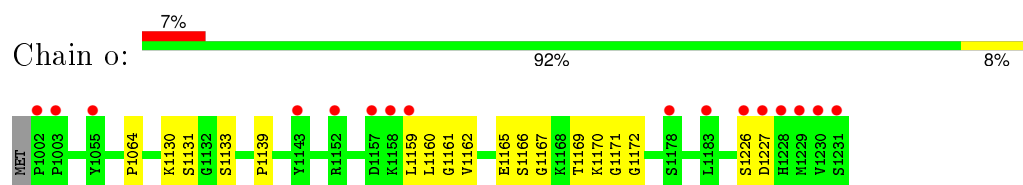
- Molecule 15: proteasome activator protein PA26



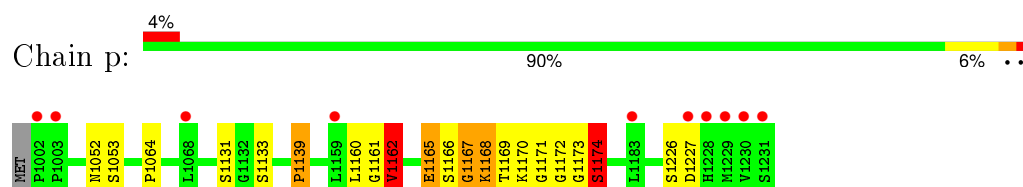
- Molecule 15: proteasome activator protein PA26



- Molecule 15: proteasome activator protein PA26



- Molecule 15: proteasome activator protein PA26



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.96 Å   232.13 Å   296.77 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.80 – 3.22 39.84 – 3.22	Depositor EDS
% Data completeness (in resolution range)	89.1 (39.80-3.22) 88.2 (39.84-3.22)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.25 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.263   ,   0.308 0.275   ,   0.312	Depositor DCC
$R_{free}$ test set	1264 reflections (0.67%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 189495 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	74222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	A	0.50	0/1959	0.70	1/2652 (0.0%)
1	O	0.49	0/1959	0.70	1/2652 (0.0%)
2	B	0.47	0/1944	0.73	0/2632
2	P	0.46	0/1944	0.72	0/2632
3	C	0.47	0/1930	0.69	0/2613
3	Q	0.47	0/1930	0.69	0/2613
4	D	0.47	0/1919	0.69	0/2598
4	R	0.45	0/1919	0.69	0/2598
5	E	0.49	0/1914	0.70	0/2579
5	S	0.47	0/1914	0.70	0/2579
6	F	0.48	0/1831	0.71	1/2473 (0.0%)
6	T	0.48	0/1831	0.70	0/2473
7	G	0.47	0/1932	0.68	0/2609
7	U	0.46	0/1932	0.67	0/2609
8	H	0.51	0/1541	0.74	0/2087
8	V	0.48	0/1541	0.73	0/2087
9	I	0.49	0/1716	0.71	0/2326
9	W	0.48	0/1716	0.70	0/2326
10	J	0.49	0/1611	0.76	2/2174 (0.1%)
10	X	0.50	0/1611	0.75	1/2174 (0.0%)
11	K	0.56	0/1613	0.74	0/2173
11	Y	0.53	0/1613	0.73	0/2173
12	L	0.54	0/1683	0.74	1/2277 (0.0%)
12	Z	0.54	0/1683	0.74	1/2277 (0.0%)
13	M	0.49	0/1795	0.73	0/2420
13	a	0.50	0/1795	0.73	0/2420
14	N	0.49	0/1855	0.75	0/2514
14	b	0.49	0/1855	0.75	0/2514
15	c	0.57	2/1786 (0.1%)	0.77	6/2415 (0.2%)
15	d	0.70	9/1786 (0.5%)	0.88	15/2415 (0.6%)
15	e	0.82	11/1786 (0.6%)	1.01	22/2415 (0.9%)
15	f	0.74	5/1786 (0.3%)	1.19	18/2415 (0.7%)
15	g	0.91	9/1786 (0.5%)	1.17	20/2415 (0.8%)
15	h	0.77	7/1786 (0.4%)	0.94	20/2415 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	i	1.22	17/1786 (1.0%)	1.43	28/2415 (1.2%)
15	j	0.56	2/1786 (0.1%)	0.77	6/2415 (0.2%)
15	k	0.69	9/1786 (0.5%)	0.88	16/2415 (0.7%)
15	l	0.81	11/1786 (0.6%)	1.01	21/2415 (0.9%)
15	m	0.73	5/1786 (0.3%)	1.18	18/2415 (0.7%)
15	n	0.91	9/1786 (0.5%)	1.17	20/2415 (0.8%)
15	o	0.76	7/1786 (0.4%)	0.94	20/2415 (0.8%)
15	p	1.23	17/1786 (1.0%)	1.43	28/2415 (1.2%)
All	All	0.63	120/75490 (0.2%)	0.85	266/102064 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	O	0	1
3	C	0	1
3	Q	0	1
14	N	0	1
15	e	0	1
15	f	0	4
15	g	0	1
15	i	0	4
15	l	0	1
15	m	0	4
15	n	0	1
15	p	0	4
All	All	0	25

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	1172	GLY	C-N	32.26	1.91	1.33
15	p	1172	GLY	C-N	32.26	1.91	1.33
15	g	1163	ASP	C-O	14.32	1.50	1.23
15	n	1163	ASP	C-O	14.30	1.50	1.23
15	i	1173	GLY	N-CA	13.87	1.66	1.46
15	p	1173	GLY	N-CA	13.85	1.66	1.46
15	g	1168	LYS	N-CA	13.72	1.73	1.46
15	n	1168	LYS	N-CA	13.70	1.73	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	n	1168	LYS	CA-C	13.62	1.88	1.52
15	g	1168	LYS	CA-C	13.60	1.88	1.52
15	n	1169	THR	N-CA	13.05	1.72	1.46
15	g	1169	THR	N-CA	13.04	1.72	1.46
15	o	1170	LYS	C-N	-12.80	1.10	1.33
15	h	1170	LYS	C-N	-12.80	1.10	1.33
15	e	1175	GLN	C-O	-12.72	0.99	1.23
15	l	1175	GLN	C-O	-12.70	0.99	1.23
15	p	1172	GLY	C-O	11.93	1.42	1.23
15	i	1172	GLY	C-O	11.86	1.42	1.23
15	m	1066	GLN	CA-CB	11.06	1.78	1.53
15	f	1066	GLN	CA-CB	11.06	1.78	1.53
15	p	1162	VAL	C-N	10.99	1.59	1.34
15	i	1162	VAL	C-N	10.88	1.59	1.34
15	p	1167	GLY	CA-C	10.31	1.68	1.51
15	n	1168	LYS	C-N	9.53	1.55	1.34
15	g	1168	LYS	C-N	9.51	1.55	1.34
15	n	1167	GLY	CA-C	8.93	1.66	1.51
15	g	1167	GLY	CA-C	8.85	1.66	1.51
15	k	1165	GLU	N-CA	8.67	1.63	1.46
15	i	1167	GLY	CA-C	8.55	1.65	1.51
15	d	1165	GLU	N-CA	8.54	1.63	1.46
15	e	1167	GLY	CA-C	8.52	1.65	1.51
15	l	1167	GLY	CA-C	8.52	1.65	1.51
15	l	1175	GLN	C-N	-8.42	1.14	1.34
15	e	1175	GLN	C-N	-8.41	1.14	1.34
15	f	1175	GLN	C-O	-8.33	1.07	1.23
15	m	1175	GLN	C-O	-8.26	1.07	1.23
15	i	1173	GLY	CA-C	-8.25	1.38	1.51
15	p	1173	GLY	CA-C	-8.25	1.38	1.51
15	f	1175	GLN	C-N	-8.08	1.15	1.34
15	p	1170	LYS	N-CA	8.08	1.62	1.46
15	i	1170	LYS	N-CA	8.02	1.62	1.46
15	e	1170	LYS	N-CA	8.01	1.62	1.46
15	l	1170	LYS	N-CA	8.01	1.62	1.46
15	m	1175	GLN	C-N	-8.01	1.15	1.34
15	p	1172	GLY	N-CA	-8.00	1.34	1.46
15	i	1172	GLY	N-CA	-7.99	1.34	1.46
15	i	1169	THR	N-CA	7.72	1.61	1.46
15	e	1169	THR	N-CA	7.67	1.61	1.46
15	p	1169	THR	N-CA	7.66	1.61	1.46
15	l	1169	THR	N-CA	7.65	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	1173	GLY	C-N	-7.54	1.16	1.34
15	p	1173	GLY	C-N	-7.48	1.16	1.34
15	h	1161	GLY	N-CA	-7.29	1.35	1.46
15	o	1161	GLY	N-CA	-7.20	1.35	1.46
15	o	1170	LYS	N-CA	7.18	1.60	1.46
15	i	1172	GLY	CA-C	-7.16	1.40	1.51
15	h	1170	LYS	N-CA	7.12	1.60	1.46
15	p	1172	GLY	CA-C	-7.10	1.40	1.51
15	e	1172	GLY	N-CA	-7.06	1.35	1.46
15	d	1165	GLU	CA-C	7.03	1.71	1.52
15	k	1165	GLU	CA-C	6.99	1.71	1.52
15	l	1172	GLY	N-CA	-6.99	1.35	1.46
15	o	1169	THR	N-CA	6.84	1.60	1.46
15	h	1169	THR	N-CA	6.82	1.59	1.46
15	h	1169	THR	CA-C	6.82	1.70	1.52
15	o	1169	THR	CA-C	6.78	1.70	1.52
15	k	1166	SER	N-CA	6.59	1.59	1.46
15	d	1171	GLY	N-CA	6.58	1.55	1.46
15	d	1171	GLY	CA-C	6.55	1.62	1.51
15	k	1171	GLY	CA-C	6.53	1.62	1.51
15	d	1166	SER	N-CA	6.53	1.59	1.46
15	e	1170	LYS	CA-C	6.52	1.70	1.52
15	l	1170	LYS	CA-C	6.51	1.69	1.52
15	p	1170	LYS	CA-C	6.51	1.69	1.52
15	g	1167	GLY	C-N	6.51	1.49	1.34
15	n	1167	GLY	C-N	6.49	1.49	1.34
15	k	1171	GLY	N-CA	6.47	1.55	1.46
15	i	1170	LYS	CA-C	6.47	1.69	1.52
15	e	1169	THR	CA-C	6.26	1.69	1.52
15	l	1169	THR	CA-C	6.26	1.69	1.52
15	i	1169	THR	CA-C	6.23	1.69	1.52
15	p	1169	THR	CA-C	6.23	1.69	1.52
15	g	1174	SER	CA-CB	-5.95	1.44	1.52
15	d	1164	ALA	C-N	5.94	1.47	1.34
15	n	1174	SER	CA-CB	-5.91	1.44	1.52
15	k	1164	ALA	C-N	5.91	1.47	1.34
15	p	1170	LYS	C-N	5.89	1.43	1.33
15	e	1170	LYS	C-N	5.88	1.43	1.33
15	i	1170	LYS	C-N	5.88	1.43	1.33
15	l	1170	LYS	C-N	5.84	1.43	1.33
15	p	1161	GLY	N-CA	-5.83	1.37	1.46
15	h	1167	GLY	CA-C	5.81	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	1161	GLY	N-CA	-5.78	1.37	1.46
15	o	1167	GLY	CA-C	5.74	1.61	1.51
15	m	1173	GLY	C-O	-5.70	1.14	1.23
15	k	1161	GLY	N-CA	5.68	1.54	1.46
15	f	1173	GLY	C-O	-5.67	1.14	1.23
15	d	1161	GLY	N-CA	5.67	1.54	1.46
15	j	1162	VAL	CA-C	5.61	1.67	1.52
15	c	1162	VAL	CA-C	5.60	1.67	1.52
15	d	1164	ALA	CA-C	5.55	1.67	1.52
15	f	1066	GLN	N-CA	5.54	1.57	1.46
15	k	1164	ALA	CA-C	5.51	1.67	1.52
15	p	1168	LYS	CA-C	5.46	1.67	1.52
15	l	1168	LYS	CA-C	5.43	1.67	1.52
15	i	1168	LYS	CA-C	5.41	1.67	1.52
15	o	1161	GLY	CA-C	-5.39	1.43	1.51
15	e	1168	LYS	CA-C	5.36	1.66	1.52
15	h	1161	GLY	CA-C	-5.36	1.43	1.51
15	d	1161	GLY	CA-C	5.33	1.60	1.51
15	j	1159	LEU	CA-C	-5.33	1.39	1.52
15	c	1159	LEU	CA-C	-5.32	1.39	1.52
15	k	1161	GLY	CA-C	5.26	1.60	1.51
15	i	1162	VAL	CA-C	5.17	1.66	1.52
15	l	1174	SER	N-CA	-5.16	1.36	1.46
15	n	1175	GLN	N-CA	-5.12	1.36	1.46
15	p	1162	VAL	CA-C	5.10	1.66	1.52
15	e	1174	SER	N-CA	-5.10	1.36	1.46
15	g	1175	GLN	N-CA	-5.07	1.36	1.46
15	m	1067	LEU	N-CA	5.00	1.56	1.46

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	n	1174	SER	N-CA-CB	-31.23	63.65	110.50
15	g	1174	SER	N-CA-CB	-31.22	63.68	110.50
15	p	1162	VAL	O-C-N	-27.33	78.97	122.70
15	i	1162	VAL	O-C-N	-27.26	79.09	122.70
15	f	1173	GLY	O-C-N	-27.22	79.15	122.70
15	m	1173	GLY	O-C-N	-27.22	79.15	122.70
15	i	1172	GLY	O-C-N	25.26	166.14	123.20
15	p	1172	GLY	O-C-N	25.22	166.08	123.20
15	m	1175	GLN	O-C-N	-23.36	85.33	122.70
15	f	1175	GLN	O-C-N	-23.33	85.37	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	p	1172	GLY	CA-C-N	-23.19	69.82	116.20
15	i	1172	GLY	CA-C-N	-23.18	69.83	116.20
15	l	1175	GLN	O-C-N	-19.81	91.01	122.70
15	e	1175	GLN	O-C-N	-19.78	91.05	122.70
15	p	1162	VAL	CA-C-N	17.28	155.22	117.20
15	i	1162	VAL	CA-C-N	17.27	155.20	117.20
15	p	1172	GLY	C-N-CA	16.87	157.73	122.30
15	i	1172	GLY	C-N-CA	16.85	157.68	122.30
15	f	1173	GLY	N-CA-C	15.14	150.96	113.10
15	m	1173	GLY	N-CA-C	15.10	150.86	113.10
15	m	1172	GLY	C-N-CA	-14.43	91.99	122.30
15	f	1172	GLY	C-N-CA	-14.40	92.06	122.30
15	p	1173	GLY	CA-C-N	-12.67	89.32	117.20
15	i	1173	GLY	CA-C-N	-12.62	89.43	117.20
15	j	1159	LEU	C-N-CA	-11.98	91.76	121.70
15	c	1159	LEU	C-N-CA	-11.94	91.85	121.70
15	g	1168	LYS	CA-C-N	11.36	142.19	117.20
15	h	1171	GLY	O-C-N	-11.35	103.91	123.20
15	o	1171	GLY	O-C-N	-11.34	103.92	123.20
15	n	1168	LYS	CA-C-N	11.34	142.14	117.20
15	o	1170	LYS	O-C-N	-11.22	104.13	123.20
15	h	1170	LYS	O-C-N	-11.20	104.17	123.20
15	n	1171	GLY	N-CA-C	-10.79	86.12	113.10
15	g	1171	GLY	N-CA-C	-10.79	86.13	113.10
15	p	1161	GLY	CA-C-N	-10.39	94.34	117.20
15	i	1161	GLY	CA-C-N	-10.39	94.35	117.20
15	i	1173	GLY	O-C-N	10.06	138.80	122.70
15	p	1173	GLY	O-C-N	10.05	138.78	122.70
15	n	1160	LEU	CB-CA-C	9.96	129.13	110.20
15	g	1160	LEU	CB-CA-C	9.96	129.12	110.20
15	p	1173	GLY	C-N-CA	-9.79	97.22	121.70
15	i	1173	GLY	C-N-CA	-9.75	97.31	121.70
15	d	1160	LEU	CB-CA-C	-9.47	92.21	110.20
15	k	1160	LEU	CB-CA-C	-9.44	92.27	110.20
15	d	1161	GLY	C-N-CA	9.00	144.21	121.70
15	k	1161	GLY	C-N-CA	8.99	144.17	121.70
15	d	1162	VAL	N-CA-C	8.65	134.35	111.00
15	k	1162	VAL	N-CA-C	8.64	134.33	111.00
15	g	1170	LYS	CB-CA-C	8.53	127.47	110.40
15	h	1171	GLY	CA-C-N	8.53	133.26	116.20
15	o	1171	GLY	CA-C-N	8.50	133.20	116.20
15	n	1170	LYS	CB-CA-C	8.49	127.38	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	n	1163	ASP	N-CA-C	8.48	133.90	111.00
15	g	1163	ASP	N-CA-C	8.48	133.88	111.00
15	i	1161	GLY	C-N-CA	8.37	142.63	121.70
15	p	1161	GLY	C-N-CA	8.37	142.62	121.70
15	l	1172	GLY	CA-C-N	-8.24	99.72	116.20
15	e	1172	GLY	CA-C-N	-8.24	99.73	116.20
15	d	1166	SER	N-CA-C	8.12	132.94	111.00
15	k	1166	SER	N-CA-C	8.11	132.91	111.00
15	h	1131	SER	N-CA-C	8.11	132.89	111.00
15	o	1131	SER	N-CA-C	8.08	132.82	111.00
15	o	1169	THR	CA-C-N	7.91	134.61	117.20
15	h	1169	THR	CA-C-N	7.89	134.55	117.20
15	i	1170	LYS	N-CA-C	7.88	132.28	111.00
15	l	1170	LYS	N-CA-C	7.88	132.26	111.00
15	h	1170	LYS	N-CA-C	7.87	132.25	111.00
15	e	1170	LYS	N-CA-C	7.87	132.24	111.00
15	o	1170	LYS	N-CA-C	7.87	132.24	111.00
15	p	1170	LYS	N-CA-C	7.86	132.22	111.00
15	g	1168	LYS	N-CA-C	7.73	131.88	111.00
15	i	1131	SER	N-CA-C	7.73	131.87	111.00
15	k	1131	SER	N-CA-C	7.72	131.85	111.00
15	p	1131	SER	N-CA-C	7.72	131.85	111.00
15	n	1168	LYS	N-CA-C	7.71	131.82	111.00
15	d	1131	SER	N-CA-C	7.70	131.78	111.00
15	i	1174	SER	N-CA-CB	7.54	121.81	110.50
15	h	1169	THR	O-C-N	-7.50	110.69	122.70
15	p	1174	SER	N-CA-CB	7.50	121.75	110.50
15	o	1169	THR	O-C-N	-7.50	110.71	122.70
15	p	1170	LYS	CB-CA-C	-7.41	95.57	110.40
15	i	1170	LYS	CB-CA-C	-7.41	95.58	110.40
15	e	1173	GLY	N-CA-C	-7.39	94.61	113.10
15	e	1170	LYS	CB-CA-C	-7.39	95.62	110.40
15	l	1170	LYS	CB-CA-C	-7.39	95.62	110.40
15	p	1174	SER	O-C-N	-7.37	110.91	122.70
15	n	1131	SER	N-CA-C	7.37	130.89	111.00
15	g	1131	SER	N-CA-C	7.36	130.88	111.00
15	g	1168	LYS	CB-CA-C	-7.36	95.67	110.40
15	n	1168	LYS	CB-CA-C	-7.36	95.68	110.40
15	l	1173	GLY	N-CA-C	-7.34	94.76	113.10
15	i	1174	SER	O-C-N	-7.33	110.98	122.70
15	l	1131	SER	N-CA-C	7.31	130.74	111.00
15	e	1131	SER	N-CA-C	7.31	130.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	j	1131	SER	N-CA-C	7.23	130.53	111.00
15	o	1172	GLY	CA-C-N	-7.22	101.76	116.20
15	h	1172	GLY	CA-C-N	-7.22	101.77	116.20
15	c	1131	SER	N-CA-C	7.21	130.48	111.00
15	m	1173	GLY	CA-C-N	7.21	133.06	117.20
15	f	1173	GLY	CA-C-N	7.19	133.01	117.20
15	g	1172	GLY	C-N-CA	-7.16	107.26	122.30
15	n	1172	GLY	C-N-CA	-7.16	107.27	122.30
15	p	1162	VAL	N-CA-CB	-7.14	95.78	111.50
15	i	1162	VAL	N-CA-CB	-7.14	95.79	111.50
15	f	1170	LYS	CB-CA-C	7.13	124.66	110.40
15	h	1160	LEU	C-N-CA	-7.13	107.33	122.30
15	o	1160	LEU	C-N-CA	-7.13	107.33	122.30
15	g	1169	THR	N-CA-CB	7.11	123.81	110.30
15	n	1169	THR	N-CA-CB	7.11	123.81	110.30
15	m	1170	LYS	CB-CA-C	7.10	124.61	110.40
15	l	1171	GLY	C-N-CA	-7.10	107.39	122.30
15	e	1171	GLY	C-N-CA	-7.09	107.42	122.30
15	o	1170	LYS	CA-C-N	7.04	130.27	116.20
15	h	1170	LYS	CA-C-N	7.03	130.25	116.20
15	g	1167	GLY	C-N-CA	7.00	139.20	121.70
15	i	1161	GLY	CA-C-O	7.00	133.20	120.60
15	n	1167	GLY	C-N-CA	6.99	139.16	121.70
15	k	1160	LEU	CA-C-N	6.97	130.14	116.20
15	p	1161	GLY	CA-C-O	6.95	133.12	120.60
15	f	1164	ALA	CA-C-N	6.95	132.48	117.20
15	d	1160	LEU	CA-C-N	6.94	130.09	116.20
15	g	1168	LYS	O-C-N	-6.94	111.60	122.70
15	m	1164	ALA	CA-C-N	6.93	132.44	117.20
15	i	1171	GLY	C-N-CA	-6.90	107.81	122.30
15	p	1171	GLY	C-N-CA	-6.90	107.82	122.30
15	n	1168	LYS	O-C-N	-6.88	111.70	122.70
15	i	1165	GLU	C-N-CA	6.86	138.84	121.70
15	l	1165	GLU	C-N-CA	6.85	138.82	121.70
15	e	1165	GLU	C-N-CA	6.84	138.80	121.70
15	p	1165	GLU	C-N-CA	6.81	138.73	121.70
15	o	1159	LEU	CB-CA-C	-6.81	97.27	110.20
15	h	1159	LEU	CB-CA-C	-6.80	97.27	110.20
15	e	1175	GLN	CA-C-O	6.78	134.33	120.10
15	e	1161	GLY	N-CA-C	6.77	130.03	113.10
15	l	1175	GLN	CA-C-O	6.76	134.30	120.10
15	l	1161	GLY	N-CA-C	6.74	129.96	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	m	1175	GLN	CB-CA-C	6.74	123.89	110.40
15	f	1175	GLN	CB-CA-C	6.74	123.88	110.40
15	d	1130	LYS	C-N-CA	-6.72	104.89	121.70
15	k	1130	LYS	C-N-CA	-6.69	104.98	121.70
15	m	1131	SER	N-CA-C	6.67	129.02	111.00
15	c	1159	LEU	CB-CA-C	-6.67	97.52	110.20
15	n	1168	LYS	CA-C-O	-6.67	106.09	120.10
15	j	1159	LEU	CB-CA-C	-6.67	97.53	110.20
15	f	1131	SER	N-CA-C	6.66	128.98	111.00
15	g	1168	LYS	CA-C-O	-6.64	106.14	120.10
15	n	1173	GLY	N-CA-C	-6.62	96.55	113.10
15	g	1173	GLY	N-CA-C	-6.61	96.56	113.10
15	g	1169	THR	CB-CA-C	-6.54	93.95	111.60
15	n	1169	THR	CB-CA-C	-6.53	93.96	111.60
15	c	1163	ASP	C-N-CA	-6.51	105.43	121.70
15	j	1163	ASP	C-N-CA	-6.48	105.49	121.70
12	Z	4	LEU	CA-CB-CG	6.43	130.09	115.30
15	f	1174	SER	CA-C-N	-6.43	103.06	117.20
15	m	1174	SER	CA-C-N	-6.42	103.07	117.20
15	l	1176	SER	N-CA-CB	-6.41	100.89	110.50
15	e	1176	SER	N-CA-CB	-6.40	100.91	110.50
15	m	1160	LEU	CA-CB-CG	-6.36	100.68	115.30
12	L	4	LEU	CA-CB-CG	6.35	129.90	115.30
15	f	1160	LEU	CA-CB-CG	-6.33	100.75	115.30
15	l	1175	GLN	CA-C-N	6.26	130.97	117.20
15	g	1174	SER	CA-C-N	-6.25	103.45	117.20
15	n	1174	SER	CA-C-N	-6.23	103.49	117.20
15	e	1175	GLN	CA-C-N	6.22	130.88	117.20
15	g	1162	VAL	C-N-CA	-6.21	106.19	121.70
15	n	1162	VAL	C-N-CA	-6.20	106.21	121.70
15	o	1161	GLY	CA-C-N	-6.09	103.81	117.20
15	h	1161	GLY	CA-C-N	-6.07	103.85	117.20
15	p	1161	GLY	O-C-N	6.06	132.39	122.70
15	f	1174	SER	N-CA-C	6.01	127.23	111.00
15	m	1169	THR	C-N-CA	-6.01	106.68	121.70
15	i	1162	VAL	C-N-CA	6.01	136.72	121.70
15	i	1161	GLY	O-C-N	6.00	132.31	122.70
15	m	1171	GLY	C-N-CA	-6.00	109.69	122.30
15	m	1174	SER	N-CA-C	6.00	127.19	111.00
15	f	1171	GLY	C-N-CA	-5.99	109.72	122.30
15	m	1174	SER	O-C-N	5.96	132.23	122.70
15	p	1162	VAL	C-N-CA	5.95	136.57	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	1169	THR	C-N-CA	-5.94	106.85	121.70
15	f	1174	SER	O-C-N	5.94	132.21	122.70
15	h	1171	GLY	N-CA-C	-5.76	98.69	113.10
15	o	1171	GLY	N-CA-C	-5.74	98.76	113.10
15	c	1168	LYS	N-CA-C	-5.72	95.54	111.00
15	j	1168	LYS	N-CA-C	-5.72	95.54	111.00
15	g	1163	ASP	CA-C-N	-5.69	104.67	117.20
15	n	1163	ASP	CA-C-N	-5.68	104.70	117.20
15	k	1165	GLU	CA-C-N	5.64	129.60	117.20
15	d	1172	GLY	N-CA-C	5.63	127.18	113.10
15	d	1165	GLU	CA-C-N	5.62	129.56	117.20
15	i	1160	LEU	CA-C-N	-5.62	104.97	116.20
15	p	1173	GLY	CA-C-O	5.62	130.71	120.60
15	p	1160	LEU	CA-C-N	-5.61	104.97	116.20
15	h	1172	GLY	O-C-N	5.61	132.74	123.20
15	k	1172	GLY	N-CA-C	5.61	127.12	113.10
15	o	1172	GLY	O-C-N	5.60	132.72	123.20
15	l	1162	VAL	CA-C-N	-5.59	104.90	117.20
15	e	1162	VAL	CA-C-N	-5.58	104.94	117.20
15	i	1173	GLY	CA-C-O	5.57	130.62	120.60
15	d	1160	LEU	N-CA-C	5.55	125.99	111.00
15	k	1160	LEU	N-CA-C	5.55	125.99	111.00
15	e	1165	GLU	N-CA-C	5.51	125.88	111.00
15	i	1165	GLU	N-CA-C	5.51	125.87	111.00
15	p	1165	GLU	N-CA-C	5.51	125.87	111.00
15	j	1131	SER	CB-CA-C	-5.50	99.65	110.10
15	l	1165	GLU	N-CA-C	5.49	125.83	111.00
15	h	1165	GLU	CA-C-N	-5.49	105.13	117.20
15	c	1131	SER	CB-CA-C	-5.48	99.70	110.10
15	o	1165	GLU	CA-C-N	-5.47	105.17	117.20
15	o	1165	GLU	C-N-CA	5.46	135.36	121.70
15	h	1165	GLU	C-N-CA	5.46	135.35	121.70
15	p	1165	GLU	CA-C-N	-5.46	105.20	117.20
15	e	1165	GLU	CA-C-N	-5.42	105.28	117.20
15	f	1164	ALA	O-C-N	-5.42	114.03	122.70
15	i	1165	GLU	CA-C-N	-5.41	105.29	117.20
15	l	1165	GLU	CA-C-N	-5.41	105.30	117.20
15	g	1165	GLU	C-N-CA	5.40	135.20	121.70
15	m	1164	ALA	O-C-N	-5.40	114.06	122.70
15	n	1165	GLU	C-N-CA	5.38	135.16	121.70
15	p	1167	GLY	N-CA-C	5.38	126.56	113.10
15	e	1170	LYS	CA-C-N	5.38	126.96	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	l	1170	LYS	CA-C-N	5.38	126.95	116.20
15	p	1170	LYS	CA-C-N	5.37	126.95	116.20
10	J	102	TYR	N-CA-C	-5.37	96.50	111.00
15	m	1171	GLY	N-CA-C	-5.37	99.67	113.10
15	i	1170	LYS	CA-C-N	5.37	126.94	116.20
15	h	1162	VAL	CA-C-N	-5.35	105.44	117.20
15	f	1171	GLY	N-CA-C	-5.35	99.73	113.10
15	o	1162	VAL	CA-C-N	-5.32	105.49	117.20
15	h	1169	THR	C-N-CA	5.30	134.94	121.70
15	o	1169	THR	C-N-CA	5.28	134.91	121.70
15	o	1166	SER	CA-C-N	5.27	126.73	116.20
15	h	1166	SER	CA-C-N	5.25	126.71	116.20
15	e	1174	SER	C-N-CA	-5.25	108.57	121.70
15	o	1165	GLU	N-CA-C	5.23	125.13	111.00
15	l	1174	SER	C-N-CA	-5.21	108.67	121.70
15	d	1131	SER	CB-CA-C	-5.21	100.20	110.10
15	l	1172	GLY	C-N-CA	5.21	133.23	122.30
15	k	1131	SER	CB-CA-C	-5.20	100.23	110.10
15	e	1172	GLY	C-N-CA	5.19	133.20	122.30
15	h	1165	GLU	N-CA-C	5.19	125.01	111.00
15	k	1131	SER	CA-C-N	-5.19	105.82	116.20
15	d	1164	ALA	C-N-CA	5.18	134.65	121.70
15	k	1164	ALA	C-N-CA	5.18	134.66	121.70
15	d	1131	SER	CA-C-N	-5.17	105.85	116.20
15	e	1172	GLY	O-C-N	5.17	131.99	123.20
15	l	1172	GLY	O-C-N	5.16	131.96	123.20
15	p	1166	SER	C-N-CA	-5.15	111.49	122.30
15	d	1165	GLU	N-CA-C	5.12	124.82	111.00
15	k	1165	GLU	N-CA-C	5.11	124.80	111.00
10	J	100	GLY	N-CA-C	-5.08	100.39	113.10
6	F	72	LEU	CA-CB-CG	5.08	126.99	115.30
15	e	1131	SER	CB-CA-C	-5.07	100.47	110.10
15	f	1165	GLU	N-CA-C	5.06	124.66	111.00
15	l	1167	GLY	N-CA-C	5.06	125.74	113.10
1	O	12	TYR	CA-C-N	-5.05	106.08	117.20
15	e	1167	GLY	N-CA-C	5.05	125.72	113.10
15	l	1131	SER	CB-CA-C	-5.05	100.51	110.10
1	A	12	TYR	CA-C-N	-5.04	106.11	117.20
15	i	1167	GLY	N-CA-C	5.04	125.69	113.10
15	m	1165	GLU	N-CA-C	5.03	124.59	111.00
10	X	100	GLY	N-CA-C	-5.01	100.56	113.10
15	d	1160	LEU	CA-CB-CG	5.01	126.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	1166	SER	CA-C-N	5.01	126.23	116.20
15	k	1160	LEU	CA-CB-CG	5.01	126.83	115.30
15	k	1175	GLN	N-CA-C	5.01	124.52	111.00
15	e	1166	SER	CA-C-N	5.00	126.21	116.20

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Mainchain
3	C	20	TYR	Sidechain
14	N	76	TYR	Sidechain
1	O	12	TYR	Mainchain
3	Q	20	TYR	Sidechain
15	e	1175	GLN	Mainchain
15	f	1173	GLY	Mainchain,Peptide
15	f	1174	SER	Mainchain
15	f	1175	GLN	Mainchain
15	g	1163	ASP	Mainchain
15	i	1139	PRO	Mainchain
15	i	1162	VAL	Mainchain,Peptide
15	i	1174	SER	Mainchain
15	l	1175	GLN	Mainchain
15	m	1173	GLY	Mainchain,Peptide
15	m	1174	SER	Mainchain
15	m	1175	GLN	Mainchain
15	n	1163	ASP	Mainchain
15	p	1139	PRO	Mainchain
15	p	1162	VAL	Mainchain,Peptide
15	p	1174	SER	Mainchain

## 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	A	1921	0	1910	232	0
1	O	1921	0	1910	229	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1907	0	1917	159	0
2	P	1907	0	1917	161	0
3	C	1900	0	1898	146	0
3	Q	1900	0	1898	142	0
4	D	1890	0	1900	89	0
4	R	1890	0	1900	92	0
5	E	1888	0	1856	106	0
5	S	1888	0	1856	104	0
6	F	1803	0	1809	110	0
6	T	1803	0	1809	107	0
7	G	1892	0	1883	156	0
7	U	1892	0	1883	152	0
8	H	1512	0	1481	161	0
8	V	1512	0	1481	151	0
9	I	1685	0	1688	104	0
9	W	1685	0	1688	119	0
10	J	1581	0	1574	75	0
10	X	1581	0	1574	76	0
11	K	1585	0	1590	80	0
11	Y	1585	0	1590	89	0
12	L	1646	0	1595	72	0
12	Z	1646	0	1595	71	0
13	M	1757	0	1711	93	0
13	a	1757	0	1711	0	0
14	N	1824	0	1832	158	0
14	b	1824	0	1832	0	0
15	c	1760	0	1784	0	0
15	d	1760	0	1784	0	0
15	e	1760	0	1783	0	0
15	f	1760	0	1783	0	37
15	g	1760	0	1784	0	0
15	h	1760	0	1783	0	0
15	i	1760	0	1782	0	0
15	j	1760	0	1784	0	0
15	k	1760	0	1784	0	0
15	l	1760	0	1783	0	0
15	m	1760	0	1783	0	0
15	n	1760	0	1784	0	0
15	o	1760	0	1783	0	0
15	p	1760	0	1782	0	37
All	All	74222	0	74254	3042	37

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 28.

All (3042) 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)
8:V:8:PHE:HE2	8:V:148:LYS:HA	1.13	1.12
3:Q:175:LEU:HD11	3:Q:199:LYS:HD2	1.33	1.11
3:C:175:LEU:HD11	3:C:199:LYS:HD2	1.33	1.10
8:H:8:PHE:HE2	8:H:148:LYS:HA	1.14	1.10
2:B:222:LEU:HD11	2:B:232:GLY:HA2	1.35	1.08
9:I:59:ILE:HG12	9:I:83:LEU:HD23	1.36	1.08
7:G:71:ARG:NH2	14:N:72:THR:HG22	1.68	1.08
2:P:222:LEU:HD11	2:P:232:GLY:HA2	1.35	1.08
1:A:204:GLU:HB3	1:A:248:ILE:HG21	1.30	1.07
7:G:71:ARG:HH21	14:N:72:THR:HG22	1.16	1.05
1:O:204:GLU:HB3	1:O:248:ILE:HG21	1.32	1.05
7:G:187:SER:HB3	7:G:190:GLU:HB2	1.40	1.04
4:R:163:THR:HG21	4:R:171:VAL:HG23	1.41	1.03
9:W:59:ILE:HG12	9:W:83:LEU:HD23	1.37	1.02
3:C:68:LYS:HG2	3:C:227:GLN:HE22	1.27	0.99
3:Q:68:LYS:HG2	3:Q:227:GLN:HE22	1.25	0.99
13:M:175:LEU:HD12	13:M:175:LEU:H	1.25	0.99
4:D:59:ILE:HD13	4:D:59:ILE:H	1.27	0.98
6:F:206:LEU:H	6:F:206:LEU:HD23	1.29	0.98
7:U:187:SER:HB3	7:U:190:GLU:HB2	1.43	0.98
13:M:173:LYS:HD3	13:M:174:TYR:H	1.27	0.98
4:D:163:THR:HG21	4:D:171:VAL:HG23	1.41	0.98
4:R:59:ILE:HD13	4:R:59:ILE:H	1.28	0.97
2:P:68:THR:HG23	2:P:71:ILE:HB	1.46	0.94
3:C:9:ARG:HE	3:C:12:ILE:HG13	1.33	0.94
3:Q:201:THR:HG22	3:Q:202:ASP:H	1.32	0.94
2:B:68:THR:HG23	2:B:71:ILE:HB	1.46	0.93
3:Q:9:ARG:HE	3:Q:12:ILE:HG13	1.32	0.93
9:I:53:GLU:O	9:I:57:GLN:HG2	1.67	0.93
1:O:114:CYS:HG	1:O:155:TYR:HD1	1.00	0.93
1:O:230:LYS:HE3	1:O:230:LYS:HA	1.51	0.93
7:G:136:ILE:HG12	7:G:149:MET:HG3	1.50	0.93
5:S:109:VAL:HB	5:S:154:GLN:HE21	1.34	0.93
3:C:217:ARG:HB3	3:C:217:ARG:HH11	1.33	0.93
7:U:136:ILE:HG12	7:U:149:MET:HG3	1.49	0.93
6:T:206:LEU:HD23	6:T:206:LEU:H	1.30	0.92
9:W:53:GLU:O	9:W:57:GLN:HG2	1.69	0.92
1:A:114:CYS:HG	1:A:155:TYR:HD1	0.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:90:ARG:HD3	9:W:68:LEU:HD13	1.50	0.91
3:C:201:THR:HG22	3:C:202:ASP:H	1.33	0.91
2:B:161:ALA:HB3	3:C:56:LEU:HD23	1.52	0.90
3:Q:217:ARG:HH11	3:Q:217:ARG:HB3	1.34	0.90
7:G:171:ALA:O	7:G:175:LEU:HB2	1.71	0.90
7:U:171:ALA:O	7:U:175:LEU:HB2	1.70	0.90
8:V:13:ILE:HG12	8:V:177:VAL:HG22	1.50	0.90
2:P:161:ALA:HB3	3:Q:56:LEU:HD23	1.53	0.90
10:J:14:MET:HE3	10:J:166:ILE:HG13	1.52	0.90
7:U:72:HIS:CD2	7:U:73:ILE:HG13	2.07	0.90
8:H:8:PHE:CE2	8:H:148:LYS:HA	2.06	0.90
3:Q:68:LYS:HG2	3:Q:227:GLN:NE2	1.85	0.90
1:A:230:LYS:HA	1:A:230:LYS:HE3	1.50	0.89
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.36	0.89
8:H:13:ILE:HG12	8:H:177:VAL:HG22	1.54	0.89
8:V:8:PHE:CE2	8:V:148:LYS:HA	2.05	0.89
5:E:109:VAL:HB	5:E:154:GLN:HE21	1.37	0.89
8:H:114:PRO:HD2	8:H:118:SER:O	1.73	0.88
3:C:68:LYS:HG2	3:C:227:GLN:NE2	1.88	0.88
4:R:203:VAL:HG21	4:R:210:ILE:HD11	1.56	0.88
2:P:57:MET:HB3	2:P:59:GLU:OE2	1.73	0.88
3:C:185:LYS:HD2	3:C:186:VAL:H	1.40	0.87
2:B:218:ASN:HD21	2:B:236:ARG:HD2	1.39	0.87
7:G:72:HIS:CD2	7:G:73:ILE:HG13	2.08	0.87
4:D:203:VAL:HG21	4:D:210:ILE:HD11	1.56	0.87
2:P:218:ASN:HD21	2:P:236:ARG:HD2	1.40	0.87
3:Q:156:ASN:HD21	4:R:79:ASN:HB3	1.38	0.87
7:G:94:GLU:HG3	7:G:114:ARG:HH11	1.40	0.87
3:C:156:ASN:HD21	4:D:79:ASN:HB3	1.38	0.87
4:R:99:THR:O	4:R:100:LEU:HD12	1.75	0.86
3:Q:185:LYS:HD2	3:Q:186:VAL:H	1.38	0.86
2:B:57:MET:HB3	2:B:59:GLU:OE2	1.75	0.86
4:R:162:GLN:HA	4:R:162:GLN:HE21	1.41	0.85
4:D:99:THR:O	4:D:100:LEU:HD12	1.75	0.85
1:A:178:ILE:O	1:A:182:LEU:HG	1.75	0.85
8:H:107:LYS:HD2	8:H:108:GLY:H	1.42	0.85
8:V:114:PRO:HD2	8:V:118:SER:O	1.76	0.85
9:W:37:ILE:HD11	9:W:43:CYS:SG	2.16	0.85
1:O:178:ILE:O	1:O:182:LEU:HG	1.76	0.85
2:P:74:VAL:HG22	2:P:75:TYR:H	1.41	0.85
4:D:162:GLN:HE21	4:D:162:GLN:HA	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:239:GLU:HA	4:R:242:GLU:HB3	1.58	0.84
4:D:239:GLU:HA	4:D:242:GLU:HB3	1.58	0.84
4:D:207:ALA:HB2	4:D:233:VAL:HG21	1.58	0.84
4:R:207:ALA:HB2	4:R:233:VAL:HG21	1.59	0.84
8:V:107:LYS:HD2	8:V:108:GLY:H	1.40	0.84
2:P:94:HIS:HD2	9:W:61:SER:HB2	1.42	0.84
2:B:211:LEU:HD12	2:B:212:ALA:N	1.93	0.83
9:I:113:ILE:HG23	9:I:119:THR:HG22	1.61	0.83
12:Z:1:THR:HA	12:Z:33:ARG:NH2	1.92	0.83
3:Q:70:ASN:ND2	3:Q:71:ASP:H	1.76	0.83
10:X:14:MET:HE3	10:X:166:ILE:HG13	1.58	0.83
14:N:32:SER:HA	14:N:190:ARG:NH1	1.92	0.83
7:U:5:THR:HG22	7:U:7:TYR:H	1.43	0.83
7:U:72:HIS:HD2	7:U:73:ILE:HG13	1.43	0.83
14:N:43:ILE:HD13	14:N:64:GLU:HG3	1.59	0.83
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.59	0.82
1:O:22:GLU:HA	2:P:26:THR:HG21	1.61	0.82
7:G:92:ARG:CZ	14:N:76:TYR:HD1	1.91	0.82
2:B:148:TYR:CE2	2:B:158:PRO:HB3	2.14	0.82
4:R:188:VAL:O	4:R:192:VAL:HG23	1.78	0.82
13:M:126:ASP:HB2	13:M:130:SER:HB3	1.62	0.82
2:B:74:VAL:HG22	2:B:75:TYR:H	1.42	0.82
3:C:217:ARG:HB3	3:C:217:ARG:NH1	1.93	0.82
2:B:90:ARG:HD3	9:I:68:LEU:HD13	1.62	0.81
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.60	0.81
1:O:44:ALA:HB2	1:O:53:VAL:HG12	1.60	0.81
6:F:176:LEU:HD22	7:G:57:LEU:HD23	1.63	0.81
1:A:44:ALA:HB2	1:A:53:VAL:HG12	1.63	0.81
1:A:22:GLU:HA	2:B:26:THR:HG21	1.62	0.81
12:L:1:THR:HA	12:L:33:ARG:NH2	1.96	0.81
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.63	0.81
9:W:113:ILE:HG23	9:W:119:THR:HG22	1.63	0.81
8:H:67:THR:HG22	8:H:73:PRO:HD3	1.61	0.81
8:V:14:LEU:HD23	8:V:100:ALA:HB3	1.62	0.81
3:Q:217:ARG:NH1	3:Q:217:ARG:HB3	1.94	0.81
2:B:94:HIS:HB3	2:B:99:ARG:HH21	1.46	0.81
4:D:188:VAL:O	4:D:192:VAL:HG23	1.80	0.81
7:G:5:THR:HG22	7:G:7:TYR:H	1.46	0.81
12:Z:1:THR:HA	12:Z:33:ARG:HH21	1.47	0.80
6:T:179:PHE:HA	6:T:182:ILE:HG13	1.62	0.80
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HA	2:B:127:VAL:HG12	1.64	0.80
11:K:43:LEU:HD13	11:K:189:ILE:HD13	1.63	0.80
1:O:131:ARG:HA	2:P:127:VAL:HG12	1.64	0.80
6:F:100:ASN:HB2	14:N:94:GLU:HG2	1.63	0.80
14:N:32:SER:HA	14:N:190:ARG:HH12	1.47	0.80
7:G:88:VAL:O	7:G:92:ARG:HG3	1.82	0.79
13:M:173:LYS:HD3	13:M:174:TYR:N	1.96	0.79
4:D:199:LEU:O	4:D:203:VAL:HG23	1.82	0.79
8:H:14:LEU:HD13	8:H:34:LEU:HD22	1.64	0.79
2:P:211:LEU:HD12	2:P:212:ALA:N	1.96	0.79
9:I:37:ILE:HD11	9:I:43:CYS:SG	2.22	0.79
5:E:233:ASN:HD22	5:E:233:ASN:N	1.81	0.79
1:O:82:VAL:CG1	1:O:142:THR:HB	2.13	0.79
14:N:152:ASN:HD22	14:N:156:ARG:NH2	1.79	0.79
7:U:88:VAL:O	7:U:92:ARG:HG3	1.83	0.79
7:G:72:HIS:HD2	7:G:73:ILE:HG13	1.45	0.79
13:M:172:LEU:H	13:M:172:LEU:HD12	1.47	0.79
2:P:148:TYR:CE2	2:P:158:PRO:HB3	2.17	0.79
13:M:28:ARG:NE	13:M:200:ASP:OD2	2.16	0.79
7:G:40:LYS:HA	7:G:45:VAL:HG12	1.63	0.79
6:F:179:PHE:HA	6:F:182:ILE:HG13	1.63	0.79
1:O:82:VAL:HG13	1:O:142:THR:HB	1.64	0.79
11:K:23:ARG:HB2	11:K:28:LEU:HD11	1.63	0.79
6:F:206:LEU:H	6:F:206:LEU:CD2	1.97	0.78
8:V:67:THR:HG22	8:V:73:PRO:HD3	1.66	0.78
3:C:70:ASN:ND2	3:C:71:ASP:H	1.80	0.78
11:Y:43:LEU:HD13	11:Y:189:ILE:HD13	1.63	0.78
5:E:233:ASN:HD22	5:E:233:ASN:H	1.32	0.78
4:R:199:LEU:O	4:R:203:VAL:HG23	1.84	0.78
1:A:82:VAL:CG1	1:A:142:THR:HB	2.14	0.78
5:S:233:ASN:N	5:S:233:ASN:HD22	1.80	0.77
9:W:112:SER:HB3	9:W:125:LEU:HD13	1.66	0.77
5:S:233:ASN:H	5:S:233:ASN:HD22	1.30	0.77
14:N:165:ILE:N	14:N:166:PRO:HD2	2.00	0.77
2:P:94:HIS:HB3	2:P:99:ARG:HH21	1.49	0.77
8:V:17:ASP:HB2	8:V:170:GLY:O	1.85	0.77
5:S:204:LEU:O	5:S:208:MET:HB2	1.84	0.77
2:P:49:LYS:HE2	2:P:58:SER:HB2	1.67	0.77
5:E:24:VAL:O	5:E:27:SER:HB3	1.85	0.77
14:N:27:LEU:HB2	14:N:192:SER:HB2	1.66	0.77
8:H:107:LYS:HD2	8:H:108:GLY:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:204:LEU:O	5:E:208:MET:HB2	1.83	0.77
8:H:14:LEU:HD23	8:H:100:ALA:HB3	1.64	0.77
8:V:14:LEU:HD13	8:V:34:LEU:HD22	1.65	0.77
1:A:82:VAL:HG13	1:A:142:THR:HB	1.67	0.77
7:U:40:LYS:HA	7:U:45:VAL:HG12	1.66	0.77
2:B:15:SER:O	3:C:27:GLU:HG3	1.84	0.77
2:B:49:LYS:HE2	2:B:58:SER:HB2	1.67	0.77
2:P:15:SER:O	3:Q:27:GLU:HG3	1.85	0.77
1:O:204:GLU:HB3	1:O:248:ILE:CG2	2.13	0.77
3:C:9:ARG:HE	3:C:12:ILE:CG1	1.98	0.77
11:Y:23:ARG:HB2	11:Y:28:LEU:HD11	1.65	0.77
6:T:206:LEU:CD2	6:T:206:LEU:H	1.98	0.77
8:V:107:LYS:HD2	8:V:108:GLY:N	1.99	0.76
6:T:176:LEU:HD22	7:U:57:LEU:HD23	1.64	0.76
6:F:201:LEU:HD11	6:F:206:LEU:HD22	1.67	0.76
5:S:24:VAL:O	5:S:27:SER:HB3	1.85	0.76
3:C:243:GLY:C	3:C:244:ILE:HD12	2.06	0.76
10:X:159:PRO:HG2	10:X:160:GLU:OE2	1.86	0.76
1:A:204:GLU:HB3	1:A:248:ILE:CG2	2.12	0.76
3:Q:9:ARG:HE	3:Q:12:ILE:CG1	1.98	0.76
2:P:44:VAL:HG23	2:P:211:LEU:HD11	1.66	0.76
12:L:1:THR:HA	12:L:33:ARG:HH21	1.49	0.76
6:T:46:LEU:HG	6:T:135:ILE:HD13	1.68	0.76
4:R:42:VAL:HG11	4:R:136:ALA:HB1	1.68	0.76
11:Y:39:SER:HB2	11:Y:40:PRO:HD2	1.68	0.76
2:P:44:VAL:HA	2:P:213:ILE:HG22	1.68	0.75
1:A:185:HIS:HA	1:A:188:LYS:NZ	2.01	0.75
10:J:129:ILE:HG22	10:J:130:ASP:N	2.01	0.75
10:J:88:GLN:HA	10:J:88:GLN:NE2	2.02	0.75
10:J:159:PRO:HG2	10:J:160:GLU:OE2	1.87	0.75
1:O:92:ASN:HD22	1:O:137:LEU:HD11	1.51	0.75
7:G:94:GLU:HG2	7:G:114:ARG:HB3	1.69	0.75
10:X:129:ILE:HG22	10:X:130:ASP:N	2.01	0.75
8:H:17:ASP:HB2	8:H:170:GLY:O	1.86	0.74
12:Z:211:ILE:HD12	12:Z:211:ILE:H	1.52	0.74
10:X:191:LYS:H	10:X:191:LYS:HD2	1.51	0.74
7:G:90:ARG:HG2	7:G:118:TYR:CD1	2.22	0.74
14:N:93:PHE:CZ	14:N:128:ARG:HG2	2.22	0.74
1:A:85:GLY:HA3	1:A:139:VAL:HG12	1.69	0.74
2:B:187:ASP:O	2:B:191:ILE:HG12	1.87	0.74
2:B:44:VAL:HG23	2:B:211:LEU:HD11	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:85:GLY:HA3	1:O:139:VAL:HG12	1.69	0.74
6:T:78:ALA:HB3	6:T:79:PRO:HD3	1.69	0.74
1:A:237:SER:O	1:A:241:ILE:HG13	1.87	0.74
10:J:191:LYS:H	10:J:191:LYS:HD2	1.53	0.74
3:C:80:LEU:H	3:C:80:LEU:HD22	1.52	0.74
2:P:244:ASN:HA	2:P:247:LEU:HD12	1.70	0.74
12:L:211:ILE:HD12	12:L:211:ILE:H	1.53	0.74
4:D:163:THR:HG21	4:D:171:VAL:CG2	2.16	0.74
3:Q:80:LEU:H	3:Q:80:LEU:HD22	1.53	0.74
5:S:182:GLU:HG2	5:S:203:ILE:HG12	1.70	0.74
7:G:134:SER:HB2	7:G:164:THR:HG21	1.70	0.74
4:D:162:GLN:NE2	4:D:163:THR:H	1.86	0.73
11:K:39:SER:HB2	11:K:40:PRO:HD2	1.70	0.73
5:E:182:GLU:HG2	5:E:203:ILE:HG12	1.68	0.73
6:F:78:ALA:HB3	6:F:79:PRO:HD3	1.70	0.73
1:A:52:VAL:HG22	1:A:227:VAL:HG13	1.68	0.73
9:W:83:LEU:O	9:W:87:LEU:HD23	1.88	0.73
9:I:112:SER:HB3	9:I:125:LEU:HD13	1.69	0.73
4:R:176:GLU:OE2	5:S:57:PRO:HD2	1.88	0.73
9:I:6:VAL:HG12	9:I:124:TYR:HB3	1.71	0.73
3:Q:243:GLY:C	3:Q:244:ILE:HD12	2.08	0.73
4:R:187:THR:HG22	4:R:189:GLU:H	1.52	0.73
1:O:237:SER:O	1:O:241:ILE:HG13	1.89	0.73
6:F:46:LEU:HG	6:F:135:ILE:HD13	1.70	0.73
9:I:83:LEU:O	9:I:87:LEU:HD23	1.87	0.73
6:T:201:LEU:HD11	6:T:206:LEU:HD22	1.68	0.73
8:V:163:ILE:HD12	8:V:170:GLY:HA2	1.71	0.73
4:R:216:LYS:HE3	4:R:220:ASP:OD2	1.89	0.73
2:B:68:THR:CG2	2:B:71:ILE:HB	2.19	0.73
7:U:94:GLU:HG2	7:U:114:ARG:HB3	1.70	0.73
4:D:42:VAL:HG11	4:D:136:ALA:HB1	1.68	0.73
2:B:44:VAL:HA	2:B:213:ILE:HG22	1.71	0.73
4:D:187:THR:HG22	4:D:189:GLU:H	1.53	0.73
2:P:74:VAL:HG22	2:P:75:TYR:N	2.03	0.73
14:N:210:LYS:O	14:N:212:LEU:HD13	1.89	0.73
4:R:162:GLN:NE2	4:R:163:THR:H	1.87	0.72
7:U:77:TYR:HE1	7:U:81:ILE:HD13	1.53	0.72
4:D:176:GLU:OE2	5:E:57:PRO:HD2	1.89	0.72
2:B:244:ASN:HA	2:B:247:LEU:HD12	1.71	0.72
7:G:121:ALA:HA	7:G:124:LEU:HD12	1.71	0.72
2:B:222:LEU:HD11	2:B:232:GLY:CA	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:134:SER:HB2	7:U:164:THR:HG21	1.70	0.72
6:T:36:VAL:HG22	6:T:160:ALA:HB2	1.71	0.72
3:C:175:LEU:HD11	3:C:199:LYS:CD	2.16	0.72
2:B:74:VAL:HG22	2:B:75:TYR:N	2.03	0.72
2:B:157:PHE:N	2:B:157:PHE:CD2	2.58	0.72
3:Q:175:LEU:HD11	3:Q:199:LYS:CD	2.17	0.72
1:O:185:HIS:HA	1:O:188:LYS:NZ	2.03	0.72
4:R:163:THR:HG21	4:R:171:VAL:CG2	2.16	0.72
13:M:175:LEU:CD1	13:M:175:LEU:H	1.99	0.72
10:X:88:GLN:HA	10:X:88:GLN:NE2	2.04	0.72
1:A:177:GLU:N	1:A:177:GLU:OE1	2.21	0.72
7:U:194:GLN:O	7:U:198:ILE:HG13	1.89	0.72
7:G:77:TYR:HE1	7:G:81:ILE:HD13	1.52	0.72
6:T:34:VAL:HG23	6:T:197:ILE:HD11	1.71	0.72
7:G:194:GLN:O	7:G:198:ILE:HG13	1.90	0.72
9:I:38:SER:OG	9:I:39:PRO:HD2	1.90	0.72
7:U:23:VAL:O	7:U:26:ALA:HB3	1.89	0.72
7:U:136:ILE:CG1	7:U:149:MET:HG3	2.19	0.72
7:U:52:LEU:HD11	7:U:206:ASN:ND2	2.05	0.72
2:P:187:ASP:O	2:P:191:ILE:HG12	1.89	0.71
9:W:6:VAL:HG12	9:W:124:TYR:HB3	1.71	0.71
11:K:67:TYR:CE1	11:K:75:LEU:HD23	2.25	0.71
6:T:194:VAL:O	6:T:197:ILE:HG22	1.90	0.71
13:M:38:ARG:NH1	13:M:221:ARG:HB3	2.04	0.71
5:S:79:SER:O	5:S:140:VAL:HG23	1.91	0.71
5:E:192:THR:HG23	5:E:195:GLU:OE2	1.90	0.71
3:C:44:ILE:HD11	3:C:146:TYR:HB3	1.73	0.71
1:A:185:HIS:HA	1:A:188:LYS:HZ1	1.55	0.71
1:O:44:ALA:CB	1:O:53:VAL:HG12	2.20	0.71
2:B:94:HIS:HD2	9:I:61:SER:HB2	1.54	0.71
7:G:23:VAL:O	7:G:26:ALA:HB3	1.91	0.71
2:P:222:LEU:HD11	2:P:232:GLY:CA	2.19	0.71
11:Y:67:TYR:CE1	11:Y:75:LEU:HD23	2.25	0.71
1:A:92:ASN:HD22	1:A:137:LEU:HD11	1.55	0.71
5:S:192:THR:HG23	5:S:195:GLU:OE2	1.91	0.71
12:L:63:CYS:O	12:L:67:GLU:HG3	1.91	0.71
2:B:48:GLU:HG2	2:B:49:LYS:N	2.05	0.71
9:I:188:ARG:O	9:I:189:ASN:HB2	1.90	0.71
7:G:243:GLN:O	7:G:246:ILE:HG22	1.89	0.71
4:D:216:LYS:HE3	4:D:220:ASP:OD2	1.91	0.71
2:P:157:PHE:CD2	2:P:157:PHE:N	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:121:ALA:HA	7:U:124:LEU:HD12	1.72	0.71
9:I:79:ALA:O	9:I:83:LEU:HG	1.90	0.70
6:F:36:VAL:HG22	6:F:160:ALA:HB2	1.72	0.70
3:C:217:ARG:CB	3:C:217:ARG:HH11	2.03	0.70
8:V:82:PHE:HB3	8:V:113:ILE:CD1	2.20	0.70
8:V:36:ARG:HB2	8:V:42:TRP:CE2	2.26	0.70
7:U:90:ARG:HG2	7:U:118:TYR:CD1	2.25	0.70
6:T:91:GLN:HG3	6:T:111:LEU:HD13	1.73	0.70
11:K:192:VAL:O	11:K:194:ASP:N	2.23	0.70
1:O:52:VAL:HG22	1:O:227:VAL:HG13	1.71	0.70
14:N:143:ALA:HB1	14:N:147:GLY:HA3	1.73	0.70
11:Y:53:THR:HG23	11:Y:54:VAL:HG13	1.72	0.70
6:F:34:VAL:HG23	6:F:197:ILE:HD11	1.74	0.70
2:B:121:ALA:HB1	2:B:129:PRO:HA	1.74	0.70
10:J:124:ASP:OD1	10:J:128:CYS:HB3	1.91	0.70
8:H:147:SER:OG	8:H:150:GLU:HB2	1.91	0.70
2:P:48:GLU:HG2	2:P:49:LYS:N	2.06	0.70
3:Q:80:LEU:H	3:Q:80:LEU:CD2	2.05	0.70
5:E:79:SER:O	5:E:140:VAL:HG23	1.91	0.70
1:O:15:HIS:HB2	1:O:18:ILE:HD13	1.74	0.70
1:A:244:ARG:O	1:A:248:ILE:HG12	1.91	0.70
3:Q:156:ASN:ND2	4:R:79:ASN:HB3	2.07	0.70
6:F:194:VAL:O	6:F:197:ILE:HG22	1.91	0.70
1:O:244:ARG:O	1:O:248:ILE:HG12	1.92	0.69
7:G:168:ARG:HG3	7:G:172:LYS:HE3	1.74	0.69
7:G:182:HIS:H	7:G:183:PRO:CD	2.04	0.69
1:A:44:ALA:CB	1:A:53:VAL:HG12	2.22	0.69
7:G:52:LEU:HD11	7:G:206:ASN:ND2	2.06	0.69
11:Y:192:VAL:O	11:Y:194:ASP:N	2.22	0.69
1:A:46:ARG:HB2	1:A:152:PRO:HB3	1.73	0.69
9:W:188:ARG:O	9:W:189:ASN:HB2	1.92	0.69
2:P:121:ALA:HB1	2:P:129:PRO:HA	1.74	0.69
8:H:82:PHE:HB3	8:H:113:ILE:CD1	2.22	0.69
2:B:176:GLU:HG2	3:C:56:LEU:HD13	1.74	0.69
11:Y:35:THR:HG22	11:Y:36:ARG:N	2.07	0.69
2:B:122:THR:HG22	2:B:123:GLN:N	2.07	0.69
7:G:187:SER:CB	7:G:190:GLU:HB2	2.21	0.69
2:B:48:GLU:OE1	2:B:200:VAL:HG22	1.92	0.69
7:G:136:ILE:CG1	7:G:149:MET:HG3	2.22	0.69
2:P:218:ASN:ND2	2:P:236:ARG:HD2	2.08	0.69
7:G:194:GLN:HA	7:G:194:GLN:HE21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:243:GLN:O	7:U:246:ILE:HG22	1.91	0.69
11:Y:5:LEU:HB2	11:Y:16:ALA:HB3	1.74	0.69
2:B:218:ASN:ND2	2:B:236:ARG:HD2	2.06	0.69
1:A:43:LEU:O	1:A:43:LEU:HD12	1.92	0.69
7:U:102:TYR:O	7:U:103:LYS:HB3	1.93	0.69
2:P:68:THR:CG2	2:P:71:ILE:HB	2.21	0.69
3:Q:217:ARG:HH11	3:Q:217:ARG:CB	2.04	0.69
5:S:51:GLU:OE2	5:S:53:ARG:HB2	1.93	0.69
11:K:53:THR:HG23	11:K:54:VAL:HG13	1.73	0.69
8:H:36:ARG:HB2	8:H:42:TRP:CE2	2.28	0.69
8:H:163:ILE:HD12	8:H:170:GLY:HA2	1.75	0.69
9:W:79:ALA:O	9:W:83:LEU:HG	1.93	0.69
5:S:59:LEU:HD13	5:S:60:GLU:N	2.08	0.69
11:Y:140:THR:CG2	11:Y:164:CYS:HB3	2.22	0.69
14:N:73:GLU:HA	14:N:76:TYR:HD2	1.57	0.69
3:Q:44:ILE:HD11	3:Q:146:TYR:HB3	1.75	0.69
7:U:24:GLU:O	7:U:27:VAL:HG23	1.93	0.69
2:B:75:TYR:HB3	2:B:134:LEU:HD22	1.74	0.69
7:U:182:HIS:H	7:U:183:PRO:CD	2.05	0.69
3:C:80:LEU:H	3:C:80:LEU:CD2	2.06	0.68
7:G:197:LYS:O	7:G:201:LEU:HD13	1.93	0.68
1:A:15:HIS:HB2	1:A:18:ILE:HD13	1.75	0.68
3:C:228:LYS:NZ	3:C:231:LYS:HE3	2.08	0.68
7:G:71:ARG:HH21	14:N:72:THR:CG2	2.00	0.68
8:V:67:THR:HG22	8:V:72:THR:HA	1.74	0.68
7:U:194:GLN:HE21	7:U:194:GLN:HA	1.59	0.68
5:S:192:THR:OG1	5:S:195:GLU:HG3	1.92	0.68
11:K:5:LEU:HB2	11:K:16:ALA:HB3	1.75	0.68
1:A:174:LYS:HD2	1:A:177:GLU:OE2	1.93	0.68
1:O:64:LEU:O	1:O:66:PRO:HD3	1.93	0.68
4:R:58:ARG:HB2	4:R:59:ILE:HD13	1.76	0.68
4:R:192:VAL:O	4:R:196:VAL:HG23	1.94	0.68
8:H:67:THR:HG22	8:H:72:THR:HA	1.74	0.68
8:H:143:ARG:HB2	8:H:143:ARG:NH1	2.08	0.68
6:F:94:TYR:CE2	6:F:98:VAL:HG21	2.29	0.68
1:O:123:ASN:ND2	2:P:83:ARG:HE	1.92	0.68
8:V:147:SER:H	8:V:150:GLU:HB3	1.59	0.68
1:A:195:ASN:HD22	1:A:196:GLU:N	1.91	0.68
1:O:46:ARG:HB2	1:O:152:PRO:HB3	1.74	0.68
14:N:104:ARG:HG3	14:N:105:SER:N	2.09	0.68
13:M:126:ASP:CB	13:M:130:SER:HB3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:14:ARG:NH2	7:U:6:GLY:HA3	2.09	0.68
7:G:102:TYR:O	7:G:103:LYS:HB3	1.92	0.68
6:F:227:GLY:O	6:F:230:VAL:HG22	1.94	0.68
1:A:123:ASN:ND2	2:B:83:ARG:HE	1.92	0.68
7:G:24:GLU:O	7:G:27:VAL:HG23	1.94	0.68
1:O:195:ASN:HD22	1:O:196:GLU:N	1.92	0.68
4:D:192:VAL:O	4:D:196:VAL:HG23	1.94	0.68
2:P:200:VAL:HG12	2:P:202:GLY:H	1.59	0.68
2:P:226:GLY:HA3	9:W:186:TYR:HB3	1.74	0.68
1:O:174:LYS:HD2	1:O:177:GLU:OE2	1.94	0.68
7:U:168:ARG:HG3	7:U:172:LYS:HE3	1.76	0.68
3:C:156:ASN:ND2	4:D:79:ASN:HB3	2.07	0.68
9:W:98:LEU:HD12	9:W:98:LEU:N	2.08	0.68
6:T:227:GLY:O	6:T:230:VAL:HG22	1.93	0.68
5:E:37:ALA:HA	5:E:50:VAL:HG12	1.75	0.68
10:J:17:LYS:HG3	10:J:156:ASN:HB3	1.74	0.68
11:K:53:THR:HG23	11:K:54:VAL:H	1.59	0.68
5:S:37:ALA:HA	5:S:50:VAL:HG12	1.76	0.68
4:R:162:GLN:HE21	4:R:162:GLN:CA	2.07	0.67
5:E:192:THR:OG1	5:E:195:GLU:HG3	1.94	0.67
14:N:197:LEU:HD23	14:N:197:LEU:C	2.14	0.67
1:A:87:ILE:HG13	1:A:91:ARG:HD2	1.76	0.67
2:B:200:VAL:HG12	2:B:202:GLY:H	1.57	0.67
2:P:75:TYR:HB3	2:P:134:LEU:HD22	1.75	0.67
8:V:143:ARG:HB2	8:V:143:ARG:NH1	2.10	0.67
1:A:200:GLU:O	1:A:204:GLU:HG3	1.94	0.67
4:D:58:ARG:HB2	4:D:59:ILE:HD13	1.77	0.67
11:Y:53:THR:HG23	11:Y:54:VAL:H	1.59	0.67
12:Z:63:CYS:O	12:Z:67:GLU:HG3	1.94	0.67
2:P:122:THR:HG22	2:P:123:GLN:N	2.09	0.67
8:V:147:SER:OG	8:V:150:GLU:HB2	1.94	0.67
1:A:14:ARG:NH2	7:G:6:GLY:HA3	2.09	0.67
6:T:34:VAL:CG2	6:T:197:ILE:HD11	2.25	0.67
2:P:176:GLU:HG2	3:Q:56:LEU:HD13	1.76	0.67
1:A:64:LEU:O	1:A:66:PRO:HD3	1.94	0.67
6:T:94:TYR:CE2	6:T:98:VAL:HG21	2.30	0.67
3:Q:222:ASP:C	3:Q:224:GLU:H	1.97	0.67
1:O:200:GLU:O	1:O:204:GLU:HG3	1.94	0.67
3:C:142:ASP:OD2	3:C:142:ASP:N	2.27	0.67
6:F:91:GLN:HG3	6:F:111:LEU:HD13	1.77	0.67
14:N:153:PRO:HA	9:W:165:ASN:ND2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:197:LYS:O	7:U:201:LEU:HD13	1.93	0.67
2:B:86:VAL:HG12	2:B:87:ASP:N	2.09	0.67
5:E:51:GLU:OE2	5:E:53:ARG:HB2	1.95	0.67
7:G:182:HIS:N	7:G:183:PRO:CD	2.58	0.67
5:S:59:LEU:HD13	5:S:60:GLU:H	1.58	0.67
8:V:133:PHE:CE2	8:V:166:ASP:HB2	2.29	0.67
9:W:38:SER:OG	9:W:39:PRO:HD2	1.95	0.67
5:E:67:ILE:HD12	5:E:218:GLN:HG2	1.77	0.67
1:O:177:GLU:OE1	1:O:177:GLU:N	2.22	0.67
3:Q:48:ALA:HB1	3:Q:65:LYS:HD3	1.77	0.67
3:Q:228:LYS:NZ	3:Q:231:LYS:HE3	2.09	0.67
7:U:187:SER:CB	7:U:190:GLU:HB2	2.23	0.66
1:O:87:ILE:HG13	1:O:91:ARG:HD2	1.77	0.66
3:Q:152:ASN:HB2	3:Q:153:PRO:CD	2.25	0.66
10:X:124:ASP:OD1	10:X:128:CYS:HB3	1.95	0.66
5:S:67:ILE:HD12	5:S:218:GLN:HG2	1.76	0.66
3:Q:142:ASP:N	3:Q:142:ASP:OD2	2.26	0.66
14:N:114:ILE:HB	14:N:130:VAL:HG13	1.77	0.66
11:K:18:SER:HB2	11:K:176:PHE:HB2	1.77	0.66
3:C:222:ASP:C	3:C:224:GLU:H	1.99	0.66
11:K:35:THR:HG22	11:K:36:ARG:N	2.10	0.66
1:A:104:PHE:CD2	1:A:112:MET:HG3	2.30	0.66
1:A:220:LYS:NZ	1:A:220:LYS:HB2	2.09	0.66
11:Y:161:LEU:O	11:Y:161:LEU:HD23	1.95	0.66
3:C:152:ASN:HB2	3:C:153:PRO:CD	2.26	0.66
10:X:17:LYS:HG3	10:X:156:ASN:HB3	1.76	0.66
5:E:59:LEU:HD13	5:E:60:GLU:N	2.11	0.66
1:O:220:LYS:NZ	1:O:220:LYS:HB2	2.10	0.66
5:S:130:GLU:HG2	5:S:131:GLU:H	1.61	0.66
4:R:56:ASP:OD1	4:R:58:ARG:HG3	1.96	0.66
5:E:130:GLU:HG2	5:E:131:GLU:H	1.60	0.66
1:O:36:ASN:C	1:O:38:THR:H	1.98	0.66
3:Q:218:LYS:HG2	3:Q:219:GLY:N	2.11	0.66
11:K:140:THR:CG2	11:K:164:CYS:HB3	2.26	0.66
12:L:191:HIS:N	12:L:191:HIS:CD2	2.63	0.66
3:C:120:GLN:O	3:C:123:THR:HB	1.96	0.66
9:I:21:THR:O	9:I:22:GLN:HB2	1.96	0.66
4:D:162:GLN:HE21	4:D:162:GLN:CA	2.07	0.66
14:N:1:THR:HG22	14:N:2:GLN:N	2.10	0.66
3:Q:70:ASN:HD22	3:Q:71:ASP:H	1.41	0.65
14:N:152:ASN:ND2	14:N:156:ARG:NH2	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:53:THR:HG23	11:Y:54:VAL:N	2.11	0.65
8:H:133:PHE:CE2	8:H:166:ASP:HB2	2.30	0.65
11:Y:140:THR:HG22	11:Y:164:CYS:HB3	1.79	0.65
7:U:182:HIS:N	7:U:183:PRO:CD	2.59	0.65
7:G:240:ASP:C	7:G:242:ALA:H	1.99	0.65
8:V:8:PHE:HE2	8:V:148:LYS:CA	2.00	0.65
8:H:59:VAL:HG11	8:H:82:PHE:CD2	2.32	0.65
5:E:59:LEU:HD11	5:E:64:ILE:HD13	1.77	0.65
8:H:8:PHE:HE2	8:H:148:LYS:CA	2.02	0.65
1:O:211:ILE:HG23	1:O:216:THR:O	1.96	0.65
8:H:67:THR:HG22	8:H:73:PRO:CD	2.27	0.65
4:R:187:THR:HG22	4:R:189:GLU:N	2.10	0.65
3:C:44:ILE:HG21	3:C:138:ALA:HB1	1.79	0.65
13:M:151:ASP:O	13:M:157:LYS:HG3	1.96	0.65
1:A:211:ILE:HG23	1:A:216:THR:O	1.96	0.65
6:F:227:GLY:O	6:F:229:ALA:N	2.30	0.65
1:A:117:LEU:O	1:A:121:MET:HG2	1.96	0.65
4:D:59:ILE:HD13	4:D:59:ILE:N	2.08	0.65
3:C:218:LYS:HG2	3:C:219:GLY:N	2.12	0.65
6:F:117:GLN:HE22	6:F:121:GLN:NE2	1.94	0.65
2:P:108:LYS:HD3	2:P:143:ASN:ND2	2.11	0.65
8:H:147:SER:H	8:H:150:GLU:HB3	1.59	0.65
4:R:59:ILE:N	4:R:59:ILE:HD13	2.09	0.65
5:S:109:VAL:HB	5:S:154:GLN:NE2	2.08	0.65
8:V:34:LEU:HD23	8:V:44:CYS:HB3	1.79	0.65
10:J:88:GLN:HA	10:J:88:GLN:HE21	1.62	0.65
5:E:108:ASN:HD21	13:M:82:LYS:NZ	1.95	0.65
1:A:36:ASN:C	1:A:38:THR:H	2.00	0.65
3:Q:39:MET:HE1	3:Q:146:TYR:HB2	1.79	0.65
11:Y:162:LYS:HB2	11:Y:162:LYS:NZ	2.12	0.65
9:W:132:LEU:HD23	9:W:132:LEU:N	2.12	0.65
1:O:164:VAL:HG22	1:O:165:GLY:H	1.61	0.64
12:Z:1:THR:HG23	12:Z:33:ARG:HH21	1.61	0.64
11:Y:3:ILE:HB	11:Y:18:SER:HB3	1.80	0.64
9:I:41:ILE:HG23	9:I:76:VAL:HG22	1.80	0.64
4:D:56:ASP:OD1	4:D:58:ARG:HG3	1.97	0.64
14:N:27:LEU:HD12	14:N:28:GLY:N	2.12	0.64
1:O:117:LEU:O	1:O:121:MET:HG2	1.97	0.64
3:Q:120:GLN:O	3:Q:123:THR:HB	1.97	0.64
13:M:156:PHE:CE2	13:M:172:LEU:HA	2.33	0.64
9:I:6:VAL:HG12	9:I:124:TYR:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:185:TRP:C	12:L:186:ILE:HD12	2.17	0.64
11:K:162:LYS:HA	11:K:195:PHE:HZ	1.62	0.64
2:P:86:VAL:HG12	2:P:87:ASP:N	2.12	0.64
2:P:64:VAL:HG11	2:P:212:ALA:HB3	1.79	0.64
2:P:28:VAL:HG22	2:P:76:SER:O	1.98	0.64
2:P:48:GLU:OE1	2:P:200:VAL:HG22	1.97	0.64
8:H:18:SER:HB2	8:H:30:VAL:HA	1.79	0.64
3:C:149:TYR:OH	4:D:59:ILE:HG13	1.98	0.64
4:D:29:ARG:HH11	4:D:29:ARG:HG2	1.63	0.64
14:N:27:LEU:HD12	14:N:28:GLY:H	1.61	0.64
4:D:187:THR:HG22	4:D:189:GLU:N	2.12	0.64
11:K:53:THR:HG23	11:K:54:VAL:N	2.13	0.64
8:V:18:SER:HB2	8:V:30:VAL:HA	1.79	0.64
4:D:50:SER:HA	4:D:53:LYS:HD2	1.79	0.64
1:A:164:VAL:HG22	1:A:165:GLY:H	1.63	0.64
2:P:218:ASN:HB3	2:P:220:ASP:OD1	1.98	0.64
8:V:107:LYS:CD	8:V:108:GLY:H	2.09	0.64
8:V:59:VAL:HG11	8:V:82:PHE:CD2	2.33	0.64
9:W:41:ILE:HG23	9:W:76:VAL:HG22	1.79	0.64
6:T:128:TYR:O	6:T:149:PRO:HB3	1.97	0.64
9:I:113:ILE:HG23	9:I:119:THR:CG2	2.28	0.64
1:O:204:GLU:HG2	1:O:244:ARG:HB3	1.78	0.64
5:S:59:LEU:HD11	5:S:64:ILE:HD13	1.78	0.64
4:R:29:ARG:HG2	4:R:29:ARG:HH11	1.62	0.64
14:N:80:LEU:HD12	14:N:80:LEU:H	1.63	0.64
6:F:34:VAL:CG2	6:F:197:ILE:HD11	2.28	0.64
7:U:192:VAL:O	7:U:195:ALA:HB3	1.98	0.64
6:T:213:ILE:HG22	6:T:214:ALA:N	2.11	0.64
9:I:132:LEU:N	9:I:132:LEU:HD23	2.13	0.64
1:A:53:VAL:CG1	1:A:144:VAL:HG11	2.27	0.64
2:P:90:ARG:NH1	9:W:68:LEU:HB3	2.13	0.64
1:O:43:LEU:HD23	1:O:178:ILE:CG2	2.27	0.64
3:Q:70:ASN:ND2	3:Q:71:ASP:N	2.45	0.64
7:G:60:PRO:O	7:G:61:GLN:HB2	1.98	0.64
14:N:44:PRO:HA	14:N:50:VAL:HA	1.79	0.64
7:U:60:PRO:O	7:U:61:GLN:HB2	1.97	0.64
3:C:48:ALA:HB1	3:C:65:LYS:HD3	1.81	0.64
1:O:188:LYS:O	1:O:190:LYS:HG2	1.98	0.63
2:B:133:SER:C	2:B:134:LEU:HD23	2.17	0.63
5:E:59:LEU:HD13	5:E:60:GLU:H	1.63	0.63
11:K:161:LEU:HD23	11:K:161:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:80:LEU:HD23	14:N:84:GLU:HB2	1.79	0.63
2:P:197:LYS:HA	2:P:204:PHE:CZ	2.33	0.63
12:Z:87:VAL:HG11	12:Z:117:SER:HA	1.79	0.63
8:H:185:ARG:HH11	8:H:185:ARG:HG3	1.62	0.63
1:A:156:LYS:HE2	1:A:166:TYR:CE2	2.33	0.63
1:A:43:LEU:HD23	1:A:178:ILE:CG2	2.27	0.63
2:P:71:ILE:HG12	2:P:138:GLY:HA3	1.81	0.63
11:Y:162:LYS:HA	11:Y:195:PHE:HZ	1.63	0.63
8:V:10:ASP:OD1	8:V:179:THR:HG22	1.98	0.63
1:A:77:ARG:HG2	1:A:77:ARG:O	1.98	0.63
1:O:94:ALA:O	1:O:98:LYS:HB2	1.98	0.63
1:A:164:VAL:HG22	1:A:165:GLY:N	2.14	0.63
8:V:36:ARG:HB2	8:V:42:TRP:CD2	2.33	0.63
11:K:162:LYS:NZ	11:K:162:LYS:HB2	2.13	0.63
12:Z:191:HIS:CD2	12:Z:191:HIS:N	2.65	0.63
7:G:71:ARG:CZ	14:N:72:THR:HG22	2.27	0.63
5:E:109:VAL:HB	5:E:154:GLN:NE2	2.12	0.63
3:Q:218:LYS:HG3	3:Q:224:GLU:O	1.98	0.63
14:N:129:TYR:CD1	14:N:130:VAL:N	2.67	0.63
10:X:141:ALA:HB2	10:X:177:ASP:HB2	1.80	0.63
14:N:206:LEU:HD23	14:N:207:THR:N	2.12	0.63
1:A:204:GLU:HG2	1:A:244:ARG:HB3	1.80	0.63
1:O:92:ASN:ND2	1:O:137:LEU:HD11	2.13	0.63
11:Y:18:SER:HB2	11:Y:176:PHE:HB2	1.79	0.63
6:F:213:ILE:HG22	6:F:214:ALA:N	2.14	0.63
5:S:10:ARG:HH11	5:S:10:ARG:HG2	1.62	0.63
9:I:98:LEU:N	9:I:98:LEU:HD12	2.13	0.63
7:G:140:VAL:HG22	7:G:145:ALA:HB2	1.81	0.63
7:U:36:SER:O	7:U:163:ALA:HB1	1.99	0.63
7:U:31:GLU:HB2	7:U:168:ARG:NH2	2.14	0.63
7:U:240:ASP:C	7:U:242:ALA:H	2.01	0.63
3:C:218:LYS:HG3	3:C:224:GLU:O	1.99	0.63
2:P:85:LEU:HD23	2:P:85:LEU:O	1.98	0.63
4:R:208:LYS:HB2	4:R:208:LYS:NZ	2.13	0.63
8:H:34:LEU:HD23	8:H:44:CYS:HB3	1.80	0.63
12:L:87:VAL:HG11	12:L:117:SER:HA	1.81	0.63
12:L:128:CYS:HB2	12:L:137:TYR:CE2	2.34	0.63
12:L:106:ARG:HH11	12:L:106:ARG:HG3	1.63	0.63
6:T:117:GLN:HE22	6:T:121:GLN:NE2	1.96	0.63
4:R:50:SER:HA	4:R:53:LYS:HD2	1.81	0.63
7:G:30:VAL:HG11	7:G:134:SER:OG	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:88:GLN:HE21	10:X:88:GLN:HA	1.63	0.63
8:H:36:ARG:HB2	8:H:42:TRP:CD2	2.33	0.63
4:D:208:LYS:NZ	4:D:208:LYS:HB2	2.14	0.63
8:V:185:ARG:HG3	8:V:185:ARG:HH11	1.64	0.63
12:Z:185:TRP:C	12:Z:186:ILE:HD12	2.19	0.63
2:B:218:ASN:HB3	2:B:220:ASP:OD1	1.99	0.63
2:B:91:LYS:C	2:B:93:ALA:H	2.02	0.63
1:O:164:VAL:HG22	1:O:165:GLY:N	2.13	0.63
3:Q:39:MET:CE	3:Q:146:TYR:HB2	2.29	0.63
2:P:123:GLN:O	2:P:124:SER:HB2	1.99	0.63
1:O:104:PHE:CD2	1:O:112:MET:HG3	2.33	0.63
8:H:97:ILE:HD12	8:H:98:ILE:N	2.13	0.62
2:B:134:LEU:HD23	2:B:134:LEU:N	2.14	0.62
12:L:1:THR:HG23	12:L:33:ARG:HH21	1.63	0.62
9:W:113:ILE:HG23	9:W:119:THR:CG2	2.29	0.62
11:Y:40:PRO:HG2	11:Y:74:GLU:OE1	1.98	0.62
2:B:110:LEU:O	2:B:114:VAL:HG23	1.98	0.62
3:C:4:ARG:HH12	4:D:3:GLY:HA3	1.63	0.62
14:N:182:ARG:HA	14:N:214:VAL:HG11	1.80	0.62
12:Z:128:CYS:HB2	12:Z:137:TYR:CE2	2.34	0.62
13:M:159:GLN:HG2	9:W:209:THR:HG21	1.81	0.62
8:H:3:ILE:HG22	8:H:16:ALA:HB1	1.81	0.62
2:B:28:VAL:HG22	2:B:76:SER:O	2.00	0.62
7:G:92:ARG:CZ	14:N:76:TYR:CD1	2.79	0.62
5:S:205:LYS:HB2	5:S:212:LEU:HD22	1.79	0.62
2:P:244:ASN:HA	2:P:247:LEU:CD1	2.28	0.62
1:O:128:TYR:HA	1:O:133:TYR:CE1	2.34	0.62
14:N:185:TYR:CE1	14:N:193:ARG:HB2	2.34	0.62
2:B:64:VAL:HG11	2:B:212:ALA:HB3	1.81	0.62
7:U:37:ILE:HA	7:U:163:ALA:HB2	1.81	0.62
5:E:205:LYS:HB2	5:E:212:LEU:HD22	1.80	0.62
7:U:182:HIS:O	7:U:184:GLU:N	2.32	0.62
3:Q:201:THR:HG22	3:Q:202:ASP:N	2.11	0.62
1:A:63:LEU:HD21	7:G:175:LEU:HD12	1.80	0.62
1:O:144:VAL:HG12	1:O:154:ILE:HG12	1.81	0.62
14:N:43:ILE:O	14:N:51:VAL:HG22	1.99	0.62
12:Z:106:ARG:HH11	12:Z:106:ARG:HG3	1.63	0.62
6:F:206:LEU:N	6:F:206:LEU:HD23	2.10	0.62
7:U:94:GLU:HG3	7:U:114:ARG:NH1	2.12	0.62
1:O:156:LYS:HE2	1:O:166:TYR:CE2	2.35	0.62
2:B:94:HIS:CB	2:B:99:ARG:HH21	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ASN:HA	2:B:247:LEU:CD1	2.29	0.62
11:K:175:ASP:HB2	11:Y:175:ASP:HB2	1.82	0.62
7:G:31:GLU:HB2	7:G:168:ARG:NH2	2.14	0.62
1:O:128:TYR:HD1	1:O:133:TYR:HH	1.46	0.62
7:G:192:VAL:O	7:G:195:ALA:HB3	1.99	0.62
2:P:145:PHE:HE1	2:P:214:ILE:HG22	1.65	0.62
2:B:197:LYS:HA	2:B:204:PHE:CZ	2.34	0.62
8:V:67:THR:HG22	8:V:73:PRO:CD	2.28	0.62
5:S:76:CYS:HB2	5:S:143:LEU:O	1.99	0.62
7:G:182:HIS:N	7:G:183:PRO:HD2	2.15	0.62
13:M:3:ASN:ND2	13:M:5:TYR:H	1.97	0.62
1:O:242:GLU:OE1	1:O:245:LEU:HD23	1.99	0.62
14:N:48:ASN:HD22	14:N:48:ASN:H	1.48	0.62
9:I:147:THR:HG23	9:I:150:GLU:OE1	1.99	0.62
7:G:36:SER:O	7:G:163:ALA:HB1	1.99	0.62
8:H:190:PRO:C	8:H:192:GLU:H	2.03	0.62
13:M:13:LEU:O	13:M:23:LEU:HD23	1.99	0.62
1:A:92:ASN:ND2	1:A:137:LEU:HD11	2.14	0.62
1:A:188:LYS:O	1:A:190:LYS:HG2	1.98	0.62
1:O:185:HIS:HA	1:O:188:LYS:HZ1	1.64	0.61
1:O:202:VAL:O	1:O:205:PHE:HB3	2.00	0.61
1:O:201:LYS:HD3	1:O:204:GLU:OE1	1.99	0.61
2:B:108:LYS:HD3	2:B:143:ASN:ND2	2.15	0.61
1:O:53:VAL:CG1	1:O:144:VAL:HG11	2.30	0.61
5:E:31:ILE:HD13	5:E:141:ALA:HB2	1.81	0.61
5:E:10:ARG:HG2	5:E:10:ARG:HH11	1.64	0.61
10:J:141:ALA:HB2	10:J:177:ASP:HB2	1.81	0.61
1:A:75:ILE:HD11	1:A:81:MET:HB3	1.81	0.61
2:B:123:GLN:O	2:B:124:SER:HB2	2.00	0.61
6:T:42:THR:HG22	6:T:218:LYS:NZ	2.15	0.61
5:E:184:LEU:HD22	6:F:56:LEU:CD2	2.30	0.61
5:S:136:ARG:HB2	5:S:137:PRO:CD	2.30	0.61
2:B:176:GLU:HA	3:C:56:LEU:HD11	1.82	0.61
9:W:71:SER:C	9:W:72:ARG:HG3	2.20	0.61
6:T:227:GLY:O	6:T:229:ALA:N	2.33	0.61
10:J:177:ASP:OD2	10:J:180:SER:HB2	2.00	0.61
5:S:184:LEU:HD22	6:T:56:LEU:CD2	2.31	0.61
6:T:26:LEU:HA	6:T:29:ILE:HD13	1.82	0.61
5:S:194:LYS:O	5:S:198:LEU:HD13	2.00	0.61
1:A:201:LYS:HD3	1:A:204:GLU:OE1	2.00	0.61
1:O:63:LEU:HD21	7:U:175:LEU:HD12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:LEU:HD12	1:O:43:LEU:O	2.00	0.61
7:G:182:HIS:O	7:G:184:GLU:N	2.33	0.61
7:U:182:HIS:N	7:U:183:PRO:HD2	2.15	0.61
14:N:226:LYS:HB3	14:N:226:LYS:NZ	2.15	0.61
12:L:176:ASN:HD21	12:L:190:ASN:HB2	1.65	0.61
13:M:195:HIS:HD2	13:M:197:GLN:H	1.47	0.61
8:V:3:ILE:HG22	8:V:16:ALA:HB1	1.82	0.61
5:E:76:CYS:HB2	5:E:143:LEU:O	2.01	0.61
11:K:140:THR:HG22	11:K:164:CYS:HB3	1.83	0.61
3:C:4:ARG:HH21	4:D:6:ARG:HG2	1.64	0.61
13:M:159:GLN:HG2	9:W:209:THR:CG2	2.31	0.61
3:Q:4:ARG:HH21	4:R:6:ARG:HG2	1.65	0.61
4:R:51:THR:HB	4:R:52:LEU:HD22	1.82	0.61
5:E:136:ARG:HB2	5:E:137:PRO:CD	2.31	0.61
8:V:6:VAL:O	8:V:12:VAL:HG23	2.00	0.61
8:V:97:ILE:HD12	8:V:98:ILE:N	2.15	0.61
1:O:77:ARG:O	1:O:77:ARG:HG2	2.01	0.61
8:H:111:TYR:HE2	8:H:121:LYS:HD2	1.65	0.61
12:L:208:ASN:O	12:L:210:VAL:N	2.34	0.61
11:Y:28:LEU:HD12	11:Y:28:LEU:N	2.15	0.61
3:C:39:MET:CE	3:C:146:TYR:HB2	2.31	0.61
1:O:75:ILE:HD11	1:O:81:MET:HB3	1.83	0.61
12:L:25:TRP:CZ3	13:M:144:SER:HA	2.36	0.61
8:H:67:THR:CG2	8:H:73:PRO:HD3	2.31	0.61
11:K:40:PRO:HG2	11:K:74:GLU:OE1	2.01	0.61
3:Q:4:ARG:HH12	4:R:3:GLY:HA3	1.65	0.61
9:I:66:HIS:O	9:I:70:THR:HG23	2.01	0.61
4:D:51:THR:HB	4:D:52:LEU:HD22	1.81	0.61
12:Z:176:ASN:HD21	12:Z:190:ASN:HB2	1.66	0.61
12:L:1:THR:CA	12:L:33:ARG:HH21	2.14	0.61
11:K:28:LEU:HD12	11:K:28:LEU:N	2.15	0.61
5:S:31:ILE:HD13	5:S:141:ALA:HB2	1.81	0.61
1:A:43:LEU:C	1:A:43:LEU:HD12	2.21	0.60
2:P:246:ARG:HH11	2:P:246:ARG:HG3	1.65	0.60
6:T:156:LEU:HD13	6:T:159:THR:HB	1.83	0.60
6:F:128:TYR:O	6:F:149:PRO:HB3	2.00	0.60
1:O:234:PHE:HD1	1:O:234:PHE:H	1.47	0.60
13:M:13:LEU:HD12	13:M:14:GLY:N	2.16	0.60
4:R:131:VAL:O	4:R:152:PRO:HG3	2.00	0.60
3:Q:11:THR:O	3:Q:11:THR:HG22	2.00	0.60
7:U:140:VAL:HG22	7:U:145:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:26:LEU:HA	6:F:29:ILE:HD13	1.83	0.60
12:Z:1:THR:CA	12:Z:33:ARG:HH21	2.12	0.60
8:V:159:LEU:O	8:V:163:ILE:HG12	2.00	0.60
4:D:131:VAL:O	4:D:152:PRO:HG3	2.01	0.60
3:Q:149:TYR:OH	4:R:59:ILE:HG13	2.00	0.60
7:G:37:ILE:HA	7:G:163:ALA:HB2	1.83	0.60
1:O:18:ILE:HD12	1:O:18:ILE:N	2.16	0.60
8:H:107:LYS:CD	8:H:108:GLY:H	2.10	0.60
2:B:246:ARG:HH11	2:B:246:ARG:HG3	1.66	0.60
1:A:94:ALA:O	1:A:98:LYS:HB2	2.01	0.60
5:S:78:MET:CE	5:S:82:THR:HG22	2.32	0.60
8:H:31:THR:HG22	8:H:33:LYS:HG2	1.82	0.60
5:E:121:LEU:HD23	5:E:121:LEU:O	2.02	0.60
9:W:21:THR:O	9:W:22:GLN:HB2	2.01	0.60
12:Z:78:ALA:O	12:Z:82:ILE:HG13	2.01	0.60
1:A:146:VAL:HA	1:A:151:GLY:O	2.02	0.60
2:B:211:LEU:HD12	2:B:212:ALA:H	1.63	0.60
9:W:6:VAL:HG12	9:W:124:TYR:CB	2.31	0.60
3:Q:44:ILE:HG21	3:Q:138:ALA:HB1	1.84	0.60
11:K:3:ILE:HB	11:K:18:SER:HB3	1.82	0.60
8:V:111:TYR:HE2	8:V:121:LYS:HD2	1.67	0.60
6:T:185:ASN:HD22	6:T:185:ASN:C	2.04	0.60
6:F:37:GLY:HA2	6:F:45:VAL:O	2.02	0.60
7:U:90:ARG:HD3	7:U:118:TYR:HE1	1.66	0.60
9:W:131:SER:O	9:W:135:MET:HB2	2.02	0.60
6:F:185:ASN:HD22	6:F:185:ASN:C	2.05	0.60
1:A:234:PHE:HD1	1:A:234:PHE:H	1.48	0.60
6:T:150:SER:O	7:U:82:PRO:HG2	2.02	0.60
1:O:146:VAL:HA	1:O:151:GLY:O	2.01	0.60
1:A:128:TYR:HA	1:A:133:TYR:CE1	2.37	0.60
2:B:28:VAL:C	2:B:30:GLN:H	2.05	0.60
7:U:30:VAL:HG11	7:U:134:SER:OG	2.01	0.60
1:A:220:LYS:HB3	1:A:242:GLU:HB2	1.84	0.60
1:O:98:LYS:HD3	8:V:68:SER:O	2.01	0.60
9:I:3:ILE:HG12	9:I:127:LEU:O	2.02	0.60
10:J:120:ILE:O	10:J:120:ILE:HG13	2.00	0.60
3:C:70:ASN:HD22	3:C:71:ASP:H	1.47	0.59
3:C:238:ILE:O	3:C:242:THR:HG23	2.02	0.59
7:U:85:ARG:HH11	7:U:85:ARG:HG2	1.66	0.59
12:Z:208:ASN:O	12:Z:210:VAL:N	2.34	0.59
7:G:70:ASP:OD1	7:G:71:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG13	1:A:227:VAL:HG22	1.83	0.59
2:B:71:ILE:HG12	2:B:138:GLY:HA3	1.84	0.59
9:I:71:SER:C	9:I:72:ARG:HG3	2.21	0.59
9:W:3:ILE:HG12	9:W:127:LEU:O	2.02	0.59
3:C:40:ALA:HB3	3:C:43:GLY:O	2.02	0.59
5:E:78:MET:CE	5:E:82:THR:HG22	2.31	0.59
8:H:6:VAL:O	8:H:12:VAL:HG23	2.03	0.59
1:O:86:PRO:C	1:O:88:PRO:HD2	2.23	0.59
9:W:41:ILE:HD11	9:W:74:PRO:HB2	1.84	0.59
1:A:53:VAL:O	1:A:225:VAL:HG13	2.02	0.59
7:U:70:ASP:OD1	7:U:71:ARG:HG2	2.03	0.59
2:P:133:SER:C	2:P:134:LEU:HD23	2.23	0.59
10:X:191:LYS:H	10:X:191:LYS:CD	2.12	0.59
6:F:156:LEU:HD13	6:F:159:THR:HB	1.83	0.59
10:J:17:LYS:HG2	10:J:156:ASN:HD22	1.67	0.59
4:R:28:LYS:O	4:R:166:ARG:HB3	2.02	0.59
6:T:158:GLY:O	6:T:159:THR:HB	2.03	0.59
10:J:107:VAL:HG22	10:J:136:ILE:HG21	1.84	0.59
9:W:7:LYS:HB3	9:W:12:VAL:HG23	1.85	0.59
4:D:103:PRO:HG2	4:D:140:PRO:CG	2.32	0.59
5:E:98:THR:CG2	5:E:102:TYR:HE1	2.15	0.59
2:B:145:PHE:HE1	2:B:214:ILE:HG22	1.68	0.59
10:J:23:ALA:CB	10:J:186:VAL:HG22	2.33	0.59
2:P:211:LEU:HD12	2:P:212:ALA:H	1.67	0.59
2:B:157:PHE:N	2:B:157:PHE:HD2	2.00	0.59
1:O:128:TYR:HD1	1:O:133:TYR:OH	1.85	0.59
14:N:130:VAL:HG13	14:N:130:VAL:O	2.02	0.59
1:O:220:LYS:HB3	1:O:242:GLU:HB2	1.85	0.59
2:P:110:LEU:O	2:P:114:VAL:HG23	2.03	0.59
2:P:176:GLU:HA	3:Q:56:LEU:HD11	1.85	0.59
5:E:233:ASN:N	5:E:233:ASN:ND2	2.51	0.59
3:C:64:GLU:HG3	3:C:65:LYS:HG3	1.85	0.59
11:K:14:ILE:O	11:K:15:LEU:HD23	2.02	0.59
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.33	0.59
6:F:42:THR:HG22	6:F:218:LYS:NZ	2.17	0.59
3:C:11:THR:O	3:C:11:THR:HG22	2.03	0.59
9:I:103:VAL:HG12	9:I:108:SER:HA	1.85	0.59
2:P:91:LYS:C	2:P:93:ALA:H	2.04	0.59
8:H:149:GLU:HG3	8:H:150:GLU:N	2.17	0.58
10:X:129:ILE:CG2	10:X:130:ASP:N	2.65	0.58
5:S:121:LEU:HD23	5:S:121:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:159:LEU:O	8:H:163:ILE:HG12	2.02	0.58
8:H:59:VAL:HG11	8:H:82:PHE:CE2	2.38	0.58
1:A:202:VAL:O	1:A:205:PHE:HB3	2.03	0.58
1:O:45:VAL:HG12	1:O:168:ALA:HB1	1.84	0.58
2:B:241:GLN:NE2	2:B:245:ASP:OD1	2.36	0.58
7:G:223:THR:HB	7:G:226:LEU:O	2.03	0.58
3:Q:169:THR:O	3:Q:173:GLN:HB2	2.03	0.58
1:A:201:LYS:HA	1:A:204:GLU:OE1	2.03	0.58
10:J:129:ILE:CG2	10:J:130:ASP:N	2.65	0.58
10:X:129:ILE:HG22	10:X:130:ASP:H	1.67	0.58
3:Q:238:ILE:O	3:Q:242:THR:HG23	2.03	0.58
3:Q:64:GLU:HG3	3:Q:65:LYS:HG3	1.86	0.58
1:O:251:GLN:O	1:O:251:GLN:HG2	2.03	0.58
10:X:191:LYS:N	10:X:191:LYS:HD2	2.18	0.58
2:P:157:PHE:N	2:P:157:PHE:HD2	2.01	0.58
1:O:117:LEU:HD12	1:O:117:LEU:O	2.03	0.58
3:C:210:ARG:HG3	3:C:210:ARG:HH11	1.68	0.58
3:Q:40:ALA:HB3	3:Q:43:GLY:O	2.03	0.58
11:Y:21:VAL:HG11	12:Z:122:LEU:HD11	1.84	0.58
1:A:128:TYR:HD1	1:A:133:TYR:OH	1.86	0.58
1:A:86:PRO:C	1:A:88:PRO:HD2	2.23	0.58
7:G:94:GLU:HG3	7:G:114:ARG:NH1	2.16	0.58
3:Q:186:VAL:O	3:Q:190:ILE:HG13	2.03	0.58
14:N:165:ILE:HD12	14:N:165:ILE:H	1.67	0.58
1:A:242:GLU:OE1	1:A:245:LEU:HD23	2.03	0.58
10:X:177:ASP:OD2	10:X:180:SER:HB2	2.03	0.58
5:S:10:ARG:NH1	5:S:10:ARG:HG2	2.19	0.58
9:W:147:THR:HG23	9:W:150:GLU:OE1	2.04	0.58
8:V:31:THR:HG22	8:V:33:LYS:HG2	1.86	0.58
8:V:4:MET:HB2	8:V:126:ILE:HG22	1.84	0.58
9:W:59:ILE:CG1	9:W:83:LEU:HD23	2.25	0.58
14:N:51:VAL:HG23	14:N:51:VAL:O	2.03	0.58
12:L:78:ALA:O	12:L:82:ILE:HG13	2.03	0.58
13:M:206:ILE:N	13:M:206:ILE:HD12	2.18	0.58
5:E:194:LYS:O	5:E:198:LEU:HD13	2.03	0.58
9:I:131:SER:O	9:I:135:MET:HB2	2.02	0.58
5:S:170:LYS:HD2	5:S:180:GLN:OE1	2.03	0.58
5:S:130:GLU:HG2	5:S:131:GLU:N	2.18	0.58
7:U:223:THR:HB	7:U:226:LEU:O	2.04	0.58
2:B:85:LEU:O	2:B:85:LEU:HD23	2.04	0.58
5:S:199:LEU:O	5:S:199:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:98:THR:CG2	5:S:102:TYR:HE1	2.16	0.58
2:P:174:PHE:HD1	2:P:195:THR:HG1	1.51	0.58
5:E:167:TYR:CD1	5:E:170:LYS:HB2	2.37	0.58
1:A:199:TRP:O	1:A:202:VAL:N	2.37	0.58
13:M:126:ASP:CG	13:M:130:SER:HB3	2.24	0.58
6:T:181:LYS:O	6:T:181:LYS:HG2	2.03	0.58
14:N:152:ASN:HD22	14:N:156:ARG:CZ	2.16	0.58
11:Y:192:VAL:C	11:Y:194:ASP:H	2.07	0.58
5:E:130:GLU:HG2	5:E:131:GLU:N	2.18	0.58
13:M:27:THR:HB	13:M:39:TYR:HA	1.86	0.58
3:Q:133:VAL:HG12	3:Q:134:SER:N	2.19	0.58
12:L:1:THR:HG23	12:L:33:ARG:HE	1.69	0.58
7:U:194:GLN:NE2	7:U:197:LYS:HD3	2.19	0.58
5:S:167:TYR:CD1	5:S:170:LYS:HB2	2.39	0.58
7:U:116:GLY:O	7:U:120:GLN:HB2	2.04	0.58
6:T:37:GLY:HA2	6:T:45:VAL:O	2.03	0.58
1:A:144:VAL:HG12	1:A:154:ILE:HG12	1.85	0.58
8:V:67:THR:CG2	8:V:73:PRO:HD3	2.33	0.58
6:F:185:ASN:ND2	6:F:185:ASN:C	2.57	0.58
13:M:27:THR:HG21	13:M:39:TYR:CD1	2.39	0.58
9:I:81:GLN:HA	9:I:81:GLN:OE1	2.03	0.58
9:W:63:ILE:HG13	9:W:82:MET:HE2	1.86	0.57
13:M:49:ASN:HD21	13:M:211:GLY:HA2	1.69	0.57
2:P:212:ALA:CB	2:P:237:LYS:HA	2.34	0.57
8:H:112:THR:O	8:H:114:PRO:HD3	2.04	0.57
13:M:124:SER:CB	13:M:137:ARG:HD2	2.34	0.57
6:T:147:PHE:HB2	6:T:153:VAL:HG22	1.85	0.57
10:X:192:ASP:O	10:X:193:GLU:O	2.22	0.57
6:F:147:PHE:HB2	6:F:153:VAL:HG22	1.85	0.57
8:V:112:THR:O	8:V:114:PRO:HD3	2.04	0.57
10:J:129:ILE:HG22	10:J:130:ASP:H	1.68	0.57
9:I:41:ILE:HD11	9:I:74:PRO:HB2	1.86	0.57
5:E:10:ARG:NH1	5:E:10:ARG:HG2	2.20	0.57
8:V:1:THR:CB	8:V:33:LYS:HZ1	2.16	0.57
5:E:170:LYS:HD2	5:E:180:GLN:OE1	2.04	0.57
9:W:103:VAL:HG12	9:W:108:SER:HA	1.87	0.57
1:A:50:CYS:HA	1:A:228:ALA:O	2.04	0.57
7:U:69:VAL:HG11	7:U:111:PHE:HE1	1.69	0.57
12:L:211:ILE:CD1	12:L:211:ILE:H	2.12	0.57
7:G:194:GLN:HA	7:G:194:GLN:NE2	2.19	0.57
6:F:137:TYR:CE1	6:F:141:GLY:HA2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:148:MET:HE3	10:X:152:LEU:HD11	1.87	0.57
8:V:190:PRO:C	8:V:192:GLU:H	2.06	0.57
10:X:23:ALA:CB	10:X:186:VAL:HG22	2.34	0.57
1:A:234:PHE:CD1	1:A:234:PHE:N	2.73	0.57
7:G:197:LYS:HZ2	7:G:201:LEU:HD21	1.69	0.57
6:T:137:TYR:CE1	6:T:141:GLY:HA2	2.38	0.57
4:R:224:LEU:HD23	4:R:229:ILE:HG12	1.87	0.57
6:F:150:SER:O	7:G:82:PRO:HG2	2.04	0.57
2:P:38:LYS:HG3	2:P:43:VAL:HG22	1.86	0.57
4:D:240:LYS:HB3	4:D:241:GLN:NE2	2.20	0.57
1:A:125:SER:HA	1:A:128:TYR:HB2	1.86	0.57
8:H:4:MET:HB2	8:H:126:ILE:HG22	1.84	0.57
1:A:52:VAL:HG22	1:A:227:VAL:HG22	1.85	0.57
2:B:212:ALA:CB	2:B:237:LYS:HA	2.35	0.57
3:C:201:THR:HG22	3:C:202:ASP:N	2.12	0.57
8:V:112:THR:HG23	8:V:112:THR:O	2.05	0.57
11:Y:35:THR:HG22	11:Y:36:ARG:H	1.67	0.57
10:X:17:LYS:HG2	10:X:156:ASN:HD22	1.69	0.57
14:N:1:THR:HG22	14:N:2:GLN:H	1.67	0.57
6:T:185:ASN:ND2	6:T:185:ASN:C	2.56	0.57
10:J:84:GLU:CD	10:J:84:GLU:H	2.07	0.57
10:X:108:VAL:HG12	10:X:109:ALA:N	2.18	0.57
10:X:120:ILE:HG13	10:X:120:ILE:O	2.05	0.57
2:B:218:ASN:CB	2:B:221:LEU:HD12	2.35	0.57
7:G:69:VAL:HG11	7:G:111:PHE:HE1	1.69	0.57
1:A:244:ARG:HD2	1:A:244:ARG:N	2.20	0.57
1:O:201:LYS:HA	1:O:204:GLU:OE1	2.04	0.57
2:B:48:GLU:CG	2:B:49:LYS:N	2.67	0.57
3:Q:185:LYS:HZ1	3:Q:186:VAL:HB	1.70	0.57
2:P:28:VAL:C	2:P:30:GLN:H	2.07	0.57
5:S:233:ASN:N	5:S:233:ASN:ND2	2.51	0.57
12:Z:211:ILE:CD1	12:Z:211:ILE:H	2.11	0.57
4:D:28:LYS:O	4:D:166:ARG:HB3	2.04	0.57
6:F:75:ALA:O	6:F:130:VAL:HG23	2.03	0.57
9:I:153:LYS:HD2	9:I:153:LYS:O	2.05	0.57
3:Q:198:SER:HA	3:Q:206:LEU:HD22	1.86	0.57
1:O:234:PHE:HD1	1:O:234:PHE:N	2.02	0.57
10:J:14:MET:HE1	10:J:166:ILE:HA	1.85	0.57
1:O:225:VAL:HB	1:O:236:LEU:HD12	1.86	0.57
1:O:87:ILE:N	1:O:88:PRO:HD2	2.20	0.57
3:C:169:THR:O	3:C:173:GLN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:VAL:HG11	12:Z:65:LEU:CD2	2.35	0.57
9:I:87:LEU:HA	9:I:94:ILE:HD11	1.87	0.57
2:B:38:LYS:HG3	2:B:43:VAL:HG22	1.87	0.57
10:X:84:GLU:CD	10:X:84:GLU:H	2.07	0.57
5:E:245:GLU:OE2	5:E:245:GLU:N	2.38	0.57
1:A:234:PHE:N	1:A:234:PHE:HD1	2.02	0.57
1:A:225:VAL:HB	1:A:236:LEU:HD12	1.86	0.57
6:F:163:ALA:O	6:F:164:ARG:HB2	2.05	0.57
2:P:94:HIS:CD2	9:W:61:SER:HB2	2.31	0.57
7:G:90:ARG:HD3	7:G:118:TYR:HE1	1.69	0.57
7:G:194:GLN:NE2	7:G:197:LYS:HD3	2.20	0.57
1:A:116:VAL:O	1:A:119:LYS:N	2.37	0.57
7:G:85:ARG:HG2	7:G:85:ARG:HH11	1.70	0.57
3:C:133:VAL:HG12	3:C:134:SER:N	2.20	0.57
14:N:16:TYR:CE2	14:N:170:VAL:HG22	2.40	0.57
1:O:52:VAL:HG13	1:O:227:VAL:HG22	1.86	0.56
14:N:43:ILE:HB	14:N:51:VAL:CG2	2.35	0.56
8:V:3:ILE:HG12	8:V:127:ALA:O	2.05	0.56
3:C:70:ASN:ND2	3:C:71:ASP:N	2.49	0.56
11:Y:35:THR:CG2	11:Y:43:LEU:HD11	2.34	0.56
6:F:62:LYS:O	6:F:73:SER:HA	2.05	0.56
7:U:178:LEU:O	7:U:182:HIS:HB2	2.05	0.56
8:H:1:THR:CB	8:H:33:LYS:HZ1	2.17	0.56
5:S:126:GLY:O	5:S:127:ALA:HB3	2.05	0.56
4:D:73:LEU:HD12	4:D:135:ILE:HG13	1.86	0.56
1:A:115:ASP:HB3	1:A:155:TYR:CE1	2.40	0.56
1:A:117:LEU:HD12	1:A:117:LEU:O	2.06	0.56
2:P:134:LEU:HD23	2:P:134:LEU:N	2.20	0.56
6:T:62:LYS:O	6:T:73:SER:HA	2.05	0.56
10:X:119:PHE:CD2	10:X:120:ILE:N	2.73	0.56
8:V:21:THR:HG21	8:V:168:SER:HA	1.87	0.56
11:Y:128:LEU:HB3	11:Y:129:PRO:HD2	1.87	0.56
4:R:103:PRO:HG2	4:R:140:PRO:CG	2.34	0.56
11:K:128:LEU:HB3	11:K:129:PRO:HD2	1.86	0.56
2:B:214:ILE:HD13	2:B:235:PHE:HA	1.87	0.56
2:P:90:ARG:HH11	9:W:68:LEU:HB3	1.70	0.56
7:U:31:GLU:HB2	7:U:168:ARG:HH22	1.71	0.56
10:J:14:MET:CE	10:J:166:ILE:HA	2.34	0.56
8:V:14:LEU:HD12	8:V:14:LEU:O	2.06	0.56
8:V:59:VAL:HG11	8:V:82:PHE:CE2	2.41	0.56
7:G:77:TYR:HB3	7:G:135:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:203:HIS:CE1	7:G:206:ASN:HB2	2.40	0.56
8:V:1:THR:HG21	8:V:33:LYS:NZ	2.20	0.56
9:W:63:ILE:HG13	9:W:82:MET:CE	2.35	0.56
9:I:63:ILE:HG13	9:I:82:MET:CE	2.35	0.56
8:H:84:GLU:OE1	8:H:84:GLU:HA	2.03	0.56
14:N:89:PRO:HD2	14:N:120:GLN:OE1	2.05	0.56
9:W:81:GLN:OE1	9:W:81:GLN:HA	2.05	0.56
11:K:35:THR:CG2	11:K:43:LEU:HD11	2.35	0.56
1:A:98:LYS:HD3	8:H:68:SER:O	2.06	0.56
6:F:185:ASN:HD22	6:F:186:PRO:N	2.04	0.56
10:X:107:VAL:HG22	10:X:136:ILE:HG21	1.86	0.56
10:J:192:ASP:O	10:J:193:GLU:O	2.24	0.56
1:A:14:ARG:HH11	1:A:14:ARG:HG3	1.69	0.56
1:A:45:VAL:HG12	1:A:168:ALA:HB1	1.87	0.56
10:X:14:MET:CE	10:X:166:ILE:HA	2.35	0.56
11:K:75:LEU:HD13	11:K:79:ALA:HB3	1.88	0.56
1:O:125:SER:HA	1:O:128:TYR:HB2	1.87	0.56
7:G:178:LEU:O	7:G:182:HIS:HB2	2.06	0.56
8:H:1:THR:N	8:H:129:SER:H	2.03	0.56
14:N:16:TYR:HB2	14:N:168:THR:O	2.06	0.56
5:S:220:SER:HA	5:S:231:TYR:HD1	1.71	0.56
9:W:87:LEU:HA	9:W:94:ILE:HD11	1.87	0.56
12:Z:1:THR:HG23	12:Z:33:ARG:HE	1.71	0.56
6:F:181:LYS:HG2	6:F:181:LYS:O	2.05	0.56
8:H:1:THR:HG21	8:H:33:LYS:NZ	2.21	0.56
2:P:243:ILE:O	2:P:245:ASP:N	2.38	0.56
2:P:241:GLN:NE2	2:P:245:ASP:OD1	2.38	0.56
3:Q:242:THR:OG1	3:Q:243:GLY:N	2.39	0.56
13:M:195:HIS:CD2	13:M:197:GLN:H	2.23	0.56
11:Y:71:GLU:O	11:Y:72:ASP:HB3	2.06	0.56
3:Q:100:LYS:HG2	3:Q:100:LYS:O	2.06	0.56
9:I:8:PHE:HD2	9:I:9:ASN:H	1.54	0.56
1:A:87:ILE:N	1:A:88:PRO:HD2	2.21	0.56
1:O:199:TRP:O	1:O:202:VAL:N	2.38	0.56
14:N:153:PRO:HA	9:W:165:ASN:HD21	1.70	0.56
11:K:28:LEU:HD12	11:K:28:LEU:H	1.69	0.56
14:N:187:ARG:HA	8:V:26:ILE:HD12	1.87	0.56
14:N:201:ASP:OD2	14:N:204:THR:HG23	2.05	0.56
3:Q:210:ARG:HH11	3:Q:210:ARG:HG3	1.71	0.56
3:C:198:SER:HA	3:C:206:LEU:HD22	1.88	0.56
14:N:68:LYS:O	14:N:72:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:156:ARG:HD2	9:W:165:ASN:HD21	1.70	0.56
14:N:27:LEU:CB	14:N:192:SER:HB2	2.36	0.56
1:O:134:MET:CE	7:U:124:LEU:HD22	2.35	0.56
3:Q:228:LYS:HZ1	3:Q:231:LYS:HE3	1.70	0.56
2:P:35:LEU:HD22	2:P:35:LEU:H	1.71	0.56
6:T:11:VAL:HG22	6:T:11:VAL:O	2.06	0.56
4:D:224:LEU:HD23	4:D:229:ILE:HG12	1.88	0.56
8:H:21:THR:HG21	8:H:168:SER:HA	1.86	0.56
5:E:126:GLY:O	5:E:127:ALA:HB3	2.05	0.56
2:P:74:VAL:CG2	2:P:75:TYR:H	2.18	0.55
2:B:241:GLN:O	2:B:243:ILE:N	2.39	0.55
7:G:58:LEU:O	7:G:59:VAL:C	2.43	0.55
11:K:161:LEU:C	11:K:161:LEU:HD23	2.27	0.55
10:X:23:ALA:HB2	10:X:186:VAL:HG22	1.87	0.55
3:Q:208:TYR:CG	3:Q:209:ASP:N	2.75	0.55
1:A:120:ARG:O	1:A:124:LEU:HB2	2.07	0.55
1:A:52:VAL:HG22	1:A:227:VAL:CG1	2.35	0.55
1:O:244:ARG:N	1:O:244:ARG:HD2	2.21	0.55
2:P:241:GLN:O	2:P:243:ILE:N	2.39	0.55
2:P:244:ASN:HA	2:P:247:LEU:CG	2.36	0.55
7:U:203:HIS:CE1	7:U:206:ASN:HB2	2.41	0.55
11:Y:161:LEU:HD23	11:Y:161:LEU:C	2.26	0.55
6:T:185:ASN:HD22	6:T:186:PRO:N	2.05	0.55
10:J:191:LYS:HD2	10:J:191:LYS:N	2.19	0.55
7:U:240:ASP:C	7:U:242:ALA:N	2.59	0.55
10:J:23:ALA:HB2	10:J:186:VAL:HG22	1.87	0.55
8:H:115:LEU:H	8:H:115:LEU:HD22	1.72	0.55
6:F:171:TYR:CD2	6:F:171:TYR:C	2.80	0.55
3:C:77:VAL:HG22	3:C:135:PHE:HE1	1.70	0.55
13:M:122:VAL:HG12	13:M:123:TYR:N	2.21	0.55
3:C:24:TYR:O	3:C:27:GLU:HB3	2.06	0.55
1:A:227:VAL:HG12	1:A:228:ALA:N	2.22	0.55
2:P:19:GLY:O	2:P:21:ILE:N	2.39	0.55
1:O:53:VAL:O	1:O:225:VAL:HG13	2.05	0.55
6:F:158:GLY:O	6:F:159:THR:HB	2.06	0.55
8:H:1:THR:OG1	8:H:2:SER:N	2.39	0.55
9:W:7:LYS:CA	9:W:12:VAL:HG23	2.36	0.55
5:S:176:SER:O	5:S:180:GLN:HB2	2.07	0.55
6:T:171:TYR:CD2	6:T:171:TYR:C	2.79	0.55
1:A:114:CYS:SG	1:A:155:TYR:HD1	2.16	0.55
11:Y:28:LEU:H	11:Y:28:LEU:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:194:ASN:HB2	14:N:212:LEU:O	2.06	0.55
7:G:240:ASP:C	7:G:242:ALA:N	2.59	0.55
5:S:64:ILE:HG22	5:S:64:ILE:O	2.06	0.55
1:A:18:ILE:HD12	1:A:18:ILE:N	2.21	0.55
8:H:190:PRO:C	8:H:192:GLU:N	2.58	0.55
7:G:150:LEU:HD12	7:G:151:GLU:H	1.72	0.55
8:H:10:ASP:OD1	8:H:179:THR:HG22	2.06	0.55
8:H:14:LEU:CD1	8:H:34:LEU:HD22	2.36	0.55
2:B:244:ASN:HA	2:B:247:LEU:CG	2.36	0.55
11:Y:75:LEU:HD13	11:Y:79:ALA:HB3	1.88	0.55
8:H:143:ARG:HB2	8:H:143:ARG:HH11	1.70	0.55
13:M:2:PHE:H	14:N:1:THR:CG2	2.19	0.55
9:W:66:HIS:O	9:W:70:THR:HG23	2.06	0.55
2:B:75:TYR:CB	2:B:134:LEU:HD22	2.36	0.55
6:T:206:LEU:HD23	6:T:206:LEU:N	2.11	0.55
7:U:194:GLN:NE2	7:U:194:GLN:HA	2.20	0.55
7:G:197:LYS:NZ	7:G:201:LEU:HD21	2.22	0.55
2:P:214:ILE:HD13	2:P:235:PHE:HA	1.88	0.55
8:H:3:ILE:HG12	8:H:127:ALA:O	2.07	0.55
1:A:14:ARG:NH1	1:A:14:ARG:HG3	2.22	0.55
11:Y:140:THR:HG21	11:Y:164:CYS:HB3	1.89	0.55
10:J:119:PHE:CD2	10:J:120:ILE:N	2.74	0.55
13:M:61:GLY:O	13:M:65:VAL:HG23	2.07	0.55
4:R:240:LYS:HB3	4:R:241:GLN:NE2	2.22	0.55
9:I:52:THR:HG22	9:I:96:ALA:HB1	1.89	0.55
1:O:52:VAL:HG22	1:O:227:VAL:HG22	1.89	0.55
7:U:77:TYR:HB3	7:U:135:THR:HG23	1.88	0.55
11:K:35:THR:HG22	11:K:36:ARG:H	1.71	0.55
3:C:242:THR:OG1	3:C:243:GLY:N	2.38	0.55
7:U:58:LEU:O	7:U:59:VAL:C	2.44	0.55
1:O:14:ARG:HG3	1:O:14:ARG:HH11	1.71	0.55
2:P:218:ASN:CB	2:P:221:LEU:HD12	2.36	0.55
11:K:196:GLN:HE21	11:K:196:GLN:HA	1.72	0.55
10:X:20:VAL:CG2	10:X:189:ILE:HB	2.37	0.55
7:U:150:LEU:HD12	7:U:151:GLU:H	1.72	0.55
3:C:198:SER:OG	3:C:199:LYS:N	2.39	0.54
1:A:134:MET:CE	7:G:124:LEU:HD22	2.37	0.54
1:A:155:TYR:CD2	1:A:165:GLY:HA2	2.42	0.54
1:O:120:ARG:O	1:O:124:LEU:HB2	2.07	0.54
12:Z:35:ILE:HD11	12:Z:45:MET:CE	2.37	0.54
6:F:11:VAL:O	6:F:11:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:21:ILE:HG22	14:N:22:ILE:N	2.23	0.54
4:R:73:LEU:HD12	4:R:135:ILE:HG13	1.89	0.54
8:V:149:GLU:HG3	8:V:150:GLU:N	2.22	0.54
2:B:28:VAL:HG21	2:B:133:SER:HB2	1.87	0.54
1:O:115:ASP:HB3	1:O:155:TYR:CE1	2.41	0.54
2:P:94:HIS:CB	2:P:99:ARG:HH21	2.17	0.54
14:N:128:ARG:HH11	14:N:138:SER:HB2	1.72	0.54
14:N:130:VAL:HB	14:N:136:THR:HG22	1.89	0.54
8:V:18:SER:OG	8:V:171:GLY:HA3	2.08	0.54
1:A:129:THR:CG2	1:A:129:THR:O	2.55	0.54
5:E:199:LEU:O	5:E:199:LEU:HD12	2.07	0.54
2:P:203:GLU:CD	2:P:203:GLU:N	2.61	0.54
9:W:153:LYS:O	9:W:153:LYS:HD2	2.07	0.54
1:O:116:VAL:O	1:O:119:LYS:N	2.38	0.54
1:A:154:ILE:HG22	1:A:166:TYR:HB2	1.88	0.54
8:H:112:THR:O	8:H:112:THR:HG23	2.06	0.54
1:O:43:LEU:HD12	1:O:43:LEU:C	2.28	0.54
11:K:28:LEU:H	11:K:28:LEU:CD1	2.20	0.54
6:T:156:LEU:HD12	6:T:159:THR:HG21	1.89	0.54
7:U:197:LYS:NZ	7:U:201:LEU:HD21	2.22	0.54
1:O:72:ILE:HA	1:O:81:MET:O	2.07	0.54
2:B:203:GLU:N	2:B:203:GLU:CD	2.61	0.54
11:Y:14:ILE:O	11:Y:15:LEU:HD23	2.08	0.54
3:C:39:MET:HE3	3:C:146:TYR:HB2	1.88	0.54
8:H:18:SER:OG	8:H:171:GLY:HA3	2.08	0.54
2:B:185:LEU:O	2:B:189:ILE:HG13	2.06	0.54
8:V:104:ASP:N	8:V:104:ASP:OD2	2.39	0.54
7:U:80:LEU:N	7:U:80:LEU:HD23	2.21	0.54
8:V:84:GLU:OE1	8:V:84:GLU:HA	2.06	0.54
10:J:20:VAL:CG2	10:J:189:ILE:HB	2.38	0.54
2:B:35:LEU:HD22	2:B:35:LEU:H	1.72	0.54
1:O:33:LYS:HD2	1:O:33:LYS:H	1.72	0.54
9:I:7:LYS:HB3	9:I:12:VAL:HG23	1.90	0.54
5:E:220:SER:HA	5:E:231:TYR:HD1	1.72	0.54
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.36	0.54
2:P:48:GLU:CG	2:P:49:LYS:N	2.68	0.54
11:K:192:VAL:C	11:K:194:ASP:H	2.07	0.54
11:Y:192:VAL:HG12	11:Y:192:VAL:O	2.08	0.54
3:C:228:LYS:HZ2	3:C:231:LYS:HE3	1.71	0.54
9:W:100:VAL:HG13	9:W:111:PHE:HB2	1.90	0.54
5:E:108:ASN:HD21	13:M:82:LYS:HZ2	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:ASP:N	8:H:104:ASP:OD2	2.39	0.54
1:O:217:GLU:OE2	1:O:217:GLU:HA	2.08	0.54
1:O:129:THR:CG2	1:O:129:THR:O	2.55	0.54
13:M:109:THR:HG23	13:M:125:PHE:HB2	1.90	0.54
1:A:124:LEU:O	1:A:128:TYR:HB2	2.07	0.54
1:A:44:ALA:O	1:A:168:ALA:HA	2.08	0.54
1:A:183:GLU:HG3	2:B:55:LEU:HD12	1.89	0.54
1:O:227:VAL:HG12	1:O:228:ALA:N	2.22	0.54
1:O:50:CYS:HA	1:O:228:ALA:O	2.07	0.54
7:G:116:GLY:O	7:G:120:GLN:HB2	2.06	0.54
8:V:155:ILE:HG22	8:V:159:LEU:HD22	1.90	0.54
2:P:45:ILE:HG13	2:P:45:ILE:O	2.06	0.54
13:M:30:ILE:HD12	13:M:30:ILE:C	2.28	0.54
2:P:185:LEU:O	2:P:189:ILE:HG13	2.07	0.54
8:H:147:SER:OG	8:H:150:GLU:CB	2.56	0.54
2:B:91:LYS:C	2:B:93:ALA:N	2.60	0.54
2:B:243:ILE:O	2:B:245:ASP:N	2.40	0.54
2:P:187:ASP:O	2:P:190:HIS:HB3	2.07	0.54
13:M:3:ASN:ND2	13:M:3:ASN:C	2.58	0.54
6:T:29:ILE:HD12	6:T:29:ILE:N	2.22	0.54
6:F:22:VAL:O	6:F:26:LEU:HD22	2.08	0.54
5:S:170:LYS:HD2	5:S:171:ALA:H	1.72	0.54
2:B:203:GLU:OE2	2:B:203:GLU:N	2.40	0.54
8:V:115:LEU:HD22	8:V:115:LEU:H	1.72	0.54
10:X:125:LEU:N	10:X:125:LEU:HD23	2.23	0.54
10:J:108:VAL:HG12	10:J:109:ALA:N	2.23	0.54
13:M:100:LYS:HE2	13:M:103:PHE:O	2.08	0.54
3:Q:198:SER:OG	3:Q:199:LYS:N	2.40	0.54
1:O:234:PHE:N	1:O:234:PHE:CD1	2.72	0.54
13:M:199:GLY:O	13:M:200:ASP:HB2	2.08	0.54
3:Q:24:TYR:O	3:Q:27:GLU:HB3	2.07	0.54
6:T:22:VAL:O	6:T:26:LEU:HD22	2.08	0.54
10:X:120:ILE:HD12	10:X:136:ILE:HG12	1.89	0.54
2:B:19:GLY:O	2:B:21:ILE:N	2.40	0.54
3:C:210:ARG:HG3	3:C:210:ARG:NH1	2.23	0.54
6:T:75:ALA:O	6:T:130:VAL:HG23	2.07	0.54
11:Y:196:GLN:HA	11:Y:196:GLN:HE21	1.72	0.54
2:P:98:LYS:HA	2:P:103:GLU:O	2.08	0.54
3:C:76:ALA:HB3	3:C:136:ILE:HB	1.90	0.54
1:A:87:ILE:HG13	1:A:91:ARG:CD	2.38	0.53
3:C:186:VAL:O	3:C:190:ILE:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:7:THR:HB	8:H:107:LYS:NZ	2.23	0.53
10:X:129:ILE:CG2	10:X:130:ASP:H	2.21	0.53
9:I:100:VAL:HG13	9:I:111:PHE:HB2	1.90	0.53
7:U:118:TYR:CE2	7:U:122:HIS:CE1	2.96	0.53
9:W:98:LEU:HD12	9:W:98:LEU:H	1.73	0.53
13:M:13:LEU:HD12	13:M:14:GLY:H	1.73	0.53
3:C:208:TYR:CG	3:C:209:ASP:N	2.75	0.53
2:B:45:ILE:O	2:B:45:ILE:HG13	2.07	0.53
9:W:146:LEU:HD12	9:W:146:LEU:N	2.22	0.53
1:O:68:THR:O	7:U:157:TRP:HE3	1.91	0.53
7:G:216:SER:HA	7:G:230:VAL:HG23	1.90	0.53
8:H:151:THR:O	8:H:154:PHE:HB3	2.08	0.53
1:O:154:ILE:HG22	1:O:166:TYR:HB2	1.89	0.53
1:O:168:ALA:O	2:P:55:LEU:HD22	2.08	0.53
1:A:80:GLY:HA3	1:A:233:PHE:CZ	2.43	0.53
2:B:226:GLY:HA3	9:I:186:TYR:HB3	1.90	0.53
3:Q:222:ASP:O	3:Q:224:GLU:N	2.40	0.53
5:E:197:GLU:O	5:E:201:LEU:HB2	2.08	0.53
10:J:38:LYS:HE3	12:Z:209:ASN:OD1	2.08	0.53
6:T:187:ASP:O	6:T:191:LYS:HG3	2.08	0.53
6:T:163:ALA:O	6:T:164:ARG:HB2	2.08	0.53
3:C:185:LYS:HZ1	3:C:186:VAL:HB	1.74	0.53
14:N:165:ILE:N	14:N:166:PRO:CD	2.71	0.53
2:B:123:GLN:O	2:B:124:SER:CB	2.57	0.53
13:M:124:SER:HB2	13:M:137:ARG:HD2	1.89	0.53
2:P:203:GLU:OE2	2:P:203:GLU:N	2.42	0.53
1:A:251:GLN:O	1:A:251:GLN:HG2	2.07	0.53
12:L:35:ILE:HD11	12:L:45:MET:CE	2.39	0.53
1:O:155:TYR:CD2	1:O:165:GLY:HA2	2.43	0.53
8:V:82:PHE:HB3	8:V:113:ILE:HD12	1.88	0.53
2:B:244:ASN:O	2:B:248:GLU:HG3	2.09	0.53
8:V:185:ARG:O	8:V:186:LEU:HD23	2.07	0.53
12:Z:99:THR:HG22	12:Z:115:VAL:O	2.09	0.53
3:Q:194:LEU:C	3:Q:196:THR:H	2.12	0.53
11:K:165:VAL:O	11:K:169:GLU:HG3	2.08	0.53
6:F:69:HIS:CD2	6:F:102:LYS:HB3	2.43	0.53
1:A:83:VAL:HG11	1:A:90:ALA:HB2	1.90	0.53
3:C:17:GLY:O	4:D:29:ARG:NH2	2.33	0.53
10:J:120:ILE:HD12	10:J:136:ILE:HG12	1.89	0.53
3:C:208:TYR:C	3:C:210:ARG:H	2.11	0.53
8:V:190:PRO:C	8:V:192:GLU:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:119:PHE:HD2	10:X:120:ILE:N	2.06	0.53
7:G:80:LEU:N	7:G:80:LEU:HD23	2.24	0.53
7:G:213:LEU:HD21	7:G:215:ILE:HD11	1.90	0.53
1:O:80:GLY:HA3	1:O:233:PHE:CZ	2.42	0.53
3:C:194:LEU:C	3:C:196:THR:H	2.12	0.53
11:K:71:GLU:O	11:K:72:ASP:HB3	2.08	0.53
8:H:14:LEU:HD12	8:H:14:LEU:O	2.09	0.53
1:O:199:TRP:O	1:O:200:GLU:C	2.47	0.53
2:P:28:VAL:HG21	2:P:133:SER:HB2	1.90	0.53
10:J:129:ILE:CG2	10:J:130:ASP:H	2.22	0.53
14:N:11:VAL:HG22	14:N:24:ALA:HB2	1.89	0.53
7:G:180:ASP:O	7:G:183:PRO:HD3	2.07	0.53
1:A:123:ASN:HD21	2:B:83:ARG:HE	1.55	0.53
8:H:25:TYR:CE1	9:I:132:LEU:HD22	2.44	0.53
8:V:1:THR:N	8:V:129:SER:H	2.07	0.53
8:V:22:THR:CG2	8:V:27:ALA:HB2	2.39	0.53
2:P:182:GLU:O	2:P:183:LEU:C	2.47	0.53
7:U:213:LEU:HD21	7:U:215:ILE:HD11	1.91	0.53
1:A:225:VAL:HG12	1:A:226:GLY:N	2.23	0.53
2:B:182:GLU:O	2:B:183:LEU:C	2.45	0.53
2:B:187:ASP:O	2:B:190:HIS:HB3	2.08	0.53
1:O:14:ARG:HG3	1:O:14:ARG:NH1	2.24	0.53
8:H:185:ARG:O	8:H:186:LEU:HD23	2.09	0.53
14:N:158:VAL:HG12	14:N:159:VAL:HG13	1.91	0.53
10:J:81:ILE:HD11	10:J:86:PHE:HA	1.90	0.53
1:A:167:LYS:O	1:A:168:ALA:HB2	2.09	0.53
2:B:190:HIS:CE1	2:B:194:LEU:HD11	2.44	0.53
1:O:167:LYS:HG2	2:P:55:LEU:O	2.09	0.53
6:T:96:SER:O	6:T:100:ASN:HA	2.07	0.53
6:F:29:ILE:N	6:F:29:ILE:HD12	2.22	0.53
11:Y:22:THR:CG2	11:Y:27:VAL:HG22	2.38	0.53
7:U:216:SER:HA	7:U:230:VAL:HG23	1.90	0.53
3:Q:76:ALA:HB3	3:Q:136:ILE:HB	1.89	0.53
8:H:22:THR:HG23	8:H:27:ALA:HB2	1.90	0.53
8:H:8:PHE:HE1	8:H:11:GLY:H	1.56	0.53
12:Z:1:THR:CB	12:Z:33:ARG:HH21	2.22	0.53
5:E:233:ASN:ND2	5:E:233:ASN:H	2.05	0.53
2:P:25:LEU:HD23	2:P:25:LEU:O	2.09	0.53
6:T:69:HIS:CD2	6:T:102:LYS:HB3	2.44	0.53
9:W:8:PHE:HD2	9:W:9:ASN:H	1.55	0.53
3:Q:77:VAL:HG22	3:Q:135:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:203:VAL:HG13	4:R:209:ASN:HB2	1.90	0.53
3:Q:185:LYS:NZ	3:Q:186:VAL:HB	2.24	0.53
14:N:51:VAL:HG12	14:N:116:VAL:HG22	1.91	0.53
1:O:124:LEU:O	1:O:128:TYR:HB2	2.08	0.53
7:U:180:ASP:O	7:U:183:PRO:HD3	2.08	0.53
9:I:146:LEU:HD12	9:I:146:LEU:N	2.24	0.53
5:S:245:GLU:OE2	5:S:245:GLU:N	2.42	0.53
1:A:33:LYS:H	1:A:33:LYS:HD2	1.74	0.53
6:F:113:CYS:SG	6:F:151:GLY:O	2.67	0.53
8:H:132:THR:O	8:V:132:THR:O	2.26	0.53
5:E:213:ASP:OD1	5:E:215:ASN:HB2	2.09	0.53
8:H:155:ILE:HG22	8:H:159:LEU:HD22	1.91	0.52
8:H:157:HIS:CE1	8:H:196:LEU:HD13	2.44	0.52
2:B:200:VAL:HG12	2:B:202:GLY:N	2.24	0.52
3:Q:42:ASP:OD1	3:Q:186:VAL:HG23	2.09	0.52
7:G:118:TYR:CE2	7:G:122:HIS:CE1	2.97	0.52
7:G:30:VAL:HG21	7:G:152:PRO:HG2	1.91	0.52
12:Z:208:ASN:C	12:Z:210:VAL:H	2.11	0.52
4:D:54:LEU:HD12	4:D:54:LEU:O	2.09	0.52
5:E:32:LYS:O	5:E:174:SER:HB3	2.09	0.52
10:X:1:SER:O	10:X:2:ASP:C	2.48	0.52
2:B:197:LYS:HA	2:B:204:PHE:CE1	2.45	0.52
1:O:114:CYS:SG	1:O:155:TYR:HD1	2.18	0.52
7:G:31:GLU:HB2	7:G:168:ARG:HH22	1.72	0.52
2:P:190:HIS:NE2	2:P:194:LEU:HD11	2.24	0.52
9:W:38:SER:HB3	9:W:41:ILE:HG13	1.91	0.52
5:S:197:GLU:O	5:S:201:LEU:HB2	2.09	0.52
3:C:77:VAL:HG12	3:C:78:ALA:N	2.24	0.52
8:H:22:THR:CG2	8:H:27:ALA:HB2	2.38	0.52
1:A:217:GLU:HA	1:A:217:GLU:OE2	2.09	0.52
4:D:48:ARG:HH21	4:D:211:GLU:HG2	1.73	0.52
7:G:47:PHE:CE2	7:G:74:GLY:HA3	2.44	0.52
9:I:59:ILE:CG1	9:I:83:LEU:HD23	2.24	0.52
2:P:218:ASN:C	2:P:220:ASP:H	2.11	0.52
11:K:23:ARG:HB2	11:K:28:LEU:CD1	2.39	0.52
10:J:191:LYS:CD	10:J:191:LYS:H	2.14	0.52
10:J:17:LYS:NZ	10:J:17:LYS:HB3	2.24	0.52
8:V:133:PHE:HE2	8:V:166:ASP:HB2	1.73	0.52
10:X:17:LYS:HB3	10:X:17:LYS:NZ	2.25	0.52
2:P:197:LYS:HA	2:P:204:PHE:CE1	2.44	0.52
12:Z:87:VAL:CG1	12:Z:117:SER:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:208:ASN:C	12:L:210:VAL:H	2.12	0.52
5:E:231:TYR:HD1	5:E:231:TYR:H	1.57	0.52
5:S:39:GLY:O	5:S:169:ALA:HA	2.09	0.52
5:E:42:THR:C	5:E:44:GLU:H	2.12	0.52
8:V:156:LYS:NZ	8:V:188:PHE:CD1	2.75	0.52
13:M:46:CYS:SG	13:M:52:MET:HB3	2.49	0.52
1:A:91:ARG:NH1	7:G:156:TYR:CE2	2.77	0.52
2:B:174:PHE:HD1	2:B:195:THR:HG1	1.58	0.52
14:N:154:LEU:HD11	9:W:136:ALA:HB1	1.91	0.52
9:W:104:ASP:O	9:W:106:THR:N	2.39	0.52
3:C:81:THR:HG22	3:C:82:ALA:N	2.25	0.52
3:C:72:LYS:HG2	3:C:225:VAL:HG21	1.90	0.52
1:O:83:VAL:HG11	1:O:90:ALA:HB2	1.91	0.52
12:L:99:THR:HG22	12:L:115:VAL:O	2.10	0.52
1:O:59:VAL:HG11	1:O:66:PRO:HG3	1.90	0.52
3:C:120:GLN:HE21	3:C:121:GLY:N	2.07	0.52
4:R:54:LEU:HD12	4:R:54:LEU:O	2.10	0.52
5:S:201:LEU:HD13	5:S:219:LEU:HD22	1.90	0.52
11:K:22:THR:CG2	11:K:27:VAL:HG22	2.39	0.52
1:O:17:THR:HG23	2:P:128:ARG:HB3	1.91	0.52
1:A:199:TRP:O	1:A:200:GLU:C	2.47	0.52
1:A:28:VAL:O	1:A:31:ALA:HB3	2.10	0.52
1:O:202:VAL:O	1:O:205:PHE:N	2.43	0.52
3:Q:187:ASP:HA	3:Q:190:ILE:CD1	2.39	0.52
3:Q:72:LYS:HG2	3:Q:225:VAL:HG21	1.92	0.52
14:N:1:THR:CG2	14:N:2:GLN:N	2.73	0.52
10:J:119:PHE:HD2	10:J:120:ILE:N	2.08	0.52
5:E:167:TYR:CE1	5:E:170:LYS:HD3	2.45	0.52
13:M:145:LEU:HD11	10:X:143:ASP:HB3	1.90	0.52
7:G:38:GLY:O	7:G:161:GLY:HA2	2.09	0.52
6:F:187:ASP:O	6:F:191:LYS:HG3	2.08	0.52
4:R:48:ARG:HH21	4:R:211:GLU:HG2	1.74	0.52
1:A:168:ALA:O	2:B:55:LEU:HD22	2.10	0.52
1:O:185:HIS:HA	1:O:188:LYS:HZ3	1.74	0.52
2:B:46:ALA:HB2	2:B:211:LEU:HD13	1.90	0.52
4:D:203:VAL:HG13	4:D:209:ASN:HB2	1.91	0.52
1:O:44:ALA:O	1:O:168:ALA:HA	2.09	0.52
7:U:194:GLN:HE21	7:U:194:GLN:CA	2.23	0.52
11:K:67:TYR:CZ	11:K:75:LEU:HD23	2.43	0.52
3:Q:131:PHE:O	3:Q:153:PRO:HB3	2.09	0.52
5:S:220:SER:HA	5:S:231:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:ASN:HD22	7:G:127:SER:N	2.08	0.52
8:H:69:GLN:HG3	8:H:70:TYR:CD1	2.45	0.52
11:K:21:VAL:HG11	12:L:122:LEU:HD11	1.92	0.52
8:V:151:THR:O	8:V:154:PHE:HB3	2.10	0.52
8:H:5:ALA:HA	8:H:14:LEU:HA	1.92	0.52
1:O:196:GLU:HG2	1:O:201:LYS:HB2	1.92	0.52
1:O:52:VAL:HG22	1:O:227:VAL:CG1	2.39	0.52
2:P:107:THR:HG21	2:P:146:SER:HB2	1.91	0.52
1:O:225:VAL:HG12	1:O:226:GLY:N	2.25	0.52
14:N:210:LYS:HE3	14:N:211:ASN:OD1	2.08	0.52
6:F:156:LEU:HD12	6:F:159:THR:HG21	1.91	0.52
1:O:123:ASN:HD21	2:P:83:ARG:HE	1.56	0.52
13:M:3:ASN:C	13:M:3:ASN:HD22	2.12	0.52
10:X:17:LYS:CG	10:X:156:ASN:HD22	2.23	0.52
10:J:20:VAL:HG22	10:J:189:ILE:HB	1.91	0.52
10:J:125:LEU:N	10:J:125:LEU:HD23	2.25	0.52
5:E:214:GLU:HG2	5:E:214:GLU:O	2.09	0.52
2:B:25:LEU:HD23	2:B:25:LEU:O	2.10	0.52
7:G:168:ARG:HG2	7:G:169:GLN:N	2.24	0.52
1:O:43:LEU:HA	1:O:169:THR:O	2.10	0.52
14:N:162:GLU:HA	14:N:165:ILE:HD11	1.91	0.52
11:K:50:ALA:O	11:K:53:THR:HG22	2.10	0.52
3:C:99:LEU:HA	3:C:104:GLU:O	2.10	0.52
12:Z:96:SER:O	12:Z:97:MET:HB3	2.10	0.52
10:J:1:SER:O	10:J:2:ASP:C	2.48	0.52
8:H:195:GLN:O	8:H:196:LEU:O	2.28	0.52
2:B:71:ILE:HD11	2:B:107:THR:HA	1.93	0.52
2:B:107:THR:HG21	2:B:146:SER:HB2	1.92	0.52
2:B:190:HIS:NE2	2:B:194:LEU:HD11	2.24	0.52
11:Y:35:THR:CG2	11:Y:36:ARG:N	2.73	0.52
14:N:146:PHE:O	14:N:149:HIS:N	2.38	0.52
3:Q:17:GLY:O	4:R:29:ARG:NH2	2.33	0.52
6:T:208:VAL:O	6:T:227:GLY:HA2	2.10	0.52
5:E:78:MET:HE1	5:E:82:THR:HG22	1.91	0.52
9:I:63:ILE:HG13	9:I:82:MET:HE2	1.92	0.52
3:C:72:LYS:HG2	3:C:225:VAL:CG2	2.40	0.52
14:N:9:THR:OG1	14:N:10:SER:N	2.32	0.52
1:A:196:GLU:HG2	1:A:201:LYS:HB2	1.91	0.51
12:Z:1:THR:CG2	12:Z:33:ARG:HH21	2.23	0.51
8:V:44:CYS:SG	8:V:98:ILE:HB	2.50	0.51
2:B:86:VAL:CG1	2:B:87:ASP:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:215:ILE:HG12	6:F:216:VAL:N	2.25	0.51
1:A:149:GLU:O	1:A:150:LEU:HG	2.10	0.51
8:V:147:SER:OG	8:V:150:GLU:CB	2.58	0.51
8:H:163:ILE:HG23	8:H:170:GLY:CA	2.38	0.51
1:A:72:ILE:HA	1:A:81:MET:O	2.10	0.51
3:Q:222:ASP:C	3:Q:224:GLU:N	2.61	0.51
3:C:222:ASP:C	3:C:224:GLU:N	2.62	0.51
7:U:60:PRO:HB3	7:U:212:GLU:OE2	2.10	0.51
1:O:101:ALA:HA	1:O:112:MET:CE	2.40	0.51
3:C:4:ARG:HH21	4:D:6:ARG:CG	2.22	0.51
3:Q:4:ARG:HH21	4:R:6:ARG:CG	2.23	0.51
2:P:91:LYS:C	2:P:93:ALA:N	2.63	0.51
13:M:16:ALA:HB2	13:M:122:VAL:HG23	1.92	0.51
7:U:150:LEU:HD12	7:U:155:SER:O	2.10	0.51
5:E:201:LEU:HD13	5:E:219:LEU:HD22	1.91	0.51
5:S:91:HIS:CG	5:S:119:LEU:HD12	2.46	0.51
6:T:144:LEU:C	6:T:145:LEU:HD12	2.31	0.51
13:M:12:ILE:HD13	13:M:110:ILE:HD12	1.92	0.51
1:A:202:VAL:O	1:A:205:PHE:N	2.43	0.51
2:B:74:VAL:CG2	2:B:75:TYR:H	2.18	0.51
2:P:46:ALA:HB2	2:P:211:LEU:HD13	1.92	0.51
2:P:75:TYR:CB	2:P:134:LEU:HD22	2.38	0.51
3:C:243:GLY:O	3:C:244:ILE:HD12	2.10	0.51
3:Q:208:TYR:C	3:Q:210:ARG:H	2.13	0.51
10:X:37:ASN:HD22	10:X:37:ASN:C	2.14	0.51
6:F:144:LEU:HD12	6:F:145:LEU:H	1.74	0.51
14:N:199:ILE:HG22	14:N:200:ILE:N	2.25	0.51
6:F:201:LEU:HD13	6:F:205:SER:HA	1.92	0.51
6:T:201:LEU:HD13	6:T:205:SER:HA	1.93	0.51
6:F:176:LEU:O	6:F:180:ILE:HG22	2.10	0.51
11:Y:67:TYR:CZ	11:Y:75:LEU:HD23	2.45	0.51
1:O:134:MET:HE3	7:U:124:LEU:HD22	1.91	0.51
11:K:192:VAL:O	11:K:192:VAL:HG12	2.10	0.51
2:P:123:GLN:O	2:P:124:SER:CB	2.58	0.51
3:C:120:GLN:NE2	3:C:120:GLN:C	2.64	0.51
14:N:1:THR:CG2	14:N:2:GLN:H	2.22	0.51
14:N:177:ILE:O	14:N:181:MET:HG2	2.10	0.51
14:N:186:TYR:CD1	9:W:139:GLU:HB3	2.45	0.51
1:A:43:LEU:HA	1:A:169:THR:O	2.10	0.51
1:A:167:LYS:HG2	2:B:55:LEU:O	2.10	0.51
2:P:44:VAL:CA	2:P:213:ILE:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:183:GLU:HG3	2:P:55:LEU:HD12	1.93	0.51
7:U:90:ARG:HD3	7:U:118:TYR:CE1	2.45	0.51
7:U:240:ASP:HA	7:U:243:GLN:HB2	1.92	0.51
8:V:143:ARG:HH11	8:V:143:ARG:HB2	1.73	0.51
10:X:119:PHE:HD2	10:X:120:ILE:H	1.57	0.51
12:Z:182:GLU:HG2	12:Z:182:GLU:O	2.11	0.51
6:T:113:CYS:SG	6:T:151:GLY:O	2.68	0.51
2:B:218:ASN:C	2:B:220:ASP:H	2.13	0.51
3:Q:243:GLY:O	3:Q:244:ILE:HD12	2.11	0.51
14:N:11:VAL:HG22	14:N:24:ALA:CB	2.40	0.51
9:I:104:ASP:O	9:I:106:THR:N	2.40	0.51
1:A:77:ARG:CG	1:A:77:ARG:O	2.56	0.51
9:W:81:GLN:O	9:W:85:GLN:HB2	2.09	0.51
8:V:22:THR:HG23	8:V:27:ALA:HB2	1.91	0.51
7:G:74:GLY:HA2	7:G:227:HIS:CD2	2.46	0.51
14:N:56:ASP:OD2	14:N:58:SER:N	2.44	0.51
14:N:233:ILE:HG13	14:N:233:ILE:O	2.10	0.51
11:K:20:ALA:HB2	11:K:177:LYS:CG	2.40	0.51
9:I:217:ILE:HD12	9:I:217:ILE:N	2.25	0.51
2:B:218:ASN:HD21	2:B:236:ARG:CD	2.18	0.51
1:A:17:THR:HG23	2:B:128:ARG:HB3	1.93	0.51
13:M:126:ASP:HB2	13:M:130:SER:CB	2.38	0.51
6:F:96:SER:O	6:F:100:ASN:HA	2.11	0.51
11:Y:28:LEU:H	11:Y:28:LEU:CD1	2.22	0.51
3:C:80:LEU:N	3:C:80:LEU:HD22	2.24	0.51
6:F:144:LEU:HD12	6:F:145:LEU:N	2.26	0.51
4:D:132:SER:HB3	4:D:164:ILE:HD12	1.93	0.51
1:O:157:THR:HA	1:O:162:TYR:O	2.11	0.51
3:C:185:LYS:NZ	3:C:186:VAL:HB	2.25	0.51
3:C:187:ASP:HA	3:C:190:ILE:CD1	2.40	0.51
1:O:167:LYS:O	1:O:168:ALA:HB2	2.11	0.51
5:S:51:GLU:HG3	5:S:208:MET:SD	2.51	0.51
3:C:222:ASP:O	3:C:224:GLU:N	2.43	0.51
3:Q:120:GLN:HE21	3:Q:121:GLY:N	2.08	0.51
9:I:8:PHE:CD2	9:I:9:ASN:N	2.79	0.51
3:C:143:ARG:HG2	11:K:73:TYR:CE1	2.46	0.51
3:Q:235:ILE:O	3:Q:237:ASP:N	2.43	0.51
8:V:14:LEU:CD1	8:V:34:LEU:HD22	2.36	0.51
7:U:30:VAL:HG21	7:U:152:PRO:HG2	1.91	0.51
11:K:140:THR:HG21	11:K:164:CYS:HB3	1.93	0.51
3:C:120:GLN:NE2	3:C:121:GLY:N	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:107:VAL:HG12	10:J:107:VAL:O	2.10	0.51
10:J:83:PRO:HB2	10:J:119:PHE:HD1	1.76	0.51
10:X:37:ASN:HB3	10:X:182:TRP:CE3	2.45	0.51
3:C:100:LYS:O	3:C:100:LYS:HG2	2.09	0.51
5:S:214:GLU:HG2	5:S:214:GLU:O	2.11	0.51
8:V:5:ALA:HA	8:V:14:LEU:HA	1.93	0.51
10:J:17:LYS:CG	10:J:156:ASN:HB3	2.41	0.51
9:I:7:LYS:CA	9:I:12:VAL:HG23	2.40	0.51
6:T:215:ILE:HG12	6:T:216:VAL:N	2.26	0.51
8:V:163:ILE:CD1	8:V:170:GLY:HA2	2.40	0.50
10:J:125:LEU:HD23	10:J:125:LEU:H	1.76	0.50
11:Y:165:VAL:O	11:Y:169:GLU:HG3	2.10	0.50
3:C:235:ILE:O	3:C:237:ASP:N	2.44	0.50
8:H:187:ILE:C	8:H:188:PHE:CD2	2.85	0.50
7:U:168:ARG:HG2	7:U:169:GLN:N	2.24	0.50
8:H:102:TYR:CD1	8:H:107:LYS:O	2.64	0.50
8:V:7:THR:HB	8:V:107:LYS:NZ	2.26	0.50
2:P:239:THR:O	2:P:243:ILE:HG13	2.11	0.50
1:A:220:LYS:HB2	1:A:220:LYS:HZ3	1.75	0.50
9:I:81:GLN:O	9:I:85:GLN:HB2	2.11	0.50
3:Q:210:ARG:NH1	3:Q:210:ARG:HG3	2.25	0.50
14:N:220:ASP:O	14:N:222:ALA:N	2.43	0.50
12:L:1:THR:CB	12:L:33:ARG:HH21	2.25	0.50
12:L:1:THR:CG2	12:L:33:ARG:HH21	2.25	0.50
2:P:246:ARG:HG3	2:P:246:ARG:NH1	2.27	0.50
14:N:80:LEU:CD2	14:N:84:GLU:HB2	2.41	0.50
8:H:185:ARG:HG3	8:H:185:ARG:NH1	2.25	0.50
8:V:1:THR:OG1	8:V:2:SER:N	2.42	0.50
8:H:156:LYS:NZ	8:H:188:PHE:CD1	2.74	0.50
7:U:74:GLY:HA2	7:U:227:HIS:CD2	2.46	0.50
7:U:47:PHE:CE2	7:U:74:GLY:HA3	2.45	0.50
6:T:82:ARG:O	6:T:86:ASN:HB2	2.11	0.50
7:G:235:LEU:O	7:G:239:ILE:HG13	2.12	0.50
1:O:126:GLN:HE21	1:O:126:GLN:C	2.15	0.50
9:W:52:THR:HG22	9:W:96:ALA:HB1	1.92	0.50
14:N:27:LEU:HD21	14:N:34:LEU:HD12	1.92	0.50
2:P:190:HIS:CE1	2:P:194:LEU:HD11	2.46	0.50
3:Q:72:LYS:HG2	3:Q:225:VAL:CG2	2.41	0.50
11:Y:18:SER:O	11:Y:34:LYS:NZ	2.41	0.50
14:N:48:ASN:HD22	14:N:48:ASN:N	2.07	0.50
5:E:170:LYS:HD2	5:E:171:ALA:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:176:SER:O	5:E:180:GLN:HB2	2.11	0.50
5:S:97:VAL:HG11	12:Z:65:LEU:HD22	1.93	0.50
5:S:231:TYR:H	5:S:231:TYR:HD1	1.59	0.50
14:N:13:SER:HB2	14:N:21:ILE:O	2.10	0.50
4:R:132:SER:HB3	4:R:164:ILE:HD12	1.92	0.50
3:Q:112:VAL:HG22	3:Q:137:TYR:CG	2.46	0.50
2:B:13:SER:HB2	2:B:21:ILE:O	13.22	0.50
2:P:244:ASN:O	2:P:248:GLU:HG3	2.11	0.50
3:Q:80:LEU:HD22	3:Q:80:LEU:N	2.24	0.50
5:E:56:SER:OG	5:E:57:PRO:HD2	2.11	0.50
2:B:241:GLN:O	2:B:244:ASN:ND2	2.45	0.50
9:I:105:PRO:O	9:I:106:THR:HG23	2.12	0.50
1:A:68:THR:O	7:G:157:TRP:HE3	1.94	0.50
3:Q:140:TYR:C	3:Q:140:TYR:CD1	2.84	0.50
8:V:58:ILE:O	8:V:61:TYR:HB3	2.11	0.50
11:Y:20:ALA:HB2	11:Y:177:LYS:CG	2.42	0.50
9:W:217:ILE:HD12	9:W:217:ILE:N	2.27	0.50
7:U:38:GLY:O	7:U:161:GLY:HA2	2.11	0.50
1:A:225:VAL:O	1:A:236:LEU:HB2	2.12	0.50
2:P:213:ILE:O	2:P:213:ILE:HD12	2.12	0.50
1:O:28:VAL:O	1:O:31:ALA:HB3	2.12	0.50
7:U:203:HIS:C	7:U:205:ASP:H	2.14	0.50
12:L:191:HIS:HD2	12:L:191:HIS:N	2.10	0.50
8:H:184:GLU:OE2	8:H:186:LEU:HD21	2.11	0.50
3:C:4:ARG:NH2	4:D:6:ARG:HG2	2.25	0.50
3:Q:4:ARG:HH21	4:R:6:ARG:HD3	1.76	0.50
10:X:20:VAL:HG22	10:X:189:ILE:HB	1.93	0.50
1:A:103:GLU:HG3	1:A:107:LYS:HD3	1.94	0.50
14:N:220:ASP:C	14:N:222:ALA:H	2.14	0.50
6:T:51:ARG:O	6:T:59:TYR:HA	2.12	0.50
10:J:37:ASN:HB3	10:J:182:TRP:CE3	2.46	0.50
6:F:39:ARG:HD3	6:F:142:ALA:HB1	1.93	0.50
3:Q:99:LEU:HA	3:Q:104:GLU:O	2.12	0.50
3:Q:185:LYS:CD	3:Q:186:VAL:H	2.18	0.50
10:X:166:ILE:HG23	10:X:167:SER:N	2.26	0.50
6:T:179:PHE:C	6:T:181:LYS:N	2.65	0.50
2:P:156:TYR:C	2:P:157:PHE:HD2	2.14	0.50
10:J:119:PHE:HD2	10:J:120:ILE:H	1.59	0.50
5:S:167:TYR:CE1	5:S:170:LYS:HD3	2.46	0.50
1:O:103:GLU:HG3	1:O:107:LYS:HD3	1.92	0.50
1:O:12:TYR:HE1	2:P:7:PHE:CE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:235:LEU:O	7:U:239:ILE:HG13	2.12	0.50
8:H:82:PHE:HB3	8:H:113:ILE:HD12	1.92	0.50
1:A:97:ALA:HB2	1:A:121:MET:CE	2.41	0.50
1:A:83:VAL:HG13	1:A:141:LEU:HD23	1.94	0.50
13:M:152:ASN:O	13:M:156:PHE:HA	2.12	0.50
1:O:87:ILE:HG13	1:O:91:ARG:CD	2.41	0.50
8:H:190:PRO:O	8:H:192:GLU:N	2.44	0.50
4:R:27:VAL:HG11	4:R:132:SER:HB2	1.94	0.50
3:C:140:TYR:CD1	3:C:140:TYR:C	2.84	0.50
1:A:128:TYR:HD1	1:A:133:TYR:HH	1.56	0.50
8:H:126:ILE:HG13	8:H:126:ILE:O	2.11	0.50
2:B:213:ILE:O	2:B:213:ILE:HD12	2.11	0.50
8:V:13:ILE:CG1	8:V:177:VAL:HG22	2.34	0.50
11:K:39:SER:CB	11:K:40:PRO:HD2	2.40	0.50
2:B:239:THR:O	2:B:243:ILE:HG13	2.11	0.50
9:I:188:ARG:O	9:I:189:ASN:CB	2.59	0.50
11:Y:50:ALA:O	11:Y:53:THR:HG22	2.12	0.50
5:S:243:LEU:C	5:S:243:LEU:HD13	2.33	0.50
9:I:8:PHE:HD2	9:I:9:ASN:N	2.10	0.50
1:O:17:THR:O	1:O:17:THR:HG22	2.12	0.50
6:T:59:TYR:CE1	6:T:209:ASP:HB3	2.47	0.50
8:H:97:ILE:HD11	8:H:99:VAL:HG23	1.94	0.49
7:G:169:GLN:N	7:G:169:GLN:OE1	2.41	0.49
1:O:92:ASN:O	1:O:95:LEU:N	2.42	0.49
7:G:90:ARG:HG2	7:G:118:TYR:CE1	2.47	0.49
3:C:80:LEU:HD23	3:C:132:GLY:O	2.12	0.49
7:U:197:LYS:HZ2	7:U:201:LEU:HD21	1.77	0.49
5:E:64:ILE:O	5:E:64:ILE:HG22	2.12	0.49
9:I:21:THR:HG22	9:I:23:GLY:O	2.12	0.49
9:I:98:LEU:H	9:I:98:LEU:HD12	1.76	0.49
3:Q:4:ARG:NH2	4:R:6:ARG:HG2	2.26	0.49
8:V:126:ILE:O	8:V:126:ILE:HG13	2.12	0.49
5:E:39:GLY:O	5:E:169:ALA:HA	2.11	0.49
14:N:26:ASN:O	14:N:39:VAL:HB	2.12	0.49
1:A:134:MET:HE3	7:G:124:LEU:HD22	1.93	0.49
2:B:44:VAL:CA	2:B:213:ILE:HG22	2.42	0.49
1:A:177:GLU:CD	1:A:177:GLU:H	2.14	0.49
2:P:71:ILE:HD11	2:P:107:THR:HA	1.94	0.49
6:T:179:PHE:CD1	6:T:180:ILE:N	2.80	0.49
4:D:187:THR:HB	4:D:190:GLU:HG2	1.93	0.49
7:G:240:ASP:HA	7:G:243:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:48:ASN:ND2	14:N:48:ASN:H	2.10	0.49
5:E:220:SER:HA	5:E:231:TYR:CD1	2.47	0.49
6:F:89:ARG:CZ	13:M:77:PHE:CD1	2.95	0.49
14:N:35:ARG:O	14:N:35:ARG:CG	2.61	0.49
13:M:147:MET:N	13:M:148:PRO:CD	2.75	0.49
7:G:108:ILE:N	7:G:109:PRO:CD	2.74	0.49
7:G:136:ILE:HD11	7:G:163:ALA:HA	1.95	0.49
7:U:169:GLN:OE1	7:U:169:GLN:N	2.38	0.49
7:G:92:ARG:NE	14:N:76:TYR:CD1	2.80	0.49
2:P:200:VAL:HG12	2:P:202:GLY:N	2.25	0.49
8:V:25:TYR:CE1	9:W:132:LEU:HD22	2.47	0.49
3:Q:120:GLN:NE2	3:Q:120:GLN:C	2.66	0.49
9:W:8:PHE:CD2	9:W:9:ASN:N	2.79	0.49
1:O:83:VAL:HG13	1:O:141:LEU:HD23	1.93	0.49
11:K:152:MET:HA	11:K:156:GLU:OE2	2.11	0.49
7:U:108:ILE:N	7:U:109:PRO:CD	2.75	0.49
5:S:32:LYS:O	5:S:174:SER:HB3	2.11	0.49
4:R:62:SER:C	4:R:64:VAL:H	2.16	0.49
6:T:39:ARG:HD3	6:T:142:ALA:HB1	1.92	0.49
11:K:51:GLY:HA3	12:L:118:ASP:O	2.11	0.49
2:B:68:THR:C	2:B:70:ASP:H	2.16	0.49
7:U:136:ILE:HD11	7:U:163:ALA:HA	1.94	0.49
1:A:230:LYS:HE3	1:A:230:LYS:CA	2.32	0.49
6:F:176:LEU:C	6:F:176:LEU:HD12	2.33	0.49
2:B:244:ASN:ND2	2:B:244:ASN:N	2.60	0.49
1:O:77:ARG:O	1:O:77:ARG:CG	2.59	0.49
12:Z:176:ASN:ND2	12:Z:187:TYR:OH	2.45	0.49
12:L:96:SER:O	12:L:97:MET:HB3	2.12	0.49
14:N:172:VAL:HA	14:N:175:GLU:HG2	1.94	0.49
8:H:137:TYR:O	8:H:139:ASP:N	2.46	0.49
7:G:168:ARG:O	7:G:171:ALA:HB3	2.12	0.49
1:O:45:VAL:HA	1:O:168:ALA:CB	2.42	0.49
10:J:88:GLN:CA	10:J:88:GLN:HE21	2.22	0.49
2:B:246:ARG:HG3	2:B:246:ARG:NH1	2.28	0.49
1:A:66:PRO:HA	1:A:69:VAL:CG2	2.42	0.49
1:A:101:ALA:HA	1:A:112:MET:CE	2.42	0.49
12:L:186:ILE:HD12	12:L:186:ILE:N	2.27	0.49
12:L:87:VAL:CG1	12:L:117:SER:HA	2.42	0.49
5:S:184:LEU:HD22	6:T:56:LEU:HD23	1.93	0.49
5:S:198:LEU:O	5:S:202:LYS:HB2	2.13	0.49
8:H:58:ILE:O	8:H:61:TYR:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:SER:C	4:D:64:VAL:H	2.16	0.49
8:V:157:HIS:CE1	8:V:196:LEU:HD13	2.47	0.49
12:Z:76:VAL:N	12:Z:108:GLU:OE1	2.44	0.49
12:L:124:GLY:HA3	12:L:127:PHE:CE2	2.47	0.49
8:V:8:PHE:HE1	8:V:11:GLY:H	1.59	0.49
1:A:225:VAL:CG1	1:A:226:GLY:N	2.76	0.49
1:A:83:VAL:HG11	1:A:90:ALA:CB	2.43	0.49
1:O:227:VAL:HB	1:O:234:PHE:CE1	2.47	0.49
4:R:34:VAL:HG12	4:R:199:LEU:HD21	1.95	0.49
7:G:72:HIS:C	7:G:72:HIS:CD2	2.85	0.49
3:Q:80:LEU:HD23	3:Q:132:GLY:O	2.12	0.49
14:N:23:ALA:O	14:N:24:ALA:HB2	2.13	0.49
7:U:90:ARG:CD	7:U:118:TYR:CE1	2.95	0.49
3:Q:81:THR:HG22	3:Q:82:ALA:N	2.27	0.49
11:K:161:LEU:HD22	11:K:195:PHE:HE2	1.77	0.49
9:I:3:ILE:HG22	9:I:16:ALA:CB	2.42	0.49
1:A:206:ALA:O	1:A:207:ILE:C	2.50	0.49
12:Z:72:GLU:HA	12:Z:72:GLU:OE2	2.12	0.49
1:A:167:LYS:HB3	1:A:167:LYS:HZ3	1.77	0.49
3:Q:185:LYS:HD2	3:Q:186:VAL:N	2.19	0.49
2:P:241:GLN:O	2:P:244:ASN:ND2	2.46	0.49
1:O:66:PRO:HA	1:O:69:VAL:CG2	2.43	0.49
7:G:60:PRO:HB3	7:G:212:GLU:OE2	2.11	0.49
5:E:184:LEU:HD22	6:F:56:LEU:HD23	1.93	0.49
5:E:126:GLY:O	5:E:127:ALA:CB	2.60	0.49
12:L:72:GLU:OE2	12:L:72:GLU:HA	2.11	0.49
10:X:81:ILE:HD11	10:X:86:PHE:HA	1.94	0.49
7:G:121:ALA:HA	7:G:124:LEU:CD1	2.42	0.49
2:B:156:TYR:C	2:B:157:PHE:HD2	2.15	0.49
10:J:17:LYS:CG	10:J:156:ASN:HD22	2.26	0.49
9:W:100:VAL:CG1	9:W:111:PHE:HB2	2.42	0.49
7:U:44:GLY:HA2	7:U:140:VAL:CG2	2.43	0.49
5:S:126:GLY:O	5:S:127:ALA:CB	2.61	0.49
6:F:123:TYR:CG	6:F:124:GLY:N	2.80	0.49
13:M:115:ASP:OD1	13:M:117:ASP:N	2.46	0.49
6:F:82:ARG:O	6:F:86:ASN:HB2	2.13	0.49
12:L:8:PHE:CE1	12:L:13:ILE:HG12	2.48	0.49
7:G:111:PHE:C	7:G:111:PHE:CD2	2.86	0.49
2:B:36:GLY:O	2:B:161:ALA:HA	2.13	0.49
8:V:82:PHE:CD1	8:V:97:ILE:HG12	2.48	0.49
7:U:194:GLN:CD	7:U:197:LYS:HD3	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:9:LEU:HD13	2:P:122:THR:O	2.13	0.49
7:U:60:PRO:O	7:U:61:GLN:CB	2.61	0.49
14:N:159:VAL:HG23	14:N:159:VAL:O	2.13	0.49
6:T:69:HIS:HE1	6:T:70:MET:CE	2.25	0.49
1:O:106:TYR:HB2	8:V:61:TYR:HD2	1.78	0.49
6:F:89:ARG:NE	13:M:77:PHE:CE1	2.81	0.49
4:D:62:SER:O	4:D:63:LYS:HB3	2.13	0.49
2:P:170:ALA:HA	2:P:173:THR:HB	1.95	0.49
7:G:98:PHE:CD1	7:G:98:PHE:C	2.86	0.49
3:C:112:VAL:HG22	3:C:137:TYR:CG	2.48	0.49
1:A:157:THR:HA	1:A:162:TYR:O	2.13	0.49
7:G:60:PRO:O	7:G:61:GLN:CB	2.61	0.49
12:Z:186:ILE:N	12:Z:186:ILE:HD12	2.28	0.49
13:M:111:ILE:HG12	13:M:123:TYR:HB2	1.95	0.49
9:I:31:CYS:SG	9:I:32:ALA:N	2.85	0.49
8:V:38:HIS:HB3	8:V:41:ILE:HB	1.95	0.49
6:T:114:ASP:O	6:T:118:LYS:HD3	2.12	0.49
13:M:36:ASN:O	13:M:37:SER:HB2	2.13	0.49
14:N:103:ARG:CZ	14:N:110:LEU:HD11	2.42	0.49
1:A:227:VAL:HB	1:A:234:PHE:CE1	2.48	0.48
8:V:97:ILE:HD11	8:V:99:VAL:HG23	1.95	0.48
1:A:104:PHE:CG	1:A:112:MET:HG3	2.48	0.48
5:S:78:MET:HE3	5:S:82:THR:HG22	1.94	0.48
8:V:185:ARG:HG3	8:V:185:ARG:NH1	2.27	0.48
11:K:22:THR:HG22	11:K:26:SER:O	2.13	0.48
6:T:215:ILE:CG1	6:T:216:VAL:N	2.76	0.48
3:C:29:ILE:C	3:C:31:HIS:H	2.17	0.48
3:Q:29:ILE:C	3:Q:31:HIS:H	2.15	0.48
1:A:163:TYR:C	1:A:163:TYR:CD1	2.84	0.48
1:O:63:LEU:O	7:U:160:LYS:HG3	2.13	0.48
3:Q:70:ASN:HD22	3:Q:71:ASP:N	2.07	0.48
6:F:179:PHE:C	6:F:181:LYS:N	2.65	0.48
7:G:203:HIS:C	7:G:205:ASP:H	2.17	0.48
8:H:133:PHE:HE2	8:H:166:ASP:HB2	1.75	0.48
3:C:4:ARG:HH21	4:D:6:ARG:HD3	1.77	0.48
2:P:145:PHE:CE1	2:P:214:ILE:HG22	2.47	0.48
8:V:69:GLN:HG3	8:V:70:TYR:CD1	2.48	0.48
11:K:25:ILE:HG12	11:Y:139:TYR:OH	2.12	0.48
5:S:42:THR:C	5:S:44:GLU:H	2.16	0.48
11:Y:1:MET:HG2	11:Y:2:ASP:H	1.78	0.48
9:I:137:VAL:O	9:I:137:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:O	1:A:95:LEU:N	2.42	0.48
8:H:4:MET:HB2	8:H:125:ALA:O	2.14	0.48
7:G:31:GLU:HG3	7:G:31:GLU:O	2.12	0.48
1:O:225:VAL:O	1:O:236:LEU:HB2	2.12	0.48
10:X:166:ILE:CG2	10:X:167:SER:N	2.77	0.48
7:G:194:GLN:HE21	7:G:194:GLN:CA	2.22	0.48
3:Q:152:ASN:HB2	3:Q:153:PRO:HD2	1.95	0.48
14:N:80:LEU:HD12	14:N:80:LEU:N	2.27	0.48
7:U:85:ARG:NH1	7:U:85:ARG:HG2	2.28	0.48
10:X:125:LEU:H	10:X:125:LEU:HD23	1.77	0.48
5:S:213:ASP:OD1	5:S:215:ASN:HB2	2.12	0.48
13:M:164:THR:O	13:M:167:LYS:HB2	2.13	0.48
14:N:141:THR:HG21	14:N:155:LEU:O	2.13	0.48
1:O:231:ASP:O	1:O:232:LYS:HB2	2.13	0.48
12:Z:38:ASN:HB2	12:Z:39:PRO:HD2	1.95	0.48
6:F:114:ASP:O	6:F:118:LYS:HD3	2.13	0.48
8:V:106:ASN:O	8:V:107:LYS:HB3	2.13	0.48
5:S:56:SER:OG	5:S:57:PRO:HD2	2.13	0.48
14:N:194:ASN:HD22	14:N:211:ASN:ND2	2.12	0.48
9:W:188:ARG:O	9:W:189:ASN:CB	2.61	0.48
2:P:86:VAL:CG1	2:P:87:ASP:N	2.76	0.48
14:N:49:THR:HG22	14:N:50:VAL:N	2.28	0.48
10:X:10:ILE:HG21	10:X:141:ALA:HB3	1.95	0.48
5:S:98:THR:CG2	5:S:102:TYR:CE1	2.96	0.48
7:U:80:LEU:CD2	7:U:80:LEU:N	2.77	0.48
11:Y:95:ARG:HG2	11:Y:95:ARG:HH11	1.78	0.48
6:T:189:LEU:HD23	6:T:189:LEU:O	2.14	0.48
4:D:160:SER:OG	4:D:181:ARG:NH1	2.46	0.48
5:E:91:HIS:CG	5:E:119:LEU:HD12	2.48	0.48
9:W:137:VAL:HG12	9:W:137:VAL:O	2.13	0.48
8:H:82:PHE:CD1	8:H:97:ILE:HG12	2.48	0.48
2:B:37:ILE:HB	2:B:44:VAL:CG1	2.43	0.48
2:P:218:ASN:HD21	2:P:236:ARG:CD	2.18	0.48
6:F:179:PHE:CD1	6:F:180:ILE:N	2.81	0.48
8:V:163:ILE:HG23	8:V:170:GLY:CA	2.36	0.48
7:G:194:GLN:CD	7:G:197:LYS:HD3	2.34	0.48
1:A:104:PHE:C	1:A:104:PHE:CD1	2.87	0.48
5:E:243:LEU:C	5:E:243:LEU:HD13	2.34	0.48
12:L:45:MET:O	12:L:45:MET:HG2	2.13	0.48
6:F:215:ILE:CG1	6:F:216:VAL:N	2.77	0.48
4:R:62:SER:O	4:R:63:LYS:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:195:GLN:O	8:V:196:LEU:O	2.31	0.48
11:K:11:ASP:O	11:K:12:SER:HB3	2.13	0.48
2:B:28:VAL:C	2:B:30:GLN:N	2.67	0.48
8:V:102:TYR:CD1	8:V:107:LYS:O	2.66	0.48
14:N:43:ILE:HB	14:N:51:VAL:HG23	1.95	0.48
14:N:43:ILE:HD13	14:N:64:GLU:CG	2.38	0.48
8:H:38:HIS:HB3	8:H:41:ILE:HB	1.96	0.48
6:T:176:LEU:O	6:T:180:ILE:HG22	2.13	0.48
11:Y:161:LEU:HD22	11:Y:195:PHE:HE2	1.77	0.48
7:G:39:ILE:HD12	7:G:195:ALA:HB2	1.96	0.48
1:O:73:PHE:N	1:O:73:PHE:CD1	2.81	0.48
12:Z:104:TYR:CE2	12:Z:110:PRO:HG3	2.49	0.48
4:D:31:THR:HB	4:D:47:GLU:CG	2.44	0.48
4:D:72:VAL:CG1	4:D:221:ILE:HD13	2.44	0.48
1:A:63:LEU:O	7:G:160:LYS:HG3	2.13	0.48
2:P:37:ILE:HB	2:P:44:VAL:CG1	2.44	0.48
2:P:218:ASN:O	2:P:220:ASP:N	2.46	0.48
10:X:14:MET:HE3	10:X:166:ILE:CG1	2.37	0.48
10:X:14:MET:HE3	10:X:166:ILE:HA	1.94	0.48
6:T:176:LEU:HD12	6:T:176:LEU:C	2.33	0.48
7:G:90:ARG:CD	7:G:118:TYR:CE1	2.96	0.48
9:I:21:THR:O	9:I:22:GLN:CB	2.61	0.48
9:W:8:PHE:HD2	9:W:9:ASN:N	2.10	0.48
8:V:187:ILE:C	8:V:188:PHE:CD2	2.87	0.48
10:J:171:LEU:HD21	10:J:199:LEU:HD13	1.95	0.48
3:C:92:ARG:NE	10:J:75:LEU:HD23	2.29	0.48
8:H:97:ILE:HD11	8:H:99:VAL:CG2	2.43	0.48
1:A:188:LYS:O	1:A:190:LYS:N	2.46	0.48
1:A:43:LEU:HD23	1:A:178:ILE:HG23	1.96	0.48
1:O:200:GLU:HG2	1:O:244:ARG:HH21	1.79	0.48
1:O:15:HIS:CB	1:O:18:ILE:HD13	2.42	0.48
8:H:12:VAL:HG22	8:H:13:ILE:N	2.29	0.48
3:C:185:LYS:HD2	3:C:186:VAL:N	2.20	0.48
1:A:126:GLN:HE21	1:A:126:GLN:C	2.16	0.48
6:F:208:VAL:O	6:F:227:GLY:HA2	2.14	0.48
3:C:65:LYS:C	3:C:66:LEU:HD12	2.34	0.48
10:X:107:VAL:O	10:X:107:VAL:HG12	2.13	0.48
6:T:69:HIS:HE1	6:T:70:MET:HE3	1.79	0.48
13:M:12:ILE:O	13:M:12:ILE:HD12	2.14	0.48
10:X:97:ARG:HG3	10:X:102:TYR:CE2	2.48	0.48
11:Y:85:ARG:O	11:Y:89:ALA:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASP:O	1:A:232:LYS:HB2	2.13	0.48
3:Q:49:GLU:O	3:Q:50:ARG:C	2.52	0.48
5:E:52:LYS:HB2	5:E:216:ASN:HA	1.95	0.48
8:V:147:SER:OG	8:V:150:GLU:N	2.36	0.48
8:H:3:ILE:HD12	8:H:44:CYS:SG	2.54	0.48
8:H:8:PHE:HD2	8:H:147:SER:O	1.97	0.48
8:H:106:ASN:O	8:H:107:LYS:HB3	2.14	0.48
2:B:94:HIS:CD2	9:I:61:SER:HB2	2.43	0.48
1:O:91:ARG:NH1	7:U:156:TYR:CE2	2.82	0.48
9:W:76:VAL:N	9:W:104:ASP:OD2	2.46	0.48
5:E:60:GLU:O	5:E:62:ASP:N	2.46	0.48
1:O:218:PHE:O	1:O:245:LEU:HD21	2.13	0.48
1:O:97:ALA:HB2	1:O:121:MET:CE	2.43	0.48
4:R:97:ARG:CZ	4:R:103:PRO:HB3	2.44	0.48
7:U:150:LEU:HD11	7:U:154:GLY:HA2	1.96	0.48
4:D:31:THR:HB	4:D:47:GLU:HG2	1.95	0.48
3:Q:182:ASP:O	3:Q:183:ASP:HB3	2.13	0.48
3:Q:192:LEU:HA	3:Q:195:LYS:HB3	1.95	0.48
10:X:171:LEU:HD21	10:X:199:LEU:HD13	1.94	0.48
5:E:103:TYR:O	13:M:88:SER:HA	2.14	0.48
13:M:85:SER:O	13:M:88:SER:N	2.46	0.48
5:S:52:LYS:HB2	5:S:216:ASN:HA	1.95	0.48
13:M:173:LYS:CD	13:M:174:TYR:N	2.74	0.48
9:I:100:VAL:CG1	9:I:111:PHE:HB2	2.44	0.48
7:G:240:ASP:O	7:G:242:ALA:N	2.46	0.48
3:Q:65:LYS:C	3:Q:66:LEU:HD12	2.35	0.48
10:X:17:LYS:CG	10:X:156:ASN:HB3	2.44	0.48
3:Q:120:GLN:NE2	3:Q:121:GLY:N	2.62	0.48
11:K:162:LYS:O	11:K:166:GLN:HG3	2.14	0.48
10:X:141:ALA:HB2	10:X:177:ASP:CB	2.43	0.48
7:U:117:GLN:O	7:U:120:GLN:HB3	2.14	0.48
4:R:73:LEU:HD23	4:R:73:LEU:C	2.34	0.48
1:A:106:TYR:HB2	8:H:61:TYR:HD2	1.78	0.48
11:Y:152:MET:HA	11:Y:156:GLU:OE2	2.14	0.48
6:F:64:ILE:HB	6:F:72:LEU:HD22	1.96	0.48
1:A:97:ALA:HB1	1:A:117:LEU:HD11	1.96	0.47
7:U:111:PHE:C	7:U:111:PHE:CD2	2.87	0.47
1:O:115:ASP:OD2	9:W:72:ARG:NH1	2.46	0.47
11:Y:35:THR:CG2	11:Y:36:ARG:H	2.27	0.47
10:X:88:GLN:HE21	10:X:88:GLN:CA	2.23	0.47
9:W:76:VAL:HG12	9:W:111:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:21:THR:HB	9:W:22:GLN:H	1.57	0.47
10:X:83:PRO:HB2	10:X:119:PHE:HD1	1.79	0.47
3:C:182:ASP:O	3:C:183:ASP:HB3	2.13	0.47
4:D:202:VAL:O	4:D:202:VAL:HG12	2.14	0.47
3:C:86:ILE:O	3:C:90:THR:HG23	2.14	0.47
11:K:1:MET:HG2	11:K:2:ASP:H	1.79	0.47
8:V:148:LYS:O	8:V:152:VAL:HG23	2.14	0.47
1:A:38:THR:CG2	1:A:85:GLY:HA2	2.44	0.47
1:A:244:ARG:HD2	1:A:244:ARG:H	1.80	0.47
1:O:185:HIS:ND1	1:O:185:HIS:O	2.47	0.47
10:J:166:ILE:HG23	10:J:167:SER:N	2.28	0.47
2:B:98:LYS:HA	2:B:103:GLU:O	2.13	0.47
1:A:73:PHE:N	1:A:73:PHE:CD1	2.82	0.47
7:G:150:LEU:HD12	7:G:155:SER:O	2.14	0.47
14:N:169:THR:O	14:N:171:GLN:N	2.47	0.47
1:O:41:ASN:O	1:O:55:SER:HA	2.14	0.47
1:O:149:GLU:O	1:O:150:LEU:HG	2.14	0.47
14:N:176:ALA:O	14:N:179:ASN:N	2.47	0.47
1:A:45:VAL:HA	1:A:168:ALA:CB	2.44	0.47
1:O:167:LYS:NZ	1:O:167:LYS:HB3	2.29	0.47
10:X:87:THR:HG23	10:X:123:PHE:CZ	2.49	0.47
5:E:143:LEU:HD11	5:E:172:ILE:HG12	1.97	0.47
5:S:130:GLU:O	5:S:131:GLU:HB2	2.14	0.47
6:T:213:ILE:CG2	6:T:214:ALA:N	2.76	0.47
7:G:39:ILE:CD1	7:G:195:ALA:HB2	2.44	0.47
6:T:144:LEU:HD12	6:T:145:LEU:N	2.29	0.47
6:T:82:ARG:HH11	6:T:82:ARG:HG3	1.79	0.47
5:S:209:GLU:HG3	5:S:210:GLU:N	2.29	0.47
9:W:175:VAL:HG12	9:W:176:CYS:N	2.29	0.47
3:C:245:THR:O	3:C:245:THR:HG22	2.14	0.47
3:Q:36:ILE:HG22	3:Q:37:GLY:N	2.30	0.47
1:A:51:THR:O	1:A:227:VAL:HG13	2.14	0.47
7:U:37:ILE:HA	7:U:163:ALA:CB	2.45	0.47
2:P:19:GLY:C	2:P:21:ILE:N	2.67	0.47
11:K:35:THR:CG2	11:K:36:ARG:N	2.76	0.47
11:Y:40:PRO:HG2	11:Y:74:GLU:CD	2.35	0.47
9:I:76:VAL:HG12	9:I:111:PHE:HE2	1.79	0.47
14:N:130:VAL:CB	14:N:136:THR:HG22	2.44	0.47
7:U:196:ALA:O	7:U:200:TYR:HD1	1.97	0.47
11:K:19:LYS:HG2	11:K:180:ILE:HG13	1.95	0.47
1:A:53:VAL:O	1:A:54:ILE:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:188:LYS:O	1:O:190:LYS:N	2.47	0.47
2:B:139:HIS:HB2	2:B:145:PHE:CD1	2.49	0.47
6:F:206:LEU:CD2	6:F:206:LEU:N	2.73	0.47
2:P:68:THR:C	2:P:70:ASP:H	2.17	0.47
7:U:72:HIS:C	7:U:72:HIS:CD2	2.87	0.47
1:O:167:LYS:HZ3	1:O:167:LYS:HB3	1.80	0.47
1:O:53:VAL:HG13	1:O:144:VAL:HG11	1.95	0.47
10:X:18:ASP:HB3	10:X:191:LYS:NZ	2.30	0.47
9:I:5:GLY:HA3	9:I:14:ILE:HG22	1.97	0.47
3:C:152:ASN:HB2	3:C:153:PRO:HD2	1.96	0.47
5:E:136:ARG:HB2	5:E:137:PRO:HD2	1.97	0.47
6:F:147:PHE:CD1	6:F:147:PHE:C	2.88	0.47
8:V:137:TYR:O	8:V:139:ASP:N	2.48	0.47
11:K:95:ARG:HH11	11:K:95:ARG:HG2	1.78	0.47
8:H:45:ARG:CB	8:H:45:ARG:NH1	2.77	0.47
12:Z:124:GLY:HA3	12:Z:127:PHE:CE2	2.49	0.47
9:I:42:TRP:HB2	9:I:178:MET:HE2	1.96	0.47
2:B:218:ASN:HB2	2:B:221:LEU:HD12	1.96	0.47
1:A:185:HIS:HA	1:A:188:LYS:HZ3	1.77	0.47
14:N:71:VAL:C	14:N:73:GLU:H	2.18	0.47
14:N:73:GLU:HA	14:N:76:TYR:CD2	2.44	0.47
11:Y:23:ARG:HB2	11:Y:28:LEU:CD1	2.40	0.47
2:B:244:ASN:HA	2:B:247:LEU:HG	1.96	0.47
6:F:159:THR:OG1	6:F:160:ALA:N	2.48	0.47
5:E:130:GLU:O	5:E:131:GLU:HB2	2.14	0.47
7:G:44:GLY:HA2	7:G:140:VAL:CG2	2.44	0.47
9:W:3:ILE:HG22	9:W:16:ALA:CB	2.44	0.47
5:S:98:THR:HG23	5:S:102:TYR:HE1	1.79	0.47
6:T:144:LEU:HD12	6:T:145:LEU:H	1.79	0.47
1:O:158:ASP:HB2	1:O:159:PRO:HD2	1.96	0.47
8:H:45:ARG:HB3	8:H:45:ARG:HH11	1.80	0.47
12:L:182:GLU:O	12:L:182:GLU:HG2	2.14	0.47
4:R:202:VAL:HG12	4:R:202:VAL:O	2.13	0.47
7:U:126:ASN:HD22	7:U:127:SER:N	2.11	0.47
11:Y:19:LYS:HG2	11:Y:180:ILE:HG13	1.95	0.47
13:M:6:GLY:O	13:M:57:PHE:HD1	1.96	0.47
8:V:8:PHE:HD2	8:V:147:SER:O	1.98	0.47
8:H:19:ARG:HB3	8:H:170:GLY:H	1.78	0.47
1:A:17:THR:O	1:A:17:THR:HG22	2.13	0.47
2:B:145:PHE:CE1	2:B:214:ILE:HG22	2.49	0.47
2:B:66:LEU:HD13	2:B:235:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:PHE:HD1	2:B:195:THR:OG1	1.97	0.47
7:U:69:VAL:O	7:U:70:ASP:HB3	2.14	0.47
2:P:36:GLY:O	2:P:161:ALA:HA	2.14	0.47
3:C:185:LYS:CD	3:C:186:VAL:H	2.20	0.47
1:O:225:VAL:CG1	1:O:226:GLY:N	2.78	0.47
11:K:28:LEU:N	11:K:28:LEU:CD1	2.77	0.47
1:O:36:ASN:C	1:O:38:THR:N	2.68	0.47
6:T:159:THR:OG1	6:T:160:ALA:N	2.48	0.47
3:C:39:MET:HE1	3:C:146:TYR:HB2	1.96	0.47
9:I:189:ASN:C	9:I:191:LEU:H	2.18	0.47
14:N:129:TYR:HD1	14:N:130:VAL:N	2.13	0.47
3:C:131:PHE:O	3:C:153:PRO:HB3	2.15	0.47
8:H:111:TYR:CE2	8:H:121:LYS:HD2	2.47	0.47
9:I:3:ILE:HD12	9:I:44:ALA:HB3	1.97	0.47
5:E:98:THR:CG2	5:E:102:TYR:CE1	2.96	0.47
2:B:170:ALA:HA	2:B:173:THR:HB	1.95	0.47
13:M:134:GLU:CD	13:M:137:ARG:HE	2.18	0.47
13:M:122:VAL:CG1	13:M:123:TYR:N	2.77	0.47
1:O:83:VAL:HG11	1:O:90:ALA:CB	2.44	0.47
1:A:12:TYR:HE1	2:B:7:PHE:CE2	2.33	0.47
13:M:29:ASN:OD1	13:M:36:ASN:HB2	2.15	0.47
4:R:72:VAL:CG1	4:R:221:ILE:HD13	2.45	0.47
8:H:131:SER:O	8:H:135:TYR:HD1	1.98	0.47
1:A:250:GLU:C	1:A:252:ASP:H	2.17	0.47
3:Q:86:ILE:O	3:Q:90:THR:HG23	2.15	0.47
3:Q:230:PHE:N	3:Q:230:PHE:CD1	2.83	0.47
5:E:38:ILE:HB	5:E:200:VAL:HG13	1.97	0.47
9:I:144:GLN:HG3	9:I:145:ASP:N	2.30	0.47
11:K:103:LEU:HD21	11:K:118:GLN:HG3	1.96	0.47
1:A:53:VAL:HG13	1:A:144:VAL:HG11	1.95	0.47
2:B:90:ARG:NH1	9:I:68:LEU:HB3	2.30	0.47
5:S:27:SER:O	5:S:30:ALA:HB3	2.15	0.47
1:A:242:GLU:O	1:A:245:LEU:HB3	2.15	0.47
10:J:10:ILE:HG21	10:J:141:ALA:HB3	1.95	0.47
4:D:97:ARG:CZ	4:D:103:PRO:HB3	2.45	0.47
9:I:137:VAL:HG21	9:I:161:ALA:CB	2.45	0.47
3:C:93:ILE:HD12	3:C:93:ILE:N	2.29	0.47
3:Q:245:THR:O	3:Q:245:THR:HG22	2.15	0.47
6:T:123:TYR:CG	6:T:124:GLY:N	2.82	0.47
7:U:98:PHE:C	7:U:98:PHE:CD1	2.87	0.47
1:O:250:GLU:C	1:O:252:ASP:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:144:GLN:HG3	9:W:145:ASP:N	2.30	0.47
8:H:5:ALA:HB2	8:H:14:LEU:HB3	1.96	0.47
14:N:151:ALA:O	14:N:152:ASN:C	2.53	0.47
2:P:48:GLU:OE1	2:P:200:VAL:HG13	2.15	0.47
2:B:243:ILE:O	2:B:246:ARG:N	2.46	0.47
1:A:101:ALA:HA	1:A:112:MET:HE2	1.97	0.47
1:A:218:PHE:O	1:A:245:LEU:HD21	2.14	0.47
1:O:218:PHE:CD2	1:O:223:LEU:HD11	2.50	0.47
1:O:242:GLU:O	1:O:245:LEU:HB3	2.15	0.47
12:Z:52:CYS:O	12:Z:56:GLU:HB2	2.15	0.47
12:L:104:TYR:CE2	12:L:110:PRO:HG3	2.50	0.47
1:A:167:LYS:NZ	1:A:167:LYS:HB3	2.30	0.47
1:A:146:VAL:HB	1:A:229:THR:O	2.15	0.47
1:O:185:HIS:C	1:O:185:HIS:ND1	2.68	0.47
2:B:64:VAL:HG11	2:B:212:ALA:CB	2.43	0.47
7:U:136:ILE:CD1	7:U:163:ALA:HA	2.45	0.47
10:J:166:ILE:CG2	10:J:167:SER:N	2.78	0.47
7:U:121:ALA:HA	7:U:124:LEU:CD1	2.43	0.47
5:S:60:GLU:O	5:S:62:ASP:N	2.48	0.47
4:R:29:ARG:HG2	4:R:29:ARG:NH1	2.28	0.47
8:H:185:ARG:C	8:H:186:LEU:HD23	2.35	0.47
8:V:185:ARG:C	8:V:186:LEU:HD23	2.36	0.47
12:L:176:ASN:ND2	12:L:190:ASN:HB2	2.28	0.47
6:F:144:LEU:C	6:F:145:LEU:HD12	2.35	0.47
6:F:74:LEU:HD22	6:F:81:ALA:CB	2.45	0.47
12:L:38:ASN:HB2	12:L:39:PRO:HD2	1.96	0.47
6:F:59:TYR:CE1	6:F:209:ASP:HB3	2.50	0.47
1:A:41:ASN:O	1:A:55:SER:HA	2.15	0.47
1:A:88:PRO:HG2	1:A:89:ASP:H	1.79	0.46
1:A:91:ARG:NH1	7:G:156:TYR:CD2	2.83	0.46
2:B:218:ASN:O	2:B:220:ASP:N	2.49	0.46
4:R:168:SER:HA	4:R:171:VAL:HG22	1.97	0.46
2:P:218:ASN:HB2	2:P:221:LEU:HD12	1.97	0.46
11:Y:28:LEU:CD1	11:Y:28:LEU:N	2.78	0.46
7:U:240:ASP:O	7:U:242:ALA:N	2.48	0.46
4:D:50:SER:HA	4:D:53:LYS:CD	2.45	0.46
12:L:176:ASN:ND2	12:L:190:ASN:HD22	2.12	0.46
9:W:21:THR:HG22	9:W:23:GLY:O	2.15	0.46
1:O:146:VAL:HB	1:O:229:THR:O	2.15	0.46
13:M:73:LYS:HE3	13:M:77:PHE:HE2	1.80	0.46
9:W:137:VAL:HG21	9:W:161:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:222:ILE:HG12	5:E:223:THR:N	2.28	0.46
8:H:34:LEU:CD2	8:H:44:CYS:HB3	2.44	0.46
1:A:185:HIS:O	1:A:185:HIS:ND1	2.49	0.46
1:A:196:GLU:HG2	1:A:201:LYS:CB	2.44	0.46
1:A:42:SER:O	1:A:170:ALA:HA	2.16	0.46
14:N:188:ASP:O	14:N:190:ARG:N	2.48	0.46
8:V:97:ILE:HD11	8:V:99:VAL:CG2	2.45	0.46
2:B:19:GLY:C	2:B:21:ILE:N	2.69	0.46
2:P:147:LEU:HD23	2:P:159:TRP:HB2	1.96	0.46
11:Y:35:THR:HG21	11:Y:43:LEU:HD11	1.97	0.46
7:G:90:ARG:HD3	7:G:118:TYR:CE1	2.49	0.46
9:W:5:GLY:HA3	9:W:14:ILE:HG22	1.98	0.46
13:M:80:ASN:O	13:M:82:LYS:N	2.47	0.46
4:D:50:SER:OG	4:D:53:LYS:HE2	2.16	0.46
8:H:111:TYR:HA	8:H:120:HIS:O	2.15	0.46
8:V:111:TYR:CE2	8:V:121:LYS:HD2	2.49	0.46
1:O:162:TYR:CD1	1:O:163:TYR:N	2.83	0.46
10:J:37:ASN:HD22	10:J:37:ASN:C	2.18	0.46
10:J:71:ASN:O	10:J:75:LEU:CD1	2.63	0.46
12:Z:8:PHE:CE1	12:Z:13:ILE:HG12	2.50	0.46
6:F:38:LEU:N	6:F:38:LEU:HD23	2.30	0.46
3:C:230:PHE:N	3:C:230:PHE:CD1	2.83	0.46
9:I:50:ALA:HB3	10:J:126:ILE:CD1	2.46	0.46
3:C:49:GLU:O	3:C:50:ARG:C	2.53	0.46
9:I:134:ALA:HB1	9:I:158:ALA:HB1	1.97	0.46
11:K:138:PHE:HD1	11:K:138:PHE:H	1.59	0.46
9:W:67:SER:HB2	9:W:72:ARG:O	2.15	0.46
2:P:244:ASN:HA	2:P:247:LEU:HG	1.97	0.46
6:F:213:ILE:CG2	6:F:214:ALA:N	2.78	0.46
8:V:184:GLU:OE2	8:V:186:LEU:HD21	2.15	0.46
5:S:97:VAL:HG21	12:Z:65:LEU:HD13	1.96	0.46
9:I:10:ASN:O	9:I:179:GLU:HG2	2.15	0.46
6:F:234:ILE:HG22	6:F:234:ILE:OXT	2.15	0.46
8:V:45:ARG:NH1	8:V:45:ARG:CB	2.78	0.46
8:V:131:SER:O	8:V:135:TYR:HD1	1.98	0.46
1:A:32:PHE:O	1:A:35:THR:N	2.40	0.46
7:U:10:SER:HB2	7:U:13:VAL:HG23	1.97	0.46
12:L:66:HIS:HD2	12:L:74:ILE:HB	1.80	0.46
1:O:196:GLU:HG2	1:O:201:LYS:CB	2.45	0.46
6:F:198:SER:HA	6:F:201:LEU:HG	1.98	0.46
8:V:12:VAL:HG22	8:V:13:ILE:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:LEU:HD23	1:O:178:ILE:HG23	1.96	0.46
2:B:9:LEU:HD13	2:B:122:THR:O	2.16	0.46
11:K:162:LYS:HZ2	11:K:162:LYS:HB2	1.80	0.46
7:U:39:ILE:CD1	7:U:195:ALA:HB2	2.45	0.46
1:O:104:PHE:CD1	1:O:104:PHE:C	2.88	0.46
2:P:174:PHE:HD1	2:P:195:THR:OG1	1.96	0.46
3:Q:235:ILE:C	3:Q:237:ASP:N	2.69	0.46
6:T:64:ILE:HB	6:T:72:LEU:HD22	1.96	0.46
5:E:61:SER:C	5:E:63:SER:H	2.18	0.46
2:P:64:VAL:HG11	2:P:212:ALA:CB	2.44	0.46
14:N:71:VAL:C	14:N:73:GLU:N	2.68	0.46
8:V:173:ILE:CG2	8:V:174:ARG:N	2.79	0.46
1:O:87:ILE:N	1:O:88:PRO:CD	2.78	0.46
7:G:201:LEU:CD1	7:G:201:LEU:H	2.28	0.46
7:U:118:TYR:CE2	7:U:122:HIS:HE1	2.33	0.46
9:W:105:PRO:O	9:W:106:THR:HG23	2.16	0.46
5:E:59:LEU:HD11	5:E:64:ILE:CD1	2.42	0.46
7:U:39:ILE:HD12	7:U:195:ALA:HB2	1.97	0.46
7:G:150:LEU:HD11	7:G:154:GLY:HA2	1.97	0.46
11:Y:22:THR:HG22	11:Y:26:SER:O	2.16	0.46
12:Z:4:LEU:C	12:Z:4:LEU:HD22	2.36	0.46
5:E:97:VAL:HG11	12:L:65:LEU:HD22	1.97	0.46
11:K:85:ARG:O	11:K:89:ALA:HB2	2.16	0.46
9:I:175:VAL:HG12	9:I:176:CYS:N	2.29	0.46
8:H:163:ILE:CD1	8:H:170:GLY:HA2	2.43	0.46
8:H:44:CYS:SG	8:H:98:ILE:HB	2.55	0.46
3:C:9:ARG:CZ	3:C:12:ILE:HD11	2.45	0.46
6:T:34:VAL:CG1	6:T:163:ALA:O	2.64	0.46
3:C:42:ASP:OD1	3:C:186:VAL:HG23	2.15	0.46
8:V:34:LEU:CD2	8:V:44:CYS:HB3	2.44	0.46
8:V:3:ILE:HD12	8:V:44:CYS:SG	2.56	0.46
1:O:38:THR:CG2	1:O:85:GLY:HA2	2.45	0.46
5:S:130:GLU:CG	5:S:131:GLU:H	2.24	0.46
2:P:66:LEU:HD13	2:P:235:PHE:CD1	2.51	0.46
8:V:4:MET:HB2	8:V:125:ALA:O	2.15	0.46
5:S:165:TYR:HB2	5:S:167:TYR:HE2	1.81	0.46
5:S:219:LEU:O	5:S:231:TYR:HB2	2.15	0.46
3:C:235:ILE:C	3:C:237:ASP:N	2.69	0.46
5:S:209:GLU:OE1	5:S:209:GLU:CA	2.63	0.46
4:R:31:THR:HB	4:R:47:GLU:HG2	1.97	0.46
3:C:175:LEU:CD1	3:C:199:LYS:HD2	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:148:LYS:O	8:H:152:VAL:HG23	2.14	0.46
2:B:147:LEU:HD23	2:B:159:TRP:HB2	1.98	0.46
1:O:42:SER:O	1:O:170:ALA:HA	2.15	0.46
6:T:46:LEU:HD22	6:T:73:SER:OG	2.16	0.46
10:J:18:ASP:HB3	10:J:191:LYS:NZ	2.30	0.46
2:P:244:ASN:ND2	2:P:244:ASN:N	2.59	0.46
6:F:46:LEU:HD22	6:F:73:SER:OG	2.15	0.46
1:O:97:ALA:HB1	1:O:117:LEU:HD11	1.98	0.46
10:J:141:ALA:HB2	10:J:177:ASP:CB	2.44	0.46
5:S:136:ARG:HB2	5:S:137:PRO:HD2	1.97	0.46
5:S:198:LEU:HB3	5:S:243:LEU:HD23	1.97	0.46
5:E:198:LEU:O	5:E:202:LYS:HB2	2.16	0.46
7:G:196:ALA:O	7:G:200:TYR:HD1	1.98	0.46
11:Y:198:GLN:HB3	11:Y:198:GLN:HE21	1.58	0.46
7:U:106:ILE:HA	7:U:107:PRO:HD3	1.72	0.46
5:E:15:PHE:CD1	5:E:21:LEU:HD21	2.50	0.46
5:S:61:SER:C	5:S:63:SER:H	2.18	0.46
1:A:162:TYR:CD1	1:A:163:TYR:N	2.84	0.46
1:A:200:GLU:HG2	1:A:244:ARG:HH21	1.79	0.46
1:O:195:ASN:O	1:O:196:GLU:HB2	2.16	0.46
1:O:185:HIS:HE2	1:O:205:PHE:HE2	1.63	0.46
3:Q:186:VAL:HG12	3:Q:190:ILE:HD11	1.98	0.46
10:X:14:MET:HE1	10:X:166:ILE:HA	1.97	0.46
8:V:16:ALA:O	8:V:17:ASP:O	2.34	0.46
5:S:204:LEU:O	5:S:205:LYS:C	2.54	0.46
11:K:40:PRO:HG2	11:K:74:GLU:CD	2.36	0.46
9:I:76:VAL:N	9:I:104:ASP:OD2	2.46	0.46
3:C:44:ILE:CG2	3:C:138:ALA:HB1	2.45	0.46
3:C:228:LYS:HZ1	3:C:231:LYS:HE3	1.80	0.46
13:M:3:ASN:HD22	13:M:4:PRO:N	2.13	0.46
13:M:4:PRO:O	14:N:104:ARG:NH1	2.46	0.46
8:V:156:LYS:HG3	8:V:175:MET:CE	2.46	0.46
1:O:158:ASP:HB2	1:O:159:PRO:CD	2.45	0.46
7:G:10:SER:HB2	7:G:13:VAL:HG23	1.97	0.46
8:V:122:LEU:HB3	8:V:123:PRO:HD2	1.97	0.46
10:J:148:MET:HE3	10:J:152:LEU:HD11	1.98	0.46
8:H:5:ALA:CB	8:H:14:LEU:HB3	2.46	0.46
1:A:53:VAL:C	1:A:54:ILE:HD12	2.36	0.46
2:B:28:VAL:HG12	2:B:29:LYS:N	2.30	0.46
4:R:59:ILE:CD1	4:R:59:ILE:H	2.08	0.46
2:P:44:VAL:HG23	2:P:213:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:19:ARG:HB3	8:V:170:GLY:H	1.81	0.46
9:I:38:SER:HB3	9:I:41:ILE:HG13	1.98	0.46
5:E:143:LEU:HD23	5:E:143:LEU:HA	1.81	0.46
1:A:15:HIS:CB	1:A:18:ILE:HD13	2.44	0.46
8:H:1:THR:H1	8:H:129:SER:H	1.63	0.46
8:H:1:THR:N	8:H:129:SER:N	2.63	0.46
5:E:165:TYR:HB2	5:E:167:TYR:HE2	1.81	0.46
6:T:144:LEU:O	6:T:145:LEU:HD12	2.16	0.46
6:F:51:ARG:O	6:F:59:TYR:HA	2.15	0.46
3:C:176:LEU:C	3:C:178:MET:N	2.70	0.46
7:G:51:LYS:HE3	7:G:63:ASN:O	2.16	0.46
1:O:176:GLN:HE21	1:O:180:THR:CG2	2.28	0.46
1:A:158:ASP:HB2	1:A:159:PRO:HD2	1.97	0.46
7:G:136:ILE:CD1	7:G:163:ALA:HA	2.46	0.46
4:D:29:ARG:NH1	4:D:29:ARG:HG2	2.29	0.46
7:G:117:GLN:O	7:G:120:GLN:HB3	2.16	0.46
7:U:201:LEU:H	7:U:201:LEU:CD1	2.29	0.46
4:R:50:SER:OG	4:R:53:LYS:HE2	2.16	0.46
8:H:156:LYS:HG3	8:H:175:MET:CE	2.46	0.46
1:O:12:TYR:CE1	2:P:7:PHE:CE2	3.03	0.46
12:L:5:ALA:HA	12:L:13:ILE:O	2.16	0.46
10:J:71:ASN:O	10:J:75:LEU:HD12	2.16	0.46
1:O:176:GLN:HE21	1:O:180:THR:HG23	1.81	0.46
5:S:142:LEU:HB2	5:S:158:ALA:HB3	1.97	0.46
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.98	0.46
8:V:66:TYR:O	8:V:67:THR:C	2.52	0.45
4:R:187:THR:HB	4:R:190:GLU:HG2	1.97	0.45
5:S:143:LEU:HD11	5:S:172:ILE:HG12	1.98	0.45
5:S:192:THR:HG1	5:S:195:GLU:HG3	1.81	0.45
1:A:59:VAL:HG11	1:A:66:PRO:HG3	1.97	0.45
9:W:50:ALA:HB2	10:X:128:CYS:HB2	1.97	0.45
6:F:82:ARG:HH11	6:F:82:ARG:HG3	1.80	0.45
4:R:31:THR:HB	4:R:47:GLU:CG	2.45	0.45
2:B:18:LEU:HD21	3:C:129:ARG:HD2	1.98	0.45
12:L:76:VAL:N	12:L:108:GLU:OE1	2.47	0.45
2:B:176:GLU:HA	3:C:56:LEU:CD1	2.45	0.45
6:T:190:ILE:O	6:T:194:VAL:HG23	2.17	0.45
9:I:67:SER:HB2	9:I:72:ARG:O	2.16	0.45
14:N:154:LEU:C	14:N:156:ARG:H	2.19	0.45
8:H:122:LEU:HB3	8:H:123:PRO:HD2	1.97	0.45
14:N:211:ASN:C	14:N:212:LEU:HD13	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:75:LEU:HD12	11:Y:80:VAL:CG2	2.46	0.45
8:V:1:THR:H1	8:V:129:SER:H	1.63	0.45
3:Q:230:PHE:N	3:Q:230:PHE:HD1	2.14	0.45
9:I:10:ASN:O	9:I:179:GLU:HA	2.16	0.45
6:F:189:LEU:HD23	6:F:189:LEU:O	2.15	0.45
4:R:160:SER:OG	4:R:181:ARG:NH1	2.49	0.45
13:M:161:GLU:OE1	13:M:171:PRO:HD2	2.16	0.45
7:U:15:SER:OG	7:U:19:ARG:HB3	2.16	0.45
2:B:200:VAL:HG12	2:B:201:GLU:N	2.31	0.45
1:O:164:VAL:CG2	1:O:165:GLY:H	2.29	0.45
12:L:211:ILE:N	12:L:211:ILE:HD12	2.28	0.45
6:T:158:GLY:O	6:T:159:THR:CB	2.64	0.45
3:Q:228:LYS:HZ2	3:Q:231:LYS:HE3	1.81	0.45
1:O:214:LEU:CD1	1:O:218:PHE:HZ	2.29	0.45
13:M:23:LEU:HD13	13:M:43:VAL:HG13	1.98	0.45
6:T:147:PHE:CD1	6:T:147:PHE:C	2.89	0.45
7:G:80:LEU:N	7:G:80:LEU:CD2	2.79	0.45
4:D:27:VAL:HG11	4:D:132:SER:HB2	1.97	0.45
14:N:101:TYR:O	14:N:102:GLN:C	2.54	0.45
8:V:6:VAL:C	8:V:12:VAL:HG23	2.37	0.45
2:P:19:GLY:O	2:P:20:GLN:C	2.54	0.45
4:D:34:VAL:HG12	4:D:199:LEU:HD21	1.98	0.45
14:N:154:LEU:HD21	9:W:136:ALA:O	2.15	0.45
1:O:36:ASN:O	1:O:38:THR:N	2.47	0.45
8:V:111:TYR:HA	8:V:120:HIS:O	2.17	0.45
5:S:213:ASP:C	5:S:215:ASN:H	2.19	0.45
3:C:192:LEU:HA	3:C:195:LYS:HB3	1.97	0.45
12:Z:66:HIS:HD2	12:Z:74:ILE:HB	1.81	0.45
4:D:151:GLU:OE1	4:D:155:ILE:HD11	2.17	0.45
1:A:166:TYR:CG	1:A:169:THR:HB	2.52	0.45
9:W:19:ARG:HD2	9:W:170:GLY:N	2.32	0.45
3:C:70:ASN:HD22	3:C:71:ASP:N	2.11	0.45
5:S:28:LEU:N	5:S:28:LEU:HD12	2.32	0.45
14:N:24:ALA:O	14:N:25:ASP:O	2.35	0.45
5:S:79:SER:HB3	5:S:172:ILE:HD12	1.99	0.45
1:A:218:PHE:CD2	1:A:223:LEU:HD11	2.52	0.45
11:Y:162:LYS:HB2	11:Y:162:LYS:HZ2	1.81	0.45
5:E:198:LEU:HB3	5:E:243:LEU:HD23	1.99	0.45
5:S:97:VAL:HG11	12:Z:65:LEU:HD21	1.98	0.45
6:F:69:HIS:HE1	6:F:70:MET:HE3	1.82	0.45
1:O:163:TYR:CD1	1:O:163:TYR:C	2.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:83:PHE:O	11:Y:86:GLN:HB3	2.16	0.45
5:E:20:ARG:O	5:E:21:LEU:HD23	2.17	0.45
10:J:62:LEU:HD23	10:J:62:LEU:HA	1.72	0.45
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.99	0.45
1:A:176:GLN:HE21	1:A:180:THR:HG23	1.82	0.45
3:C:9:ARG:NE	3:C:12:ILE:HD11	2.32	0.45
4:R:185:PRO:HB3	4:R:190:GLU:HG3	1.98	0.45
6:F:94:TYR:CD2	6:F:94:TYR:C	2.90	0.45
4:D:73:LEU:C	4:D:73:LEU:HD23	2.37	0.45
5:E:209:GLU:OE1	5:E:209:GLU:CA	2.65	0.45
1:A:87:ILE:N	1:A:88:PRO:CD	2.79	0.45
4:D:168:SER:HA	4:D:171:VAL:HG22	1.98	0.45
4:R:199:LEU:C	4:R:201:GLU:H	2.20	0.45
9:I:4:VAL:HA	9:I:125:LEU:O	2.17	0.45
3:Q:218:LYS:HG3	3:Q:224:GLU:C	2.36	0.45
8:V:190:PRO:O	8:V:192:GLU:N	2.49	0.45
4:D:73:LEU:HD12	4:D:135:ILE:CG1	2.47	0.45
1:O:68:THR:O	7:U:157:TRP:CE3	2.69	0.45
9:I:55:VAL:HG13	9:I:56:THR:N	2.31	0.45
1:A:185:HIS:ND1	1:A:185:HIS:C	2.70	0.45
2:B:48:GLU:OE1	2:B:200:VAL:HG13	2.16	0.45
7:U:113:ASP:O	7:U:114:ARG:C	2.54	0.45
2:P:28:VAL:C	2:P:30:GLN:N	2.69	0.45
13:M:222:ASP:CG	9:W:19:ARG:HH22	2.20	0.45
14:N:48:ASN:ND2	14:N:48:ASN:N	2.64	0.45
6:T:22:VAL:O	6:T:25:ALA:HB3	2.17	0.45
12:L:176:ASN:ND2	12:L:187:TYR:OH	2.49	0.45
9:W:21:THR:O	9:W:22:GLN:CB	2.65	0.45
14:N:186:TYR:HD1	9:W:139:GLU:HB3	1.81	0.45
12:Z:7:ARG:O	12:Z:8:PHE:HB3	2.17	0.45
11:Y:103:LEU:HD21	11:Y:118:GLN:HG3	1.99	0.45
11:Y:92:ILE:HA	11:Y:92:ILE:HD12	1.82	0.45
9:W:10:ASN:O	9:W:179:GLU:HA	2.15	0.45
3:C:141:ASP:OD2	3:C:147:GLN:NE2	2.50	0.45
5:S:35:SER:OG	5:S:66:LYS:HE2	2.16	0.45
7:U:168:ARG:O	7:U:171:ALA:HB3	2.16	0.45
11:K:35:THR:HG21	11:K:43:LEU:HD11	1.99	0.45
2:B:19:GLY:O	2:B:20:GLN:C	2.55	0.45
1:O:88:PRO:HG2	1:O:89:ASP:H	1.81	0.45
7:U:90:ARG:HG2	7:U:118:TYR:CE1	2.51	0.45
6:F:227:GLY:C	6:F:229:ALA:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:GLN:HE21	4:D:54:LEU:HD21	1.82	0.45
11:Y:51:GLY:HA3	12:Z:118:ASP:O	2.16	0.45
5:E:61:SER:C	5:E:63:SER:N	2.70	0.45
7:G:129:ARG:HA	7:G:130:PRO:HD3	1.83	0.45
5:E:235:LYS:O	5:E:238:GLU:HG2	2.17	0.45
3:Q:93:ILE:HD12	3:Q:93:ILE:N	2.32	0.45
14:N:127:LEU:HG	14:N:142:LEU:HD12	1.98	0.45
1:A:50:CYS:SG	1:A:202:VAL:HG21	2.57	0.45
1:O:185:HIS:NE2	1:O:205:PHE:HE2	2.15	0.45
1:O:188:LYS:C	1:O:190:LYS:H	2.21	0.45
1:O:185:HIS:NE2	1:O:205:PHE:CE2	2.85	0.45
5:S:233:ASN:H	5:S:233:ASN:ND2	2.04	0.45
2:P:200:VAL:HG12	2:P:201:GLU:N	2.32	0.45
6:T:94:TYR:CD2	6:T:94:TYR:C	2.91	0.45
2:P:139:HIS:HB2	2:P:145:PHE:CD1	2.52	0.45
12:Z:45:MET:HG2	12:Z:45:MET:O	2.15	0.45
3:Q:183:ASP:O	3:Q:184:MET:C	2.55	0.45
6:F:64:ILE:HG21	6:F:85:SER:HB2	1.99	0.45
5:E:142:LEU:HB2	5:E:158:ALA:HB3	1.99	0.45
5:E:236:THR:O	5:E:240:ILE:HG13	2.17	0.45
1:O:206:ALA:O	1:O:207:ILE:C	2.54	0.45
7:U:175:LEU:O	7:U:179:VAL:HG23	2.17	0.44
5:E:51:GLU:HG3	5:E:208:MET:SD	2.57	0.44
8:V:2:SER:OG	8:V:162:ALA:HB1	2.17	0.44
9:W:216:SER:C	9:W:217:ILE:HD12	2.38	0.44
3:C:183:ASP:O	3:C:184:MET:C	2.56	0.44
10:J:13:ALA:HB2	10:J:22:ILE:HD12	1.98	0.44
3:Q:106:ILE:HA	3:Q:107:PRO:HD3	1.87	0.44
1:A:36:ASN:C	1:A:38:THR:N	2.69	0.44
1:A:36:ASN:O	1:A:38:THR:N	2.49	0.44
8:H:137:TYR:CE2	8:H:157:HIS:HB3	2.52	0.44
8:H:173:ILE:CG2	8:H:174:ARG:N	2.79	0.44
1:A:184:ASN:O	1:A:188:LYS:HG3	2.17	0.44
1:A:52:VAL:HG22	1:A:227:VAL:CG2	2.48	0.44
2:B:28:VAL:O	2:B:30:GLN:N	2.51	0.44
2:B:39:ALA:HB3	2:B:42:GLY:O	2.16	0.44
1:A:176:GLN:HE21	1:A:180:THR:CG2	2.30	0.44
4:D:168:SER:O	4:D:172:ARG:HB2	2.17	0.44
7:G:113:ASP:O	7:G:114:ARG:C	2.55	0.44
2:P:28:VAL:HG12	2:P:29:LYS:N	2.32	0.44
8:H:123:PRO:HB2	8:H:124:TYR:HD1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ALA:HA	2:B:118:MET:HB2	1.99	0.44
5:E:140:VAL:HG22	5:E:141:ALA:N	2.32	0.44
11:K:196:GLN:HE21	11:K:196:GLN:CA	2.30	0.44
3:Q:191:GLU:HG2	3:Q:195:LYS:HE2	1.99	0.44
5:S:61:SER:C	5:S:63:SER:N	2.70	0.44
3:C:36:ILE:HG22	3:C:37:GLY:N	2.32	0.44
13:M:92:ASN:OD1	13:M:92:ASN:C	2.56	0.44
13:M:165:ASN:HD22	13:M:165:ASN:HA	1.58	0.44
11:Y:138:PHE:H	11:Y:138:PHE:HD1	1.64	0.44
5:E:35:SER:OG	5:E:66:LYS:HE2	2.17	0.44
10:J:95:TYR:C	10:J:97:ARG:N	2.70	0.44
9:W:67:SER:O	9:W:71:SER:N	2.50	0.44
1:O:181:ASN:OD1	1:O:209:HIS:CD2	2.71	0.44
1:O:42:SER:HA	1:O:54:ILE:O	2.17	0.44
4:D:239:GLU:HA	4:D:242:GLU:CB	2.40	0.44
11:K:161:LEU:HD22	11:K:195:PHE:CE2	2.52	0.44
5:E:201:LEU:HA	5:E:201:LEU:HD12	1.78	0.44
12:L:35:ILE:HG21	12:L:56:GLU:HB3	1.98	0.44
1:A:33:LYS:N	1:A:33:LYS:HD2	2.32	0.44
12:L:97:MET:O	12:L:116:ASP:HA	2.17	0.44
9:I:11:GLY:HA3	9:I:178:MET:O	2.17	0.44
6:F:51:ARG:HG2	6:F:52:ASN:N	2.32	0.44
3:C:191:GLU:HG2	3:C:195:LYS:HE2	2.00	0.44
12:Z:206:SER:O	12:Z:207:PHE:HB2	2.17	0.44
12:L:4:LEU:C	12:L:4:LEU:HD22	2.38	0.44
1:A:181:ASN:OD1	1:A:209:HIS:CD2	2.71	0.44
12:L:206:SER:O	12:L:207:PHE:HB2	2.17	0.44
4:R:75:PHE:HB3	4:R:133:THR:HG22	1.99	0.44
9:I:67:SER:OG	9:I:68:LEU:N	2.50	0.44
6:F:179:PHE:C	6:F:181:LYS:H	2.21	0.44
1:O:240:ASN:O	1:O:243:GLU:HB2	2.18	0.44
4:D:185:PRO:HB3	4:D:190:GLU:HG3	1.99	0.44
14:N:210:LYS:O	14:N:212:LEU:CD1	2.63	0.44
7:U:203:HIS:O	7:U:205:ASP:N	2.50	0.44
2:B:84:VAL:C	2:B:86:VAL:N	2.70	0.44
9:W:3:ILE:HD12	9:W:44:ALA:HB3	1.99	0.44
5:E:98:THR:HG23	5:E:102:TYR:HE1	1.81	0.44
3:Q:173:GLN:HE21	4:R:54:LEU:HD21	1.83	0.44
12:Z:35:ILE:HG21	12:Z:56:GLU:HB3	1.99	0.44
3:Q:77:VAL:HG12	3:Q:78:ALA:N	2.31	0.44
3:C:20:TYR:O	3:C:21:GLN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:38:LEU:N	6:T:38:LEU:HD23	2.32	0.44
11:Y:11:ASP:O	11:Y:12:SER:HB3	2.17	0.44
7:G:104:THR:HA	7:G:105:PRO:HD2	1.83	0.44
1:A:133:TYR:O	1:A:134:MET:HB3	2.18	0.44
1:A:185:HIS:NE2	1:A:205:PHE:HE2	2.15	0.44
2:B:36:GLY:HA2	2:B:44:VAL:O	2.18	0.44
9:W:54:ALA:O	9:W:57:GLN:HB2	2.18	0.44
1:O:166:TYR:CG	1:O:169:THR:HB	2.53	0.44
4:R:239:GLU:HA	4:R:242:GLU:CB	2.40	0.44
9:I:19:ARG:HD2	9:I:170:GLY:N	2.33	0.44
8:H:66:TYR:O	8:H:67:THR:C	2.56	0.44
11:K:35:THR:CG2	11:K:36:ARG:H	2.30	0.44
13:M:156:PHE:HE2	13:M:172:LEU:HA	1.81	0.44
14:N:25:ASP:C	14:N:25:ASP:OD2	2.56	0.44
5:E:56:SER:HG	5:E:57:PRO:HD2	1.82	0.44
11:Y:3:ILE:O	11:Y:4:ILE:HD13	2.18	0.44
6:T:217:GLY:O	6:T:218:LYS:C	2.55	0.44
6:F:23:GLU:HA	6:F:26:LEU:HD23	2.00	0.44
8:V:187:ILE:O	8:V:187:ILE:HG23	2.17	0.44
13:M:6:GLY:O	13:M:57:PHE:CD1	2.70	0.44
12:Z:12:ILE:HG22	12:Z:13:ILE:N	2.32	0.44
3:C:230:PHE:N	3:C:230:PHE:HD1	2.15	0.44
7:G:51:LYS:O	7:G:211:PHE:HB2	2.18	0.44
11:K:198:GLN:HB3	11:K:198:GLN:HE21	1.58	0.44
4:R:151:GLU:OE1	4:R:155:ILE:HD11	2.18	0.44
3:Q:111:LEU:HD22	3:Q:111:LEU:O	2.18	0.44
9:W:31:CYS:SG	9:W:32:ALA:N	2.90	0.44
8:V:46:SER:O	8:V:52:THR:HG21	2.17	0.44
5:S:20:ARG:O	5:S:21:LEU:HD23	2.18	0.44
3:Q:91:ALA:HB2	3:Q:115:LEU:HD21	1.99	0.44
7:G:69:VAL:O	7:G:70:ASP:HB3	2.18	0.44
1:A:188:LYS:C	1:A:190:LYS:H	2.19	0.44
1:A:185:HIS:NE2	1:A:205:PHE:CE2	2.86	0.44
3:C:9:ARG:NH2	3:C:12:ILE:HD11	2.33	0.44
2:P:212:ALA:O	2:P:213:ILE:HG23	2.18	0.44
6:T:74:LEU:HD22	6:T:81:ALA:CB	2.48	0.44
9:I:5:GLY:CA	9:I:14:ILE:HG22	2.47	0.44
5:S:143:LEU:HA	5:S:143:LEU:HD23	1.83	0.44
9:I:189:ASN:C	9:I:191:LEU:N	2.71	0.44
9:W:189:ASN:C	9:W:191:LEU:H	2.20	0.44
11:Y:161:LEU:HD22	11:Y:195:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:176:ASN:ND2	12:Z:190:ASN:HB2	2.30	0.44
3:C:208:TYR:C	3:C:210:ARG:N	2.71	0.44
3:Q:133:VAL:CG1	3:Q:134:SER:N	2.81	0.44
3:C:135:PHE:O	3:C:150:THR:HA	2.17	0.44
1:A:103:GLU:CG	1:A:107:LYS:HD3	2.48	0.44
8:V:137:TYR:CE2	8:V:157:HIS:HB3	2.52	0.44
8:H:151:THR:HG23	8:H:152:VAL:N	2.32	0.44
2:P:176:GLU:HA	3:Q:56:LEU:CD1	2.47	0.44
4:D:99:THR:C	4:D:100:LEU:HD12	2.38	0.44
6:T:179:PHE:C	6:T:181:LYS:H	2.20	0.44
10:J:87:THR:HG23	10:J:123:PHE:CZ	2.53	0.44
8:V:10:ASP:CG	8:V:179:THR:HG22	2.38	0.44
5:E:213:ASP:C	5:E:215:ASN:H	2.21	0.44
8:V:156:LYS:HD2	8:V:188:PHE:CE1	2.53	0.44
7:G:38:GLY:N	7:G:162:ALA:O	2.50	0.44
11:Y:172:MET:HA	11:Y:173:PRO:HD3	1.80	0.44
8:H:131:SER:O	8:H:135:TYR:CD1	2.71	0.44
12:Z:64:ARG:NH2	12:Z:68:LEU:HD21	2.33	0.44
9:W:134:ALA:HB1	9:W:158:ALA:HB1	1.98	0.44
6:T:17:GLY:HA3	7:U:29:ALA:HB2	2.00	0.44
1:A:46:ARG:HD2	1:A:152:PRO:HB2	2.00	0.44
14:N:152:ASN:ND2	14:N:156:ARG:HH21	2.15	0.44
6:T:156:LEU:HD23	7:U:58:LEU:HD23	2.00	0.44
4:D:159:TRP:CZ2	5:E:59:LEU:HD23	2.53	0.44
2:P:84:VAL:C	2:P:86:VAL:N	2.71	0.44
6:F:217:GLY:O	6:F:218:LYS:C	2.56	0.44
14:N:16:TYR:CZ	14:N:170:VAL:HG13	2.52	0.44
6:F:69:HIS:HE1	6:F:70:MET:CE	2.30	0.44
6:T:51:ARG:HG2	6:T:52:ASN:N	2.32	0.44
12:L:12:ILE:HG22	12:L:13:ILE:N	2.32	0.44
12:L:7:ARG:O	12:L:8:PHE:HB3	2.18	0.44
11:K:138:PHE:N	11:K:138:PHE:CD1	2.84	0.44
8:V:123:PRO:HB2	8:V:124:TYR:HD1	1.83	0.44
14:N:216:ASN:HD22	14:N:216:ASN:HA	1.59	0.44
5:E:241:LYS:HB3	5:E:241:LYS:NZ	2.33	0.44
6:T:50:LYS:HD3	6:T:212:SER:OG	2.17	0.44
3:C:106:ILE:HA	3:C:107:PRO:HD3	1.87	0.44
12:L:3:THR:HB	12:L:16:VAL:HG12	2.00	0.44
10:X:7:ASN:HA	10:X:29:GLY:O	2.17	0.44
9:W:42:TRP:HB2	9:W:178:MET:HE2	2.00	0.44
1:A:75:ILE:HG21	1:A:117:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:O	1:A:196:GLU:HB2	2.17	0.44
2:B:68:THR:O	2:B:70:ASP:N	2.51	0.44
7:G:175:LEU:O	7:G:179:VAL:HG23	2.17	0.44
8:H:105:LYS:O	8:H:107:LYS:N	2.50	0.44
5:E:27:SER:O	5:E:30:ALA:HB3	2.18	0.44
1:A:243:GLU:O	1:A:246:VAL:N	2.49	0.44
6:T:94:TYR:C	6:T:94:TYR:HD2	2.22	0.44
14:N:79:PRO:HG2	14:N:80:LEU:HD12	2.00	0.44
9:W:7:LYS:HA	9:W:12:VAL:HG23	2.00	0.44
7:G:216:SER:CA	7:G:230:VAL:HG23	2.47	0.44
7:U:216:SER:CA	7:U:230:VAL:HG23	2.47	0.44
3:Q:135:PHE:O	3:Q:150:THR:HA	2.17	0.44
7:G:236:GLN:O	7:G:239:ILE:N	2.50	0.44
1:O:126:GLN:C	1:O:126:GLN:NE2	2.71	0.44
5:E:209:GLU:HG3	5:E:210:GLU:N	2.32	0.44
9:W:11:GLY:HA3	9:W:178:MET:O	2.18	0.44
4:D:4:TYR:CD2	4:D:13:PRO:HD3	2.53	0.44
3:Q:176:LEU:C	3:Q:178:MET:N	2.70	0.44
1:O:50:CYS:SG	1:O:202:VAL:HG21	2.57	0.43
6:T:34:VAL:HG12	6:T:163:ALA:O	2.18	0.43
7:U:31:GLU:HG3	7:U:31:GLU:O	2.17	0.43
8:V:5:ALA:HB2	8:V:14:LEU:HB3	2.00	0.43
8:V:5:ALA:CB	8:V:14:LEU:HB3	2.48	0.43
5:S:59:LEU:HD11	5:S:64:ILE:CD1	2.45	0.43
13:M:2:PHE:CB	14:N:1:THR:HG23	2.48	0.43
14:N:80:LEU:O	14:N:82:ASP:N	2.51	0.43
12:Z:191:HIS:HD2	12:Z:191:HIS:N	2.11	0.43
4:D:103:PRO:HG2	4:D:140:PRO:HG2	2.00	0.43
3:Q:208:TYR:O	3:Q:210:ARG:N	2.51	0.43
10:X:125:LEU:CD2	10:X:125:LEU:H	2.31	0.43
10:J:148:MET:HE2	10:J:172:ASN:HB2	2.00	0.43
6:T:234:ILE:OXT	6:T:234:ILE:HG22	2.17	0.43
12:Z:81:LYS:HG3	12:Z:85:ASN:HD21	1.83	0.43
3:C:91:ALA:HB2	3:C:115:LEU:HD21	2.00	0.43
4:D:59:ILE:CD1	4:D:59:ILE:H	2.06	0.43
5:E:204:LEU:O	5:E:205:LYS:C	2.55	0.43
11:Y:75:LEU:HD12	11:Y:80:VAL:HG23	2.00	0.43
9:W:7:LYS:CB	9:W:12:VAL:HG23	2.46	0.43
3:C:208:TYR:O	3:C:210:ARG:N	2.51	0.43
11:K:22:THR:HG23	11:K:27:VAL:HG22	2.00	0.43
7:G:126:ASN:ND2	7:G:126:ASN:C	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:116:ASP:OD1	12:L:116:ASP:C	2.56	0.43
5:S:209:GLU:HA	5:S:209:GLU:OE1	2.18	0.43
2:P:18:LEU:HD21	3:Q:129:ARG:HD2	2.00	0.43
10:X:71:ASN:O	10:X:75:LEU:CD1	2.66	0.43
4:R:168:SER:O	4:R:172:ARG:HB2	2.18	0.43
4:R:203:VAL:CG1	4:R:209:ASN:HB2	2.48	0.43
2:P:241:GLN:C	2:P:243:ILE:N	2.71	0.43
2:P:243:ILE:O	2:P:246:ARG:N	2.47	0.43
9:W:5:GLY:CA	9:W:14:ILE:HG22	2.48	0.43
14:N:197:LEU:HD23	14:N:198:ALA:N	2.32	0.43
1:A:220:LYS:HG2	1:A:242:GLU:OE2	2.18	0.43
1:O:75:ILE:HG21	1:O:117:LEU:HD21	2.00	0.43
12:Z:176:ASN:ND2	12:Z:190:ASN:HD22	2.16	0.43
8:V:126:ILE:HD12	8:V:134:ILE:HG13	2.00	0.43
7:U:116:GLY:O	7:U:120:GLN:N	2.35	0.43
7:G:126:ASN:HD22	7:G:126:ASN:C	2.22	0.43
12:Z:97:MET:O	12:Z:116:ASP:HA	2.17	0.43
8:H:187:ILE:O	8:H:187:ILE:HG23	2.18	0.43
1:A:68:THR:O	7:G:157:TRP:CE3	2.72	0.43
12:L:32:LYS:HE2	13:M:132:GLU:OE2	2.18	0.43
2:P:34:SER:HB3	2:P:47:THR:OG1	2.19	0.43
11:Y:55:GLN:HG3	12:Z:88:TYR:CD2	2.54	0.43
10:X:13:ALA:HB2	10:X:22:ILE:HD12	1.99	0.43
2:P:217:GLU:OE1	2:P:231:LYS:HB2	2.18	0.43
8:V:151:THR:HG23	8:V:152:VAL:N	2.33	0.43
2:B:211:LEU:HD12	2:B:212:ALA:O	2.18	0.43
6:F:34:VAL:CG1	6:F:163:ALA:O	2.66	0.43
3:C:201:THR:CG2	3:C:202:ASP:H	2.14	0.43
4:D:100:LEU:O	4:D:102:ASP:N	2.47	0.43
4:R:50:SER:HA	4:R:53:LYS:CD	2.47	0.43
9:I:216:SER:C	9:I:217:ILE:HD12	2.39	0.43
6:F:89:ARG:NE	13:M:77:PHE:CD1	2.86	0.43
3:Q:36:ILE:CG2	3:Q:37:GLY:N	2.82	0.43
9:W:10:ASN:O	9:W:179:GLU:HG2	2.19	0.43
5:S:15:PHE:CD1	5:S:21:LEU:HD21	2.53	0.43
8:H:134:ILE:O	8:H:138:CYS:SG	2.76	0.43
8:H:82:PHE:CE1	8:H:97:ILE:HG12	2.54	0.43
4:D:199:LEU:C	4:D:201:GLU:H	2.22	0.43
9:I:67:SER:O	9:I:71:SER:N	2.51	0.43
6:F:100:ASN:CB	14:N:94:GLU:HG2	2.43	0.43
5:E:24:VAL:O	5:E:28:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:123:PHE:N	10:X:123:PHE:CD1	2.86	0.43
14:N:187:ARG:NH2	9:W:135:MET:SD	2.91	0.43
5:E:219:LEU:O	5:E:231:TYR:HB2	2.18	0.43
14:N:37:ASN:C	14:N:39:VAL:H	2.20	0.43
12:Z:38:ASN:HB2	12:Z:39:PRO:CD	2.48	0.43
11:Y:138:PHE:N	11:Y:138:PHE:CD1	2.86	0.43
9:W:97:TYR:CD1	9:W:97:TYR:N	2.85	0.43
3:Q:175:LEU:CD1	3:Q:199:LYS:HD2	2.24	0.43
8:H:126:ILE:HD12	8:H:134:ILE:HG13	2.00	0.43
1:A:158:ASP:HB2	1:A:159:PRO:CD	2.47	0.43
1:A:188:LYS:C	1:A:190:LYS:N	2.72	0.43
2:B:40:THR:HG21	2:B:182:GLU:HA	2.00	0.43
4:D:162:GLN:NE2	4:D:163:THR:N	2.62	0.43
2:P:36:GLY:HA2	2:P:44:VAL:O	2.18	0.43
6:F:179:PHE:O	6:F:181:LYS:N	2.52	0.43
8:V:15:GLY:O	8:V:16:ALA:HB2	2.18	0.43
14:N:146:PHE:O	14:N:147:GLY:C	2.55	0.43
14:N:49:THR:HG22	14:N:50:VAL:H	1.83	0.43
10:J:23:ALA:HB1	10:J:186:VAL:HG22	2.00	0.43
12:Z:116:ASP:OD1	12:Z:118:ASP:HB2	2.18	0.43
1:O:103:GLU:CG	1:O:107:LYS:HD3	2.49	0.43
14:N:15:LYS:HD3	14:N:140:PRO:HA	2.00	0.43
12:L:4:LEU:HD12	12:L:161:ILE:HD11	2.00	0.43
2:P:18:LEU:CD2	3:Q:129:ARG:HD2	2.49	0.43
10:J:8:GLY:HA2	10:J:140:THR:HG21	2.00	0.43
1:A:26:TYR:O	1:A:29:GLU:N	2.52	0.43
1:A:42:SER:HA	1:A:54:ILE:O	2.17	0.43
9:I:54:ALA:O	9:I:57:GLN:HB2	2.19	0.43
1:O:44:ALA:HA	1:O:53:VAL:HA	2.01	0.43
4:R:239:GLU:H	4:R:239:GLU:HG3	1.55	0.43
4:R:233:VAL:O	4:R:237:GLU:HG2	2.19	0.43
12:L:1:THR:HG23	12:L:33:ARG:NH2	2.32	0.43
1:A:240:ASN:O	1:A:243:GLU:HB2	2.18	0.43
3:Q:79:GLY:O	3:Q:80:LEU:C	2.57	0.43
7:G:24:GLU:HA	7:G:27:VAL:HG23	2.01	0.43
3:C:218:LYS:HG3	3:C:224:GLU:C	2.37	0.43
5:E:64:ILE:N	5:E:64:ILE:CD1	2.81	0.43
7:G:218:CYS:HA	7:G:223:THR:HG21	2.01	0.43
1:O:104:PHE:CG	1:O:112:MET:HG3	2.53	0.43
8:V:1:THR:N	8:V:129:SER:N	2.66	0.43
11:K:83:PHE:O	11:K:86:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:55:VAL:HG13	9:W:56:THR:N	2.33	0.43
7:G:15:SER:OG	7:G:19:ARG:HB3	2.18	0.43
4:D:75:PHE:HB3	4:D:133:THR:HG22	2.00	0.43
1:A:24:ARG:O	1:A:25:LEU:HB2	2.18	0.43
1:A:75:ILE:HD11	1:A:81:MET:CB	2.47	0.43
1:O:200:GLU:HG2	1:O:244:ARG:NH2	2.33	0.43
2:B:190:HIS:O	2:B:192:ALA:N	2.52	0.43
1:O:164:VAL:CG2	1:O:165:GLY:N	2.81	0.43
1:O:53:VAL:C	1:O:54:ILE:HD12	2.39	0.43
8:V:15:GLY:HA2	8:V:174:ARG:O	2.19	0.43
1:O:133:TYR:O	1:O:134:MET:HB3	2.18	0.43
1:O:46:ARG:HD2	1:O:152:PRO:HB2	2.01	0.43
14:N:114:ILE:HB	14:N:130:VAL:CG1	2.48	0.43
6:T:23:GLU:HA	6:T:26:LEU:HD23	1.99	0.43
10:J:84:GLU:N	10:J:84:GLU:CD	2.72	0.43
3:Q:207:THR:HB	3:Q:209:ASP:OD1	2.19	0.43
11:Y:86:GLN:O	11:Y:89:ALA:HB3	2.19	0.43
8:V:45:ARG:HH11	8:V:45:ARG:HB3	1.83	0.43
1:A:32:PHE:HA	1:A:35:THR:HG23	2.01	0.43
4:R:37:LYS:HG2	4:R:160:SER:O	2.18	0.43
10:J:97:ARG:HG3	10:J:102:TYR:CE2	2.54	0.43
3:C:111:LEU:HD22	3:C:111:LEU:O	2.19	0.43
9:W:220:ILE:HG23	10:X:46:GLY:O	2.19	0.43
6:F:197:ILE:HG23	6:F:198:SER:N	2.34	0.43
1:O:230:LYS:HE3	1:O:230:LYS:CA	2.33	0.43
14:N:152:ASN:O	14:N:156:ARG:HG3	2.19	0.43
2:B:241:GLN:C	2:B:243:ILE:N	2.71	0.43
2:P:190:HIS:O	2:P:192:ALA:N	2.52	0.43
7:U:44:GLY:HA3	7:U:218:CYS:O	2.18	0.43
6:F:74:LEU:HD12	6:F:74:LEU:C	2.40	0.43
11:Y:103:LEU:HA	11:Y:103:LEU:HD23	1.84	0.43
4:D:84:ILE:N	4:D:84:ILE:HD12	2.34	0.43
10:X:62:LEU:HD23	10:X:62:LEU:HA	1.75	0.43
4:R:84:ILE:N	4:R:84:ILE:CD1	2.82	0.43
7:U:51:LYS:HE3	7:U:63:ASN:O	2.19	0.43
13:M:176:SER:O	13:M:177:VAL:C	2.56	0.43
8:V:8:PHE:CD1	8:V:8:PHE:C	2.91	0.43
1:A:210:MET:O	1:A:211:ILE:C	2.57	0.43
3:Q:9:ARG:NE	3:Q:12:ILE:HD11	2.34	0.43
4:D:203:VAL:CG1	4:D:209:ASN:HB2	2.48	0.43
12:Z:19:ARG:N	12:Z:33:ARG:HH12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:126:ASP:CB	13:M:130:SER:H	2.32	0.43
9:W:4:VAL:HA	9:W:125:LEU:O	2.18	0.43
10:X:191:LYS:N	10:X:191:LYS:CD	2.81	0.43
13:M:3:ASN:HD22	13:M:4:PRO:CD	2.32	0.43
1:A:112:MET:HA	1:A:113:PRO:HD3	1.76	0.43
1:O:214:LEU:HD12	1:O:218:PHE:HZ	1.83	0.43
1:O:220:LYS:HZ3	1:O:220:LYS:HB2	1.80	0.43
7:U:44:GLY:HA2	7:U:140:VAL:HG23	2.00	0.43
2:B:170:ALA:O	2:B:173:THR:N	2.49	0.43
4:D:225:SER:O	4:D:229:ILE:HG13	2.19	0.43
6:T:82:ARG:NH1	6:T:82:ARG:HG3	2.34	0.43
9:I:144:GLN:HE21	9:I:144:GLN:HB2	1.69	0.43
11:K:138:PHE:HB3	12:Z:134:THR:OG1	2.19	0.43
12:L:134:THR:OG1	11:Y:138:PHE:HB3	2.19	0.43
3:C:160:TRP:CG	3:C:163:ILE:HB	2.53	0.43
8:H:147:SER:OG	8:H:150:GLU:N	2.36	0.42
8:H:157:HIS:CD2	8:V:140:LYS:NZ	2.87	0.42
1:A:200:GLU:HG2	1:A:244:ARG:NH2	2.33	0.42
10:J:123:PHE:CD1	10:J:123:PHE:N	2.87	0.42
1:O:30:TYR:O	1:O:31:ALA:C	2.56	0.42
7:U:134:SER:CB	7:U:164:THR:HG21	2.46	0.42
9:I:38:SER:OG	9:I:39:PRO:CD	2.63	0.42
2:B:111:VAL:HG22	2:B:136:ILE:HD12	2.01	0.42
9:W:38:SER:O	9:W:39:PRO:C	2.57	0.42
1:O:220:LYS:HB2	1:O:220:LYS:HZ2	1.81	0.42
9:W:132:LEU:N	9:W:132:LEU:CD2	2.80	0.42
9:I:132:LEU:N	9:I:132:LEU:CD2	2.81	0.42
9:I:52:THR:HG22	9:I:96:ALA:CB	2.49	0.42
1:O:33:LYS:HD2	1:O:33:LYS:N	2.32	0.42
3:C:109:GLU:CD	3:C:113:ARG:HH21	2.23	0.42
2:B:92:VAL:O	2:B:96:SER:HB2	2.19	0.42
3:Q:20:TYR:O	3:Q:21:GLN:C	2.56	0.42
9:I:94:ILE:HG13	9:I:94:ILE:O	2.19	0.42
1:O:244:ARG:HD2	1:O:244:ARG:H	1.82	0.42
2:B:161:ALA:HB3	3:C:56:LEU:CD2	2.38	0.42
9:I:5:GLY:O	9:I:124:TYR:HA	2.19	0.42
6:F:94:TYR:HD2	6:F:94:TYR:C	2.21	0.42
7:G:85:ARG:HG2	7:G:85:ARG:NH1	2.33	0.42
12:Z:116:ASP:C	12:Z:116:ASP:OD1	2.58	0.42
8:H:156:LYS:HD2	8:H:188:PHE:CE1	2.54	0.42
8:H:188:PHE:N	8:H:188:PHE:CD2	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:64:ILE:HG21	6:T:85:SER:HB2	2.01	0.42
11:K:86:GLN:O	11:K:89:ALA:HB3	2.19	0.42
2:B:18:LEU:CD2	3:C:129:ARG:HD2	2.48	0.42
14:N:15:LYS:HG3	14:N:127:LEU:HD22	2.01	0.42
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.84	0.42
11:K:78:GLN:C	11:K:78:GLN:CD	2.77	0.42
14:N:63:ILE:O	14:N:66:LEU:HB2	2.19	0.42
5:S:38:ILE:HB	5:S:200:VAL:HG13	2.01	0.42
1:A:44:ALA:O	1:A:168:ALA:CA	2.68	0.42
1:O:184:ASN:O	1:O:188:LYS:HG3	2.18	0.42
6:T:179:PHE:O	6:T:181:LYS:N	2.52	0.42
6:F:158:GLY:O	6:F:159:THR:CB	2.67	0.42
3:Q:208:TYR:C	3:Q:210:ARG:N	2.72	0.42
12:L:52:CYS:O	12:L:56:GLU:HB2	2.20	0.42
7:G:213:LEU:CD2	7:G:215:ILE:HD11	2.49	0.42
8:V:188:PHE:CD2	8:V:188:PHE:N	2.86	0.42
10:J:125:LEU:CD2	10:J:125:LEU:H	2.32	0.42
4:R:27:VAL:CG1	4:R:132:SER:HB2	2.49	0.42
9:I:10:ASN:HA	9:I:180:ILE:HD12	2.01	0.42
5:E:97:VAL:HG11	12:L:65:LEU:CD2	2.50	0.42
9:W:10:ASN:HA	9:W:180:ILE:HD12	2.01	0.42
8:H:46:SER:O	8:H:52:THR:HG21	2.19	0.42
13:M:108:HIS:CD2	13:M:139:GLY:HA3	2.54	0.42
8:H:81:VAL:O	8:H:85:LEU:HG	2.19	0.42
4:D:122:GLN:HB2	4:D:123:SER:H	1.64	0.42
1:O:51:THR:O	1:O:227:VAL:HG13	2.19	0.42
7:G:37:ILE:HA	7:G:163:ALA:CB	2.47	0.42
8:H:6:VAL:C	8:H:12:VAL:HG23	2.39	0.42
3:Q:190:ILE:H	3:Q:190:ILE:HG13	1.56	0.42
14:N:71:VAL:O	14:N:73:GLU:N	2.52	0.42
14:N:27:LEU:HD13	14:N:36:PHE:O	2.20	0.42
10:X:87:THR:HG22	10:X:129:ILE:HD13	2.02	0.42
7:G:81:ILE:HA	7:G:81:ILE:HD13	1.92	0.42
7:U:52:LEU:HD11	7:U:206:ASN:HD22	1.82	0.42
5:E:79:SER:HB3	5:E:172:ILE:HD12	2.00	0.42
8:H:1:THR:H2	8:H:128:GLY:CA	2.32	0.42
12:Z:208:ASN:C	12:Z:210:VAL:N	2.73	0.42
10:X:107:VAL:HG22	10:X:136:ILE:CG2	2.50	0.42
5:S:201:LEU:HA	5:S:201:LEU:HD12	1.74	0.42
9:I:8:PHE:HB2	9:I:146:LEU:O	2.20	0.42
6:F:82:ARG:NH1	6:F:82:ARG:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:45:ARG:CB	8:H:45:ARG:HH11	2.33	0.42
11:Y:19:LYS:CG	11:Y:180:ILE:HG13	2.48	0.42
6:F:3:ARG:HD3	6:F:3:ARG:H	1.85	0.42
8:H:9:LYS:HB2	8:H:146:MET:O	2.19	0.42
6:F:41:ASN:HB2	6:F:183:ASP:OD1	2.19	0.42
8:H:16:ALA:O	8:H:17:ASP:O	2.38	0.42
12:L:19:ARG:N	12:L:33:ARG:HH12	2.17	0.42
8:V:173:ILE:HG22	8:V:174:ARG:N	2.34	0.42
8:H:122:LEU:HD11	14:N:36:PHE:HE1	1.84	0.42
6:F:36:VAL:CG1	6:F:37:GLY:N	2.82	0.42
13:M:3:ASN:HD22	13:M:4:PRO:HD2	1.84	0.42
1:A:214:LEU:CD1	1:A:218:PHE:HZ	2.32	0.42
8:H:2:SER:OG	8:H:162:ALA:HB1	2.19	0.42
2:P:38:LYS:HA	2:P:43:VAL:HG22	2.00	0.42
6:T:171:TYR:C	6:T:171:TYR:HD2	2.23	0.42
1:A:12:TYR:CE1	2:B:7:PHE:CE2	3.07	0.42
10:X:95:TYR:C	10:X:97:ARG:N	2.72	0.42
3:C:176:LEU:O	3:C:178:MET:N	2.52	0.42
5:E:209:GLU:OE1	5:E:209:GLU:HA	2.19	0.42
4:R:84:ILE:N	4:R:84:ILE:HD12	2.34	0.42
7:U:51:LYS:O	7:U:211:PHE:HB2	2.19	0.42
9:I:97:TYR:CD1	9:I:97:TYR:N	2.86	0.42
11:K:92:ILE:HD12	11:K:92:ILE:HA	1.81	0.42
11:K:168:LEU:O	11:K:172:MET:HB2	2.19	0.42
9:I:148:LYS:O	9:I:152:ILE:HG13	2.19	0.42
5:S:222:ILE:HG12	5:S:223:THR:N	2.29	0.42
9:W:148:LYS:O	9:W:152:ILE:HG13	2.20	0.42
6:T:198:SER:HA	6:T:201:LEU:HG	2.00	0.42
1:O:131:ARG:O	1:O:132:ALA:HB3	2.19	0.42
14:N:25:ASP:HA	14:N:195:PHE:HB3	2.00	0.42
7:G:203:HIS:O	7:G:205:ASP:N	2.53	0.42
1:O:26:TYR:O	1:O:29:GLU:N	2.53	0.42
14:N:114:ILE:HG22	14:N:115:ILE:N	2.35	0.42
10:X:17:LYS:HG3	10:X:156:ASN:CB	2.47	0.42
10:J:94:LEU:HD11	10:J:106:PRO:HG3	2.02	0.42
4:R:225:SER:O	4:R:229:ILE:HG13	2.20	0.42
4:R:103:PRO:HG2	4:R:140:PRO:HG3	2.02	0.42
8:H:187:ILE:O	8:H:188:PHE:HD2	2.03	0.42
11:Y:139:TYR:CE2	11:Y:172:MET:HG3	2.55	0.42
3:C:181:LYS:O	3:C:184:MET:HB2	2.19	0.42
8:V:45:ARG:HH11	8:V:45:ARG:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:131:SER:O	8:V:135:TYR:CD1	2.72	0.42
12:L:9:GLN:HB3	12:L:9:GLN:HE21	1.64	0.42
10:X:8:GLY:HA2	10:X:140:THR:HG21	2.01	0.42
9:W:90:TYR:O	9:W:91:GLN:C	2.58	0.42
8:H:174:ARG:HG2	8:H:174:ARG:HH11	1.85	0.42
1:A:141:LEU:HB2	1:A:157:THR:CG2	2.50	0.42
3:Q:9:ARG:CZ	3:Q:12:ILE:HD11	2.49	0.42
4:R:99:THR:C	4:R:100:LEU:HD12	2.39	0.42
13:M:126:ASP:HB2	13:M:130:SER:N	2.33	0.42
11:K:75:LEU:HD12	11:K:80:VAL:HG23	2.02	0.42
6:F:156:LEU:HD23	7:G:58:LEU:HD23	2.02	0.42
9:W:76:VAL:HG11	9:W:109:HIS:HB2	2.00	0.42
1:O:101:ALA:HA	1:O:112:MET:HE2	2.01	0.42
10:X:148:MET:HE3	10:X:152:LEU:CD1	2.49	0.42
4:D:84:ILE:N	4:D:84:ILE:CD1	2.82	0.42
12:Z:3:THR:HB	12:Z:16:VAL:HG12	2.02	0.42
14:N:3:GLN:HG2	14:N:4:PRO:N	2.34	0.42
1:O:76:SER:C	1:O:78:THR:H	2.23	0.42
4:R:217:PRO:O	4:R:218:ASP:HB2	2.19	0.42
1:A:163:TYR:O	1:A:164:VAL:HB	2.20	0.42
1:O:188:LYS:C	1:O:190:LYS:N	2.73	0.42
2:P:212:ALA:HB2	2:P:237:LYS:HA	2.01	0.42
4:D:233:VAL:O	4:D:237:GLU:HG2	2.20	0.42
1:A:126:GLN:NE2	1:A:126:GLN:C	2.73	0.42
4:R:159:TRP:CZ2	5:S:59:LEU:HD23	2.55	0.42
3:Q:39:MET:HE3	3:Q:146:TYR:HB2	2.02	0.42
6:T:227:GLY:C	6:T:229:ALA:H	2.23	0.42
8:H:189:TYR:HA	8:H:190:PRO:HD3	1.85	0.42
10:J:84:GLU:HA	10:J:119:PHE:HE1	1.85	0.42
4:D:103:PRO:HG2	4:D:140:PRO:HG3	2.02	0.42
6:F:42:THR:HG22	6:F:218:LYS:HZ1	1.85	0.42
3:C:207:THR:HB	3:C:209:ASP:OD1	2.19	0.42
10:X:84:GLU:HA	10:X:119:PHE:HE1	1.85	0.42
4:D:212:ILE:O	4:D:224:LEU:HB2	2.20	0.42
6:F:171:TYR:HD2	6:F:171:TYR:C	2.23	0.42
5:S:214:GLU:OE2	5:S:214:GLU:N	2.52	0.42
7:G:108:ILE:N	7:G:109:PRO:HD3	2.35	0.42
3:Q:29:ILE:C	3:Q:31:HIS:N	2.73	0.42
11:Y:55:GLN:HG3	12:Z:88:TYR:CE2	2.55	0.42
13:M:135:GLN:HG2	13:M:135:GLN:O	2.20	0.42
13:M:136:CYS:SG	13:M:150:LEU:HD23	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LEU:O	2:B:158:PRO:HA	2.19	0.42
3:C:186:VAL:HG12	3:C:190:ILE:HD11	2.02	0.42
11:Y:184:VAL:HG22	11:Y:189:ILE:HG12	2.02	0.42
1:O:89:ASP:O	1:O:92:ASN:HB3	2.20	0.42
1:O:91:ARG:NH1	7:U:156:TYR:CD2	2.88	0.42
5:S:64:ILE:N	5:S:64:ILE:CD1	2.83	0.42
11:K:3:ILE:O	11:K:4:ILE:HD13	2.20	0.42
2:B:170:ALA:O	2:B:173:THR:HB	2.20	0.42
14:N:119:VAL:HG23	14:N:200:ILE:HG22	2.01	0.42
9:I:137:VAL:HG21	9:I:161:ALA:HB2	2.02	0.42
11:K:19:LYS:CG	11:K:180:ILE:HG13	2.50	0.42
4:R:133:THR:O	4:R:149:GLN:HA	2.20	0.42
11:Y:78:GLN:CD	11:Y:78:GLN:C	2.78	0.42
8:V:48:SER:OG	8:V:49:ALA:N	2.53	0.42
2:P:111:VAL:HG22	2:P:136:ILE:HD12	2.01	0.42
8:H:4:MET:SD	8:H:159:LEU:CD1	3.08	0.42
8:H:157:HIS:O	8:H:160:SER:HB3	2.20	0.42
1:A:164:VAL:CG2	1:A:165:GLY:H	2.32	0.42
1:O:182:LEU:CD2	1:O:209:HIS:HD2	2.33	0.42
9:I:73:GLU:HA	9:I:74:PRO:HD3	1.83	0.42
3:Q:43:GLY:HA2	3:Q:216:ILE:O	2.19	0.42
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.55	0.42
1:O:21:PRO:HA	2:P:23:TYR:CG	2.55	0.42
14:N:35:ARG:HG2	14:N:35:ARG:O	2.20	0.42
3:Q:195:LYS:HG2	3:Q:195:LYS:O	2.20	0.42
7:U:126:ASN:C	7:U:126:ASN:ND2	2.73	0.42
7:U:95:ALA:O	7:U:98:PHE:HB3	2.19	0.42
8:V:45:ARG:HB2	8:V:45:ARG:NH1	2.35	0.42
5:S:40:ILE:HD12	5:S:200:VAL:HG23	2.02	0.42
8:H:46:SER:HB3	8:H:96:GLY:HA3	2.02	0.42
6:T:3:ARG:HD3	6:T:3:ARG:H	1.85	0.42
7:U:104:THR:HA	7:U:105:PRO:HD2	1.82	0.42
7:U:217:TRP:CH2	7:U:222:GLU:HB3	2.55	0.42
8:V:81:VAL:O	8:V:85:LEU:HG	2.20	0.42
9:W:121:VAL:HG22	9:W:122:GLY:N	2.34	0.42
12:L:64:ARG:NH2	12:L:68:LEU:HD21	2.35	0.42
8:H:4:MET:SD	8:H:159:LEU:HD13	2.61	0.41
7:G:36:SER:O	7:G:163:ALA:CB	2.67	0.41
1:O:53:VAL:O	1:O:54:ILE:HD12	2.19	0.41
14:N:196:SER:OG	14:N:210:LYS:HD2	2.19	0.41
11:K:75:LEU:HD12	11:K:80:VAL:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:53:THR:CG2	11:K:54:VAL:N	2.82	0.41
14:N:226:LYS:HZ3	14:N:226:LYS:HB3	1.81	0.41
9:W:7:LYS:HA	9:W:12:VAL:HA	2.02	0.41
2:P:40:THR:HG21	2:P:182:GLU:HA	2.02	0.41
6:T:215:ILE:CG1	6:T:216:VAL:H	2.33	0.41
6:T:39:ARG:HD2	6:T:40:SER:O	2.19	0.41
9:W:175:VAL:CG1	9:W:176:CYS:N	2.82	0.41
11:Y:19:LYS:HD3	11:Y:180:ILE:HG13	2.01	0.41
5:E:61:SER:O	5:E:63:SER:N	2.53	0.41
1:A:135:ARG:HG3	1:A:135:ARG:NH1	2.35	0.41
1:O:32:PHE:HA	1:O:35:THR:HG23	2.02	0.41
12:Z:21:THR:HG21	12:Z:170:TYR:HD1	1.85	0.41
1:A:178:ILE:HD13	1:A:210:MET:CE	2.51	0.41
9:W:94:ILE:HG13	9:W:94:ILE:O	2.20	0.41
6:T:197:ILE:HG23	6:T:198:SER:N	2.35	0.41
3:C:202:ASP:O	3:C:203:SER:C	2.58	0.41
12:Z:1:THR:HG23	12:Z:33:ARG:NH2	2.30	0.41
2:P:147:LEU:O	2:P:158:PRO:HA	2.20	0.41
5:E:28:LEU:HD12	5:E:28:LEU:N	2.34	0.41
7:G:90:ARG:CD	7:G:118:TYR:HE1	2.32	0.41
1:O:243:GLU:O	1:O:246:VAL:N	2.52	0.41
14:N:11:VAL:O	14:N:143:ALA:HA	2.19	0.41
14:N:195:PHE:HB2	14:N:196:SER:H	1.52	0.41
14:N:209:LYS:HG2	14:N:212:LEU:HD11	2.03	0.41
9:I:76:VAL:HG11	9:I:109:HIS:HB2	2.01	0.41
9:W:189:ASN:C	9:W:191:LEU:N	2.73	0.41
5:S:78:MET:HE1	5:S:82:THR:HG22	2.00	0.41
4:R:73:LEU:HD12	4:R:135:ILE:CG1	2.50	0.41
1:O:126:GLN:HE21	1:O:127:ILE:N	2.18	0.41
7:U:126:ASN:C	7:U:126:ASN:HD22	2.24	0.41
12:L:38:ASN:HB2	12:L:39:PRO:CD	2.50	0.41
5:S:61:SER:O	5:S:63:SER:N	2.53	0.41
2:P:34:SER:HB3	2:P:47:THR:CB	2.50	0.41
7:G:67:GLN:HG2	14:N:77:ASP:OD1	2.20	0.41
6:T:107:ARG:HA	6:T:110:HIS:CD2	2.55	0.41
6:F:126:ARG:HH11	6:F:126:ARG:HG3	1.83	0.41
14:N:227:GLY:H	8:V:32:ASP:CG	2.23	0.41
12:L:21:THR:HG21	12:L:170:TYR:HD1	1.84	0.41
8:H:144:GLU:O	8:H:145:ASN:HB3	2.20	0.41
3:Q:159:GLY:O	4:R:56:ASP:HB2	2.20	0.41
4:D:203:VAL:HG21	4:D:210:ILE:CD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:151:ALA:C	14:N:153:PRO:HD2	2.41	0.41
1:A:237:SER:HB2	1:A:240:ASN:HB2	2.02	0.41
10:J:18:ASP:HB3	10:J:191:LYS:HZ3	1.85	0.41
1:A:16:ILE:HG13	1:A:16:ILE:H	1.56	0.41
1:A:66:PRO:HA	1:A:69:VAL:HG23	2.02	0.41
3:C:133:VAL:CG1	3:C:134:SER:N	2.82	0.41
3:C:77:VAL:CG1	3:C:78:ALA:N	2.84	0.41
2:P:128:ARG:HG3	2:P:128:ARG:HH11	1.86	0.41
7:U:38:GLY:N	7:U:162:ALA:O	2.48	0.41
13:M:87:ASN:CG	13:M:88:SER:N	2.73	0.41
8:H:45:ARG:NH1	8:H:45:ARG:HB2	2.35	0.41
3:Q:236:LYS:O	3:Q:240:VAL:HG23	2.21	0.41
4:R:96:HIS:CG	4:R:104:VAL:HG12	2.55	0.41
12:L:81:LYS:HD2	12:L:81:LYS:HA	1.92	0.41
12:Z:9:GLN:HB3	12:Z:9:GLN:HE21	1.64	0.41
7:U:83:ASP:CG	7:U:129:ARG:HH22	2.23	0.41
4:R:4:TYR:CD2	4:R:13:PRO:HD3	2.55	0.41
5:S:46:VAL:CG2	5:S:153:TYR:HB3	2.50	0.41
7:G:168:ARG:O	7:G:172:LYS:HG3	2.20	0.41
7:G:113:ASP:O	7:G:116:GLY:N	2.53	0.41
7:U:5:THR:HG23	7:U:7:TYR:HD2	1.85	0.41
5:S:24:VAL:O	5:S:28:LEU:HD13	2.20	0.41
2:B:122:THR:O	2:B:124:SER:N	2.53	0.41
2:P:35:LEU:N	2:P:35:LEU:HD22	2.34	0.41
11:Y:22:THR:HG23	11:Y:27:VAL:HG22	2.01	0.41
5:E:42:THR:C	5:E:44:GLU:N	2.73	0.41
11:Y:172:MET:CE	11:Y:174:MET:HB2	2.50	0.41
9:I:175:VAL:CG1	9:I:176:CYS:N	2.83	0.41
8:H:173:ILE:HG22	8:H:174:ARG:N	2.35	0.41
8:H:8:PHE:C	8:H:8:PHE:CD1	2.91	0.41
1:A:236:LEU:HA	1:A:236:LEU:HD23	1.78	0.41
7:U:36:SER:O	7:U:163:ALA:CB	2.67	0.41
8:H:13:ILE:CG1	8:H:177:VAL:HG22	2.37	0.41
1:O:210:MET:O	1:O:211:ILE:C	2.58	0.41
7:G:118:TYR:CE2	7:G:122:HIS:HE1	2.36	0.41
7:U:24:GLU:HA	7:U:27:VAL:HG23	2.01	0.41
9:W:104:ASP:OD1	9:W:106:THR:OG1	2.34	0.41
7:G:44:GLY:HA3	7:G:218:CYS:O	2.21	0.41
14:N:169:THR:O	14:N:172:VAL:N	2.53	0.41
11:Y:10:GLN:HB2	11:Y:152:MET:O	2.20	0.41
4:D:133:THR:O	4:D:149:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:129:ARG:HA	7:U:130:PRO:HD3	1.83	0.41
10:J:7:ASN:HA	10:J:29:GLY:O	2.20	0.41
2:P:39:ALA:HB3	2:P:42:GLY:O	2.20	0.41
12:Z:173:GLY:O	12:Z:193:VAL:HB	2.19	0.41
8:H:172:VAL:HG23	8:H:173:ILE:O	2.20	0.41
1:A:195:ASN:HD22	1:A:195:ASN:C	2.23	0.41
1:A:30:TYR:O	1:A:31:ALA:C	2.56	0.41
1:A:43:LEU:C	1:A:43:LEU:CD1	2.89	0.41
2:B:113:GLU:OE1	2:B:116:LYS:HE2	2.21	0.41
7:U:135:THR:O	7:U:149:MET:HA	2.19	0.41
1:O:178:ILE:HD13	1:O:210:MET:CE	2.50	0.41
6:T:46:LEU:HG	6:T:135:ILE:CD1	2.46	0.41
1:A:237:SER:HB2	1:A:240:ASN:CB	2.51	0.41
2:P:150:VAL:HG13	2:P:156:TYR:HB3	2.02	0.41
12:L:186:ILE:HG22	12:L:188:HIS:CD2	2.55	0.41
12:Z:106:ARG:NH1	12:Z:106:ARG:HG3	2.32	0.41
13:M:125:PHE:CD2	13:M:131:TYR:HB3	2.56	0.41
7:G:95:ALA:O	7:G:98:PHE:HB3	2.19	0.41
9:W:137:VAL:HG21	9:W:161:ALA:HB2	2.02	0.41
14:N:63:ILE:O	14:N:66:LEU:N	2.54	0.41
7:U:56:LYS:HD3	7:U:56:LYS:HA	1.93	0.41
11:Y:158:LEU:HA	11:Y:158:LEU:HD23	1.91	0.41
2:P:109:LEU:HD23	2:P:109:LEU:HA	1.81	0.41
1:A:92:ASN:C	1:A:92:ASN:OD1	2.99	0.41
8:H:15:GLY:HA2	8:H:174:ARG:O	2.20	0.41
9:I:83:LEU:HD12	9:I:113:ILE:HD11	2.02	0.41
1:A:21:PRO:HA	2:B:23:TYR:CD1	2.56	0.41
2:B:212:ALA:O	2:B:213:ILE:HG23	2.21	0.41
10:J:14:MET:HE3	10:J:166:ILE:CG1	2.34	0.41
8:V:105:LYS:HG2	8:V:106:ASN:N	2.35	0.41
8:H:67:THR:HA	8:H:71:GLY:O	2.20	0.41
8:V:172:VAL:HG23	8:V:173:ILE:O	2.21	0.41
10:J:87:THR:HG22	10:J:129:ILE:HD13	2.03	0.41
9:I:38:SER:O	9:I:39:PRO:C	2.59	0.41
3:Q:218:LYS:HB2	3:Q:225:VAL:HA	2.03	0.41
6:F:111:LEU:HA	6:F:111:LEU:HD23	1.85	0.41
7:U:218:CYS:HA	7:U:223:THR:HG21	2.03	0.41
1:O:103:GLU:HA	8:V:61:TYR:HE2	1.85	0.41
9:W:215:GLU:O	9:W:216:SER:HB3	2.21	0.41
12:L:116:ASP:OD1	12:L:118:ASP:HB2	2.20	0.41
9:I:50:ALA:CB	10:J:126:ILE:HG13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:172:MET:HE3	11:K:174:MET:HB2	2.03	0.41
13:M:63:ALA:O	13:M:67:ARG:HB2	2.21	0.41
7:G:209:LYS:O	7:G:210:ASP:C	2.59	0.41
5:E:46:VAL:CG2	5:E:153:TYR:HB3	2.51	0.41
3:C:236:LYS:O	3:C:240:VAL:HG23	2.21	0.41
3:Q:233:GLN:O	3:Q:234:GLU:C	2.59	0.41
9:I:84:LYS:HE2	9:I:119:THR:HG23	2.01	0.41
1:A:158:ASP:OD2	1:A:162:TYR:HB3	2.21	0.41
13:M:222:ASP:HB2	9:W:19:ARG:NH2	2.36	0.41
11:Y:39:SER:CB	11:Y:40:PRO:HD2	2.39	0.41
14:N:210:LYS:HD2	14:N:211:ASN:H	1.86	0.41
14:N:197:LEU:CD2	14:N:197:LEU:C	2.85	0.41
1:O:220:LYS:HG2	1:O:242:GLU:OE2	2.20	0.41
9:I:215:GLU:O	9:I:216:SER:HB3	2.21	0.41
3:Q:15:PRO:HA	4:R:22:TYR:CG	2.56	0.41
13:M:57:PHE:O	13:M:58:ALA:C	2.58	0.41
13:M:24:ALA:HB1	13:M:202:LEU:HD11	2.01	0.41
14:N:218:LYS:HE2	9:W:142:TRP:O	2.20	0.41
2:B:217:GLU:OE1	2:B:231:LYS:HB2	2.20	0.41
9:I:90:TYR:O	9:I:91:GLN:C	2.58	0.41
14:N:54:SER:HB3	14:N:113:ALA:HB3	2.03	0.41
8:H:137:TYR:O	8:H:138:CYS:C	2.59	0.41
8:H:97:ILE:HG23	8:H:113:ILE:O	2.21	0.41
1:A:44:ALA:HA	1:A:53:VAL:HA	2.02	0.41
1:A:21:PRO:HA	2:B:23:TYR:CG	2.55	0.41
2:P:161:ALA:HB3	3:Q:56:LEU:CD2	2.38	0.41
3:C:190:ILE:H	3:C:190:ILE:HG13	1.57	0.41
1:O:178:ILE:HD13	1:O:210:MET:HE1	2.03	0.41
1:O:44:ALA:O	1:O:168:ALA:CA	2.69	0.41
9:W:84:LYS:HE2	9:W:119:THR:HG23	2.02	0.41
8:H:122:LEU:HB3	8:H:123:PRO:CD	2.50	0.41
6:T:74:LEU:HD12	6:T:74:LEU:C	2.42	0.41
3:C:79:GLY:O	3:C:80:LEU:C	2.59	0.41
2:P:244:ASN:HD22	2:P:244:ASN:N	2.19	0.41
14:N:210:LYS:O	14:N:211:ASN:O	2.38	0.41
9:W:5:GLY:O	9:W:124:TYR:HA	2.21	0.41
1:A:123:ASN:HD21	2:B:83:ARG:NE	2.18	0.41
2:P:122:THR:O	2:P:124:SER:N	2.53	0.41
11:Y:162:LYS:O	11:Y:166:GLN:HG3	2.20	0.41
14:N:182:ARG:HG3	14:N:214:VAL:CG1	2.51	0.41
3:Q:4:ARG:HH21	4:R:6:ARG:CD	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:GLY:HA2	3:C:216:ILE:O	2.20	0.41
7:U:119:VAL:O	7:U:120:GLN:C	2.59	0.41
8:H:115:LEU:N	8:H:115:LEU:HD22	2.34	0.41
14:N:21:ILE:CG2	14:N:22:ILE:N	2.84	0.41
2:B:35:LEU:HD22	2:B:35:LEU:N	2.36	0.41
11:K:20:ALA:HB2	11:K:177:LYS:HB2	2.03	0.41
3:Q:6:TYR:CD2	3:Q:15:PRO:HD3	2.56	0.41
11:Y:9:VAL:HB	11:Y:10:GLN:H	1.72	0.41
9:W:144:GLN:HE21	9:W:144:GLN:HB2	1.65	0.41
12:Z:5:ALA:HA	12:Z:13:ILE:O	2.20	0.41
12:L:4:LEU:HD12	12:L:161:ILE:CD1	2.51	0.41
8:V:46:SER:HB3	8:V:96:GLY:HA3	2.02	0.41
6:T:17:GLY:CA	7:U:29:ALA:HB2	2.51	0.41
6:F:97:LEU:HD11	13:M:70:ASN:OD1	2.21	0.41
3:C:96:GLN:HA	3:C:96:GLN:NE2	2.36	0.41
11:Y:120:ASP:C	11:Y:120:ASP:OD1	2.59	0.41
2:P:104:TYR:OH	9:W:64:GLU:OE1	2.39	0.41
3:C:233:GLN:O	3:C:234:GLU:C	2.58	0.41
8:V:9:LYS:HB2	8:V:146:MET:O	2.21	0.41
13:M:192:THR:HG23	13:M:198:VAL:O	2.21	0.41
3:Q:96:GLN:NE2	3:Q:96:GLN:HA	2.36	0.41
14:N:228:TYR:HE2	8:V:35:THR:CG2	2.34	0.41
4:D:127:ARG:HA	4:D:128:PRO:HD3	1.93	0.41
8:H:163:ILE:H	8:H:163:ILE:HG12	1.68	0.41
9:I:87:LEU:HD12	9:I:115:ALA:O	2.21	0.41
2:B:207:ASP:C	2:B:209:ILE:H	2.24	0.41
3:Q:202:ASP:O	3:Q:203:SER:C	2.59	0.41
9:W:67:SER:OG	9:W:68:LEU:N	2.54	0.41
7:G:136:ILE:HG12	7:G:149:MET:CG	2.36	0.41
7:U:168:ARG:O	7:U:172:LYS:HG3	2.21	0.41
8:V:163:ILE:H	8:V:163:ILE:HG12	1.70	0.41
8:V:174:ARG:HG2	8:V:174:ARG:HH11	1.86	0.41
13:M:172:LEU:N	13:M:172:LEU:HD12	2.22	0.41
1:O:237:SER:HB2	1:O:240:ASN:HB2	2.02	0.41
4:R:166:ARG:HG2	4:R:166:ARG:NH1	2.36	0.41
6:F:144:LEU:O	6:F:145:LEU:HD12	2.21	0.41
11:Y:103:LEU:HD23	11:Y:118:GLN:HA	2.03	0.41
7:G:66:ILE:O	7:G:229:PHE:HZ	2.03	0.41
6:T:126:ARG:HH11	6:T:126:ARG:HG3	1.86	0.41
6:T:140:SER:HB2	6:T:143:HIS:NE2	2.36	0.41
7:U:237:GLU:O	7:U:241:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:107:ARG:HA	6:F:110:HIS:CD2	2.56	0.41
12:L:205:GLY:HA3	11:Y:149:ARG:HH21	1.86	0.41
2:B:34:SER:OG	2:B:76:SER:HB2	2.21	0.40
1:O:63:LEU:CD2	7:U:175:LEU:HD12	2.50	0.40
4:R:100:LEU:O	4:R:101:GLU:HB2	2.21	0.40
13:M:152:ASN:C	13:M:152:ASN:HD22	2.23	0.40
12:Z:211:ILE:HD12	12:Z:211:ILE:N	2.29	0.40
14:N:25:ASP:HA	14:N:195:PHE:CB	2.51	0.40
7:G:44:GLY:HA2	7:G:140:VAL:HG23	2.02	0.40
12:L:106:ARG:NH1	12:L:106:ARG:HG3	2.32	0.40
10:X:108:VAL:CG1	10:X:109:ALA:N	2.84	0.40
3:Q:194:LEU:C	3:Q:196:THR:N	2.74	0.40
7:U:213:LEU:CD2	7:U:215:ILE:HD11	2.50	0.40
1:O:158:ASP:OD2	1:O:162:TYR:HB3	2.21	0.40
10:X:66:PHE:CZ	10:X:90:VAL:HB	2.56	0.40
14:N:126:PHE:C	14:N:126:PHE:CD1	2.94	0.40
12:L:36:GLU:O	12:L:37:ILE:C	2.59	0.40
2:P:92:VAL:O	2:P:96:SER:HB2	2.21	0.40
3:Q:141:ASP:OD2	3:Q:147:GLN:NE2	2.54	0.40
8:H:154:PHE:O	8:H:155:ILE:C	2.57	0.40
4:R:171:VAL:HG23	4:R:172:ARG:N	2.37	0.40
2:B:44:VAL:HG23	2:B:213:ILE:CG2	2.51	0.40
3:C:9:ARG:HE	3:C:12:ILE:CD1	2.34	0.40
1:O:18:ILE:CD1	1:O:18:ILE:N	2.83	0.40
1:O:18:ILE:HG23	2:P:20:GLN:NE2	2.36	0.40
7:G:92:ARG:NE	14:N:76:TYR:CE1	2.89	0.40
8:H:38:HIS:CE1	8:H:67:THR:HG21	2.56	0.40
2:B:244:ASN:N	2:B:244:ASN:HD22	2.19	0.40
6:F:157:TYR:CE1	7:G:59:VAL:HG22	2.56	0.40
6:F:227:GLY:C	6:F:229:ALA:N	2.73	0.40
1:A:220:LYS:HB2	1:A:220:LYS:HZ2	1.85	0.40
5:E:64:ILE:N	5:E:64:ILE:HD12	2.36	0.40
1:O:112:MET:HA	1:O:113:PRO:HD3	1.77	0.40
10:J:106:PRO:O	10:J:107:VAL:HG23	2.21	0.40
3:C:194:LEU:C	3:C:196:THR:N	2.74	0.40
7:U:236:GLN:O	7:U:239:ILE:N	2.53	0.40
5:E:39:GLY:HA2	5:E:47:VAL:O	2.20	0.40
8:V:122:LEU:HB3	8:V:123:PRO:CD	2.50	0.40
1:O:176:GLN:NE2	1:O:180:THR:HG23	2.36	0.40
7:G:83:ASP:CG	7:G:129:ARG:HH22	2.24	0.40
12:L:4:LEU:CD1	12:L:161:ILE:HD11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:71:ASN:O	10:X:75:LEU:HD12	2.20	0.40
11:K:139:TYR:CE2	11:K:172:MET:HG3	2.56	0.40
8:V:65:LEU:HG	8:V:65:LEU:O	2.22	0.40
5:S:235:LYS:O	5:S:238:GLU:HG2	2.21	0.40
6:F:140:SER:HB2	6:F:143:HIS:NE2	2.36	0.40
1:A:210:MET:C	1:A:212:ASP:N	2.73	0.40
7:G:176:GLU:O	7:G:179:VAL:HB	2.21	0.40
8:V:82:PHE:CE1	8:V:97:ILE:HG12	2.56	0.40
1:O:123:ASN:HD21	2:P:83:ARG:NE	2.17	0.40
9:W:73:GLU:HA	9:W:74:PRO:HD3	1.86	0.40
13:M:124:SER:OG	13:M:137:ARG:HD2	2.21	0.40
10:X:23:ALA:HB1	10:X:186:VAL:HG22	2.04	0.40
10:X:37:ASN:ND2	10:X:37:ASN:H	2.20	0.40
1:O:127:ILE:HG13	1:O:127:ILE:H	1.59	0.40
8:V:137:TYR:O	8:V:138:CYS:C	2.60	0.40
2:P:47:THR:HG21	2:P:63:LYS:HE2	2.02	0.40
7:U:209:LYS:O	7:U:210:ASP:C	2.59	0.40
4:D:194:LEU:HA	4:D:197:ARG:CD	2.52	0.40
7:G:49:VAL:HG22	7:G:50:GLU:N	2.37	0.40
8:H:151:THR:O	8:H:154:PHE:N	2.52	0.40
2:P:218:ASN:HA	2:P:219:PRO:HD2	1.90	0.40
1:O:237:SER:HB2	1:O:240:ASN:CB	2.51	0.40
11:Y:194:ASP:HA	11:Y:197:ALA:HB3	2.03	0.40
1:A:98:LYS:NZ	8:H:68:SER:O	2.40	0.40
9:I:63:ILE:HG13	9:I:82:MET:HE1	2.03	0.40
9:I:7:LYS:HA	9:I:12:VAL:HG23	2.03	0.40
1:A:103:GLU:HA	8:H:61:TYR:HE2	1.85	0.40
7:U:108:ILE:N	7:U:109:PRO:HD3	2.35	0.40
7:G:64:VAL:HG12	7:G:66:ILE:H	1.86	0.40
13:M:17:GLY:HA3	13:M:20:PHE:CE1	2.56	0.40
4:R:39:LYS:O	4:R:40:ASN:HB3	2.21	0.40
1:A:89:ASP:O	1:A:92:ASN:HB3	2.21	0.40
8:H:15:GLY:O	8:H:16:ALA:HB2	2.21	0.40
7:G:119:VAL:O	7:G:120:GLN:C	2.59	0.40
1:A:126:GLN:HE21	1:A:127:ILE:N	2.19	0.40
6:T:62:LYS:HE3	6:T:74:LEU:O	2.22	0.40
7:U:133:VAL:O	7:U:152:PRO:HD3	2.22	0.40
6:T:137:TYR:CE2	6:T:218:LYS:HA	2.57	0.40
4:D:52:LEU:N	4:D:52:LEU:HD22	2.37	0.40
5:S:98:THR:HG22	5:S:102:TYR:CE1	2.57	0.40
8:V:156:LYS:NZ	8:V:188:PHE:HD1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:17:THR:CG2	1:O:17:THR:O	2.69	0.40
8:H:156:LYS:HG3	8:H:175:MET:HE1	2.02	0.40
6:F:39:ARG:HD2	6:F:40:SER:O	2.21	0.40
3:Q:188:ASP:O	3:Q:191:GLU:HB3	2.21	0.40
3:C:93:ILE:H	3:C:93:ILE:HD12	1.85	0.40
12:L:105:THR:OG1	12:L:108:GLU:HG2	2.21	0.40
10:J:95:TYR:C	10:J:97:ARG:H	2.25	0.40
12:Z:64:ARG:CZ	12:Z:68:LEU:HD21	2.51	0.40
7:U:204:GLU:HG3	7:U:204:GLU:O	2.22	0.40
4:R:194:LEU:HA	4:R:197:ARG:CD	2.52	0.40
3:C:15:PRO:HA	4:D:22:TYR:CG	2.56	0.40

All (37) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:1065:GLU:C	15:p:1167:GLY:CA[1_554]	0.47	1.73
15:f:1065:GLU:CD	15:p:1165:GLU:OE1[1_554]	0.71	1.49
15:f:1067:LEU:N	15:p:1167:GLY:O[1_554]	0.86	1.34
15:f:1066:GLN:N	15:p:1167:GLY:CA[1_554]	0.94	1.26
15:f:1066:GLN:N	15:p:1167:GLY:C[1_554]	1.01	1.19
15:f:1065:GLU:OE1	15:p:1165:GLU:OE1[1_554]	1.21	0.99
15:f:1065:GLU:OE2	15:p:1165:GLU:OE1[1_554]	1.24	0.96
15:f:1070:VAL:CG2	15:p:1168:LYS:NZ[1_554]	1.24	0.96
15:f:1065:GLU:O	15:p:1167:GLY:N[1_554]	1.33	0.87
15:f:1066:GLN:CB	15:p:1168:LYS:N[1_554]	1.43	0.77
15:f:1066:GLN:CG	15:p:1168:LYS:CB[1_554]	1.47	0.73
15:f:1065:GLU:OE2	15:p:1165:GLU:CD[1_554]	1.48	0.72
15:f:1066:GLN:OE1	15:p:1168:LYS:O[1_554]	1.50	0.70
15:f:1065:GLU:C	15:p:1167:GLY:N[1_554]	1.51	0.69
15:f:1065:GLU:O	15:p:1167:GLY:CA[1_554]	1.58	0.62
15:f:1065:GLU:OE2	15:p:1165:GLU:OE2[1_554]	1.59	0.61
15:f:1066:GLN:CA	15:p:1167:GLY:C[1_554]	1.60	0.60
15:f:1169:THR:OG1	15:p:1052:ASN:O[1_554]	1.60	0.60
15:f:1066:GLN:CA	15:p:1168:LYS:N[1_554]	1.65	0.55
15:f:1065:GLU:CA	15:p:1167:GLY:CA[1_554]	1.75	0.45
15:f:1067:LEU:N	15:p:1167:GLY:C[1_554]	1.75	0.45
15:f:1066:GLN:N	15:p:1168:LYS:N[1_554]	1.77	0.43
15:f:1066:GLN:CB	15:p:1168:LYS:CA[1_554]	1.78	0.42
15:f:1066:GLN:OE1	15:p:1168:LYS:C[1_554]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:1066:GLN:C	15:p:1167:GLY:C[1_554]	1.86	0.34
15:f:1066:GLN:C	15:p:1167:GLY:O[1_554]	1.86	0.34
15:f:1065:GLU:CD	15:p:1165:GLU:CD[1_554]	1.86	0.34
15:f:1070:VAL:CG2	15:p:1168:LYS:CE[1_554]	1.89	0.31
15:f:1065:GLU:C	15:p:1167:GLY:C[1_554]	1.96	0.24
15:f:1070:VAL:CB	15:p:1168:LYS:NZ[1_554]	2.01	0.19
15:f:1066:GLN:N	15:p:1167:GLY:N[1_554]	2.05	0.15
15:f:1066:GLN:CD	15:p:1168:LYS:CB[1_554]	2.06	0.14
15:f:1065:GLU:CG	15:p:1165:GLU:OE1[1_554]	2.07	0.13
15:f:1066:GLN:CB	15:p:1168:LYS:CB[1_554]	2.08	0.12
15:f:1169:THR:OG1	15:p:1053:SER:CA[1_554]	2.11	0.09
15:f:1066:GLN:N	15:p:1167:GLY:O[1_554]	2.13	0.07
15:f:1067:LEU:CA	15:p:1167:GLY:O[1_554]	2.17	0.03

## 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	A	241/252 (96%)	175 (73%)	53 (22%)	13 (5%)	2	19
1	O	241/252 (96%)	174 (72%)	54 (22%)	13 (5%)	2	19
2	B	247/250 (99%)	192 (78%)	39 (16%)	16 (6%)	1	13
2	P	247/250 (99%)	193 (78%)	38 (15%)	16 (6%)	1	13
3	C	241/258 (93%)	192 (80%)	35 (14%)	14 (6%)	2	17
3	Q	241/258 (93%)	192 (80%)	35 (14%)	14 (6%)	2	17
4	D	239/254 (94%)	203 (85%)	28 (12%)	8 (3%)	5	32
4	R	239/254 (94%)	203 (85%)	28 (12%)	8 (3%)	5	32
5	E	243/260 (94%)	204 (84%)	27 (11%)	12 (5%)	3	21
5	S	243/260 (94%)	201 (83%)	30 (12%)	12 (5%)	3	21
6	F	232/234 (99%)	192 (83%)	33 (14%)	7 (3%)	5	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	232/234 (99%)	191 (82%)	33 (14%)	8 (3%)	5	31
7	G	241/288 (84%)	188 (78%)	37 (15%)	16 (7%)	1	12
7	U	241/288 (84%)	188 (78%)	37 (15%)	16 (7%)	1	12
8	H	194/196 (99%)	143 (74%)	38 (20%)	13 (7%)	1	12
8	V	194/196 (99%)	142 (73%)	37 (19%)	15 (8%)	1	8
9	I	220/222 (99%)	173 (79%)	37 (17%)	10 (4%)	3	24
9	W	220/222 (99%)	174 (79%)	35 (16%)	11 (5%)	3	21
10	J	202/205 (98%)	173 (86%)	24 (12%)	5 (2%)	7	41
10	X	202/205 (98%)	174 (86%)	23 (11%)	5 (2%)	7	41
11	K	196/198 (99%)	171 (87%)	20 (10%)	5 (3%)	7	40
11	Y	196/198 (99%)	170 (87%)	21 (11%)	5 (3%)	7	40
12	L	210/212 (99%)	183 (87%)	24 (11%)	3 (1%)	14	57
12	Z	210/212 (99%)	185 (88%)	22 (10%)	3 (1%)	14	57
13	M	220/222 (99%)	193 (88%)	24 (11%)	3 (1%)	14	57
13	a	220/222 (99%)	192 (87%)	25 (11%)	3 (1%)	14	57
14	N	231/233 (99%)	176 (76%)	39 (17%)	16 (7%)	1	11
14	b	231/233 (99%)	176 (76%)	39 (17%)	16 (7%)	1	11
15	c	228/231 (99%)	207 (91%)	14 (6%)	7 (3%)	5	34
15	d	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	7	40
15	e	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	7	40
15	f	228/231 (99%)	200 (88%)	17 (8%)	11 (5%)	3	22
15	g	228/231 (99%)	202 (89%)	18 (8%)	8 (4%)	4	31
15	h	228/231 (99%)	209 (92%)	15 (7%)	4 (2%)	11	51
15	i	228/231 (99%)	207 (91%)	16 (7%)	5 (2%)	8	45
15	j	228/231 (99%)	207 (91%)	14 (6%)	7 (3%)	5	34
15	k	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	7	40
15	l	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	7	40
15	m	228/231 (99%)	199 (87%)	18 (8%)	11 (5%)	3	22
15	n	228/231 (99%)	202 (89%)	18 (8%)	8 (4%)	4	31
15	o	228/231 (99%)	209 (92%)	15 (7%)	4 (2%)	11	51
15	p	228/231 (99%)	207 (91%)	16 (7%)	5 (2%)	8	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9506/9802 (97%)	7986 (84%)	1140 (12%)	380 (4%)	4 27

All (380) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	LEU
1	A	168	ALA
1	A	221	ASN
1	A	232	LYS
2	B	123	GLN
2	B	124	SER
2	B	244	ASN
3	C	4	ARG
3	C	20	TYR
3	C	183	ASP
3	C	203	SER
3	C	221	ASN
4	D	40	ASN
4	D	56	ASP
4	D	205	THR
5	E	61	SER
5	E	127	ALA
5	E	130	GLU
5	E	209	GLU
5	E	249	ALA
6	F	142	ALA
6	F	218	LYS
6	F	228	GLU
7	G	182	HIS
7	G	183	PRO
7	G	184	GLU
8	H	17	ASP
8	H	97	ILE
8	H	105	LYS
8	H	106	ASN
8	H	137	TYR
8	H	138	CYS
9	I	91	GLN
9	I	189	ASN
10	J	193	GLU
11	K	193	ASP
12	L	209	ASN

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Mol	Chain	Res	Type
14	N	25	ASP
14	N	81	ALA
14	N	130	VAL
14	N	211	ASN
14	N	221	PHE
1	O	150	LEU
1	O	168	ALA
1	O	221	ASN
1	O	232	LYS
2	P	123	GLN
2	P	124	SER
2	P	244	ASN
3	Q	4	ARG
3	Q	20	TYR
3	Q	183	ASP
3	Q	203	SER
3	Q	221	ASN
4	R	40	ASN
4	R	56	ASP
4	R	205	THR
5	S	127	ALA
5	S	130	GLU
5	S	209	GLU
5	S	249	ALA
6	T	142	ALA
6	T	218	LYS
6	T	228	GLU
7	U	182	HIS
7	U	183	PRO
7	U	184	GLU
8	V	17	ASP
8	V	97	ILE
8	V	105	LYS
8	V	106	ASN
8	V	137	TYR
8	V	138	CYS
9	W	189	ASN
10	X	193	GLU
11	Y	193	ASP
12	Z	209	ASN
14	b	25	ASP
14	b	81	ALA

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Mol	Chain	Res	Type
14	b	130	VAL
14	b	211	ASN
14	b	221	PHE
15	c	1133	SER
15	c	1139	PRO
15	c	1162	VAL
15	c	1164	ALA
15	d	1133	SER
15	d	1139	PRO
15	e	1133	SER
15	e	1139	PRO
15	f	1133	SER
15	f	1139	PRO
15	f	1162	VAL
15	f	1174	SER
15	g	1133	SER
15	g	1139	PRO
15	g	1162	VAL
15	g	1163	ASP
15	g	1164	ALA
15	g	1170	LYS
15	h	1133	SER
15	h	1139	PRO
15	i	1133	SER
15	i	1139	PRO
15	i	1162	VAL
15	j	1133	SER
15	j	1139	PRO
15	j	1162	VAL
15	j	1164	ALA
15	k	1133	SER
15	k	1139	PRO
15	l	1133	SER
15	l	1139	PRO
15	m	1133	SER
15	m	1139	PRO
15	m	1162	VAL
15	m	1174	SER
15	m	1175	GLN
15	n	1133	SER
15	n	1139	PRO
15	n	1162	VAL

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Mol	Chain	Res	Type
15	n	1163	ASP
15	n	1164	ALA
15	n	1170	LYS
15	o	1133	SER
15	o	1139	PRO
15	p	1133	SER
15	p	1139	PRO
15	p	1162	VAL
1	A	37	GLN
1	A	151	GLY
1	A	164	VAL
1	A	190	LYS
1	A	243	GLU
2	B	20	GLN
2	B	31	GLY
2	B	182	GLU
2	B	242	GLU
2	B	243	ILE
3	C	184	MET
3	C	223	GLY
5	E	131	GLU
5	E	134	MET
5	E	206	GLN
5	E	244	LYS
6	F	118	LYS
6	F	159	THR
7	G	71	ARG
7	G	72	HIS
7	G	186	LEU
7	G	188	ALA
7	G	204	GLU
7	G	207	LYS
8	H	74	SER
9	I	22	GLN
9	I	95	GLY
9	I	221	CYS
13	M	81	ASP
14	N	24	ALA
14	N	132	LEU
14	N	152	ASN
14	N	189	ALA
1	O	37	GLN

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Mol	Chain	Res	Type
1	O	151	GLY
1	O	164	VAL
1	O	175	GLN
1	O	190	LYS
1	O	243	GLU
2	P	20	GLN
2	P	31	GLY
2	P	182	GLU
2	P	242	GLU
2	P	243	ILE
3	Q	184	MET
3	Q	223	GLY
3	Q	236	LYS
5	S	61	SER
5	S	131	GLU
5	S	134	MET
5	S	206	GLN
5	S	244	LYS
6	T	118	LYS
6	T	159	THR
7	U	71	ARG
7	U	72	HIS
7	U	152	PRO
7	U	185	GLY
7	U	186	LEU
7	U	188	ALA
7	U	204	GLU
7	U	207	LYS
8	V	74	SER
9	W	22	GLN
9	W	91	GLN
9	W	95	GLY
9	W	221	CYS
13	a	81	ASP
14	b	24	ALA
14	b	132	LEU
14	b	152	ASN
14	b	189	ALA
15	c	1163	ASP
15	c	1166	SER
15	e	1174	SER
15	f	1164	ALA

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Mol	Chain	Res	Type
15	f	1170	LYS
15	f	1175	GLN
15	j	1163	ASP
15	j	1166	SER
15	l	1174	SER
15	m	1164	ALA
15	m	1170	LYS
1	A	175	GLN
1	A	189	SER
3	C	80	LEU
3	C	209	ASP
3	C	236	LYS
5	E	189	SER
7	G	70	ASP
7	G	152	PRO
7	G	185	GLY
7	G	224	ASN
8	H	9	LYS
8	H	33	LYS
8	H	191	ASP
9	I	48	THR
9	I	145	ASP
10	J	5	SER
11	K	141	PHE
14	N	76	TYR
14	N	151	ALA
14	N	170	VAL
1	O	77	ARG
1	O	189	SER
3	Q	80	LEU
3	Q	209	ASP
7	U	224	ASN
8	V	9	LYS
9	W	145	ASP
10	X	5	SER
11	Y	141	PHE
13	a	37	SER
14	b	76	TYR
14	b	151	ALA
14	b	170	VAL
15	d	1162	VAL
15	d	1176	SER

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Mol	Chain	Res	Type
15	f	1166	SER
15	f	1173	GLY
15	f	1176	SER
15	g	1166	SER
15	k	1162	VAL
15	k	1176	SER
15	m	1166	SER
15	m	1173	GLY
15	m	1176	SER
15	n	1166	SER
1	A	77	ARG
1	A	200	GLU
2	B	29	LYS
2	B	79	GLY
3	C	233	GLN
4	D	58	ARG
4	D	78	LEU
5	E	214	GLU
6	F	117	GLN
6	F	232	LYS
8	H	68	SER
8	H	145	ASN
9	I	17	ASP
9	I	49	ALA
11	K	50	ALA
12	L	97	MET
12	L	165	ALA
13	M	37	SER
13	M	58	ALA
1	O	200	GLU
2	P	79	GLY
3	Q	195	LYS
3	Q	233	GLN
4	R	58	ARG
4	R	78	LEU
4	R	122	GLN
5	S	189	SER
5	S	214	GLU
6	T	232	LYS
7	U	70	ASP
7	U	210	ASP
8	V	33	LYS

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Mol	Chain	Res	Type
8	V	68	SER
8	V	145	ASN
8	V	191	ASP
9	W	17	ASP
9	W	48	THR
9	W	49	ALA
11	Y	192	VAL
12	Z	97	MET
12	Z	165	ALA
13	a	58	ALA
14	b	9	THR
2	B	69	PRO
2	B	122	THR
2	B	208	THR
2	B	219	PRO
3	C	177	GLN
3	C	234	GLU
4	D	122	GLN
7	G	210	ASP
11	K	192	VAL
2	P	29	LYS
2	P	122	THR
2	P	208	THR
2	P	219	PRO
3	Q	234	GLU
4	R	200	LEU
6	T	117	GLN
8	V	50	ALA
11	Y	50	ALA
15	d	1226	SER
15	e	1226	SER
15	i	1226	SER
15	k	1226	SER
15	l	1226	SER
15	p	1226	SER
2	B	191	ILE
3	C	195	LYS
4	D	200	LEU
5	E	62	ASP
7	G	241	PHE
9	I	39	PRO
10	J	2	ASP

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Mol	Chain	Res	Type
14	N	9	THR
2	P	69	PRO
2	P	158	PRO
2	P	191	ILE
3	Q	30	SER
5	S	62	ASP
6	T	5	ASN
7	U	241	PHE
9	W	21	THR
9	W	39	PRO
10	X	2	ASP
15	h	1226	SER
15	o	1226	SER
2	B	158	PRO
11	K	9	VAL
11	Y	9	VAL
15	i	1064	PRO
15	p	1064	PRO
4	D	202	VAL
7	G	84	GLY
10	J	100	GLY
10	J	107	VAL
14	N	177	ILE
4	R	202	VAL
8	V	30	VAL
14	b	11	VAL
14	b	22	ILE
14	b	177	ILE
15	c	1064	PRO
15	d	1064	PRO
15	e	1162	VAL
15	f	1064	PRO
15	h	1064	PRO
15	j	1064	PRO
15	k	1064	PRO
15	l	1162	VAL
15	m	1064	PRO
15	o	1064	PRO
8	H	30	VAL
14	N	11	VAL
7	U	84	GLY
10	X	100	GLY

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Mol	Chain	Res	Type
10	X	107	VAL
15	e	1064	PRO
15	l	1064	PRO
15	n	1064	PRO
14	N	22	ILE
8	V	189	TYR
15	g	1064	PRO

### 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	A	207/210 (99%)	185 (89%)	22 (11%)	8	34
1	O	207/210 (99%)	186 (90%)	21 (10%)	9	37
2	B	208/209 (100%)	188 (90%)	20 (10%)	10	39
2	P	208/209 (100%)	189 (91%)	19 (9%)	12	42
3	C	203/216 (94%)	181 (89%)	22 (11%)	8	34
3	Q	203/216 (94%)	181 (89%)	22 (11%)	8	34
4	D	213/226 (94%)	196 (92%)	17 (8%)	15	52
4	R	213/226 (94%)	196 (92%)	17 (8%)	15	52
5	E	201/215 (94%)	188 (94%)	13 (6%)	21	61
5	S	201/215 (94%)	187 (93%)	14 (7%)	19	58
6	F	193/193 (100%)	174 (90%)	19 (10%)	10	38
6	T	193/193 (100%)	173 (90%)	20 (10%)	9	35
7	G	201/239 (84%)	182 (90%)	19 (10%)	11	40
7	U	201/239 (84%)	183 (91%)	18 (9%)	12	43
8	H	162/162 (100%)	145 (90%)	17 (10%)	8	35
8	V	162/162 (100%)	144 (89%)	18 (11%)	8	32
9	I	181/181 (100%)	164 (91%)	17 (9%)	11	41
9	W	181/181 (100%)	164 (91%)	17 (9%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	172/173 (99%)	163 (95%)	9 (5%)	29	69
10	X	172/173 (99%)	163 (95%)	9 (5%)	29	69
11	K	175/175 (100%)	157 (90%)	18 (10%)	9	36
11	Y	175/175 (100%)	158 (90%)	17 (10%)	10	39
12	L	169/169 (100%)	159 (94%)	10 (6%)	24	65
12	Z	169/169 (100%)	158 (94%)	11 (6%)	21	61
13	M	185/185 (100%)	164 (89%)	21 (11%)	7	31
13	a	185/185 (100%)	163 (88%)	22 (12%)	6	28
14	N	199/199 (100%)	185 (93%)	14 (7%)	19	58
14	b	199/199 (100%)	184 (92%)	15 (8%)	17	55
15	c	188/189 (100%)	182 (97%)	6 (3%)	46	80
15	d	188/189 (100%)	186 (99%)	2 (1%)	80	93
15	e	188/189 (100%)	186 (99%)	2 (1%)	80	93
15	f	188/189 (100%)	182 (97%)	6 (3%)	46	80
15	g	188/189 (100%)	184 (98%)	4 (2%)	61	87
15	h	188/189 (100%)	186 (99%)	2 (1%)	80	93
15	i	188/189 (100%)	186 (99%)	2 (1%)	80	93
15	j	188/189 (100%)	182 (97%)	6 (3%)	46	80
15	k	188/189 (100%)	186 (99%)	2 (1%)	80	93
15	l	188/189 (100%)	186 (99%)	2 (1%)	80	93
15	m	188/189 (100%)	182 (97%)	6 (3%)	46	80
15	n	188/189 (100%)	184 (98%)	4 (2%)	61	87
15	o	188/189 (100%)	186 (99%)	2 (1%)	80	93
15	p	188/189 (100%)	186 (99%)	2 (1%)	80	93
All	All	7970/8150 (98%)	7444 (93%)	526 (7%)	21	61

All (526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	56	GLN
1	A	65	ASP
1	A	73	PHE
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	126	GLN
1	A	128	TYR
1	A	131	ARG
1	A	133	TYR
1	A	150	LEU
1	A	153	SER
1	A	163	TYR
1	A	167	LYS
1	A	193	HIS
1	A	195	ASN
1	A	212	ASP
1	A	220	LYS
1	A	221	ASN
1	A	230	LYS
1	A	234	PHE
1	A	250	GLU
2	B	10	THR
2	B	26	THR
2	B	28	VAL
2	B	35	LEU
2	B	55	LEU
2	B	59	GLU
2	B	68	THR
2	B	118	MET
2	B	134	LEU
2	B	150	VAL
2	B	157	PHE
2	B	173	THR
2	B	178	ARG
2	B	182	GLU
2	B	184	GLU
2	B	204	PHE
2	B	211	LEU
2	B	220	ASP
2	B	244	ASN
2	B	245	ASP
3	C	10	THR
3	C	26	LEU
3	C	53	THR
3	C	70	ASN
3	C	81	THR

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Mol	Chain	Res	Type
3	C	86	ILE
3	C	111	LEU
3	C	115	LEU
3	C	120	GLN
3	C	134	SER
3	C	142	ASP
3	C	150	THR
3	C	158	THR
3	C	175	LEU
3	C	183	ASP
3	C	185	LYS
3	C	190	ILE
3	C	192	LEU
3	C	202	ASP
3	C	217	ARG
3	C	221	ASN
3	C	224	GLU
4	D	9	SER
4	D	24	LEU
4	D	29	ARG
4	D	49	ARG
4	D	52	LEU
4	D	54	LEU
4	D	59	ILE
4	D	105	THR
4	D	118	GLN
4	D	132	SER
4	D	162	GLN
4	D	166	ARG
4	D	208	LYS
4	D	211	GLU
4	D	215	VAL
4	D	218	ASP
4	D	239	GLU
5	E	48	LEU
5	E	76	CYS
5	E	78	MET
5	E	110	GLU
5	E	119	LEU
5	E	154	GLN
5	E	184	LEU
5	E	221	CYS

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Mol	Chain	Res	Type
5	E	222	ILE
5	E	226	ASP
5	E	232	ASP
5	E	233	ASN
5	E	245	GLU
6	F	3	ARG
6	F	10	THR
6	F	31	GLN
6	F	62	LYS
6	F	72	LEU
6	F	90	GLN
6	F	93	ASN
6	F	94	TYR
6	F	100	ASN
6	F	107	ARG
6	F	117	GLN
6	F	147	PHE
6	F	166	GLN
6	F	171	TYR
6	F	176	LEU
6	F	185	ASN
6	F	189	LEU
6	F	206	LEU
6	F	228	GLU
7	G	19	ARG
7	G	27	VAL
7	G	28	LYS
7	G	42	ASN
7	G	72	HIS
7	G	76	VAL
7	G	80	LEU
7	G	81	ILE
7	G	97	SER
7	G	120	GLN
7	G	126	ASN
7	G	127	SER
7	G	147	LEU
7	G	152	PRO
7	G	189	ARG
7	G	208	GLU
7	G	217	TRP
7	G	224	ASN

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Mol	Chain	Res	Type
7	G	243	GLN
8	H	8	PHE
8	H	21	THR
8	H	36	ARG
8	H	39	ASP
8	H	72	THR
8	H	82	PHE
8	H	83	LYS
8	H	84	GLU
8	H	88	GLU
8	H	92	ASN
8	H	104	ASP
8	H	118	SER
8	H	132	THR
8	H	137	TYR
8	H	149	GLU
8	H	153	ASP
8	H	172	VAL
9	I	10	ASN
9	I	21	THR
9	I	33	LYS
9	I	39	PRO
9	I	41	ILE
9	I	72	ARG
9	I	81	GLN
9	I	82	MET
9	I	85	GLN
9	I	98	LEU
9	I	104	ASP
9	I	132	LEU
9	I	144	GLN
9	I	146	LEU
9	I	153	LYS
9	I	177	VAL
9	I	178	MET
10	J	37	ASN
10	J	64	GLU
10	J	90	VAL
10	J	123	PHE
10	J	125	LEU
10	J	133	LYS
10	J	138	SER

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Mol	Chain	Res	Type
10	J	171	LEU
10	J	191	LYS
11	K	7	ILE
11	K	8	ARG
11	K	11	ASP
11	K	22	THR
11	K	28	LEU
11	K	36	ARG
11	K	75	LEU
11	K	78	GLN
11	K	86	GLN
11	K	91	SER
11	K	110	LYS
11	K	111	LYS
11	K	136	SER
11	K	162	LYS
11	K	194	ASP
11	K	195	PHE
11	K	196	GLN
11	K	198	GLN
12	L	4	LEU
12	L	9	GLN
12	L	21	THR
12	L	25	TRP
12	L	33	ARG
12	L	86	LEU
12	L	104	TYR
12	L	105	THR
12	L	111	THR
12	L	211	ILE
13	M	3	ASN
13	M	18	GLU
13	M	23	LEU
13	M	27	THR
13	M	31	THR
13	M	48	ASP
13	M	49	ASN
13	M	52	MET
13	M	67	ARG
13	M	85	SER
13	M	109	THR
13	M	135	GLN

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Mol	Chain	Res	Type
13	M	144	SER
13	M	151	ASP
13	M	152	ASN
13	M	165	ASN
13	M	172	LEU
13	M	174	TYR
13	M	175	LEU
13	M	214	LYS
13	M	221	ARG
14	N	34	LEU
14	N	48	ASN
14	N	85	GLU
14	N	102	GLN
14	N	104	ARG
14	N	111	TRP
14	N	132	LEU
14	N	138	SER
14	N	140	PRO
14	N	171	GLN
14	N	184	LEU
14	N	212	LEU
14	N	216	ASN
14	N	226	LYS
1	O	39	ASN
1	O	56	GLN
1	O	65	ASP
1	O	73	PHE
1	O	117	LEU
1	O	124	LEU
1	O	126	GLN
1	O	128	TYR
1	O	131	ARG
1	O	133	TYR
1	O	150	LEU
1	O	153	SER
1	O	163	TYR
1	O	167	LYS
1	O	193	HIS
1	O	195	ASN
1	O	220	LYS
1	O	221	ASN
1	O	230	LYS

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Mol	Chain	Res	Type
1	O	234	PHE
1	O	250	GLU
2	P	10	THR
2	P	26	THR
2	P	28	VAL
2	P	35	LEU
2	P	55	LEU
2	P	59	GLU
2	P	68	THR
2	P	118	MET
2	P	134	LEU
2	P	150	VAL
2	P	157	PHE
2	P	173	THR
2	P	178	ARG
2	P	182	GLU
2	P	184	GLU
2	P	204	PHE
2	P	220	ASP
2	P	244	ASN
2	P	245	ASP
3	Q	10	THR
3	Q	26	LEU
3	Q	53	THR
3	Q	70	ASN
3	Q	81	THR
3	Q	86	ILE
3	Q	111	LEU
3	Q	115	LEU
3	Q	120	GLN
3	Q	134	SER
3	Q	142	ASP
3	Q	150	THR
3	Q	158	THR
3	Q	175	LEU
3	Q	183	ASP
3	Q	185	LYS
3	Q	190	ILE
3	Q	192	LEU
3	Q	202	ASP
3	Q	217	ARG
3	Q	221	ASN

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Mol	Chain	Res	Type
3	Q	224	GLU
4	R	9	SER
4	R	24	LEU
4	R	29	ARG
4	R	49	ARG
4	R	52	LEU
4	R	54	LEU
4	R	59	ILE
4	R	105	THR
4	R	118	GLN
4	R	132	SER
4	R	162	GLN
4	R	166	ARG
4	R	208	LYS
4	R	211	GLU
4	R	215	VAL
4	R	218	ASP
4	R	239	GLU
5	S	48	LEU
5	S	76	CYS
5	S	78	MET
5	S	110	GLU
5	S	119	LEU
5	S	154	GLN
5	S	180	GLN
5	S	184	LEU
5	S	221	CYS
5	S	222	ILE
5	S	226	ASP
5	S	232	ASP
5	S	233	ASN
5	S	245	GLU
6	T	3	ARG
6	T	10	THR
6	T	31	GLN
6	T	62	LYS
6	T	72	LEU
6	T	90	GLN
6	T	93	ASN
6	T	94	TYR
6	T	100	ASN
6	T	107	ARG

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Mol	Chain	Res	Type
6	T	117	GLN
6	T	147	PHE
6	T	157	TYR
6	T	166	GLN
6	T	171	TYR
6	T	176	LEU
6	T	185	ASN
6	T	189	LEU
6	T	206	LEU
6	T	228	GLU
7	U	19	ARG
7	U	27	VAL
7	U	42	ASN
7	U	72	HIS
7	U	76	VAL
7	U	80	LEU
7	U	81	ILE
7	U	97	SER
7	U	120	GLN
7	U	126	ASN
7	U	127	SER
7	U	147	LEU
7	U	152	PRO
7	U	189	ARG
7	U	208	GLU
7	U	217	TRP
7	U	224	ASN
7	U	243	GLN
8	V	4	MET
8	V	8	PHE
8	V	21	THR
8	V	36	ARG
8	V	39	ASP
8	V	72	THR
8	V	82	PHE
8	V	83	LYS
8	V	84	GLU
8	V	88	GLU
8	V	92	ASN
8	V	104	ASP
8	V	118	SER
8	V	132	THR

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Mol	Chain	Res	Type
8	V	137	TYR
8	V	149	GLU
8	V	153	ASP
8	V	172	VAL
9	W	10	ASN
9	W	21	THR
9	W	33	LYS
9	W	39	PRO
9	W	41	ILE
9	W	72	ARG
9	W	81	GLN
9	W	82	MET
9	W	85	GLN
9	W	98	LEU
9	W	104	ASP
9	W	132	LEU
9	W	144	GLN
9	W	146	LEU
9	W	153	LYS
9	W	177	VAL
9	W	178	MET
10	X	37	ASN
10	X	64	GLU
10	X	90	VAL
10	X	123	PHE
10	X	125	LEU
10	X	133	LYS
10	X	138	SER
10	X	171	LEU
10	X	191	LYS
11	Y	7	ILE
11	Y	8	ARG
11	Y	11	ASP
11	Y	22	THR
11	Y	36	ARG
11	Y	75	LEU
11	Y	78	GLN
11	Y	86	GLN
11	Y	91	SER
11	Y	110	LYS
11	Y	111	LYS
11	Y	136	SER

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Mol	Chain	Res	Type
11	Y	162	LYS
11	Y	194	ASP
11	Y	195	PHE
11	Y	196	GLN
11	Y	198	GLN
12	Z	4	LEU
12	Z	9	GLN
12	Z	21	THR
12	Z	25	TRP
12	Z	33	ARG
12	Z	86	LEU
12	Z	104	TYR
12	Z	105	THR
12	Z	111	THR
12	Z	152	ASP
12	Z	211	ILE
13	a	3	ASN
13	a	18	GLU
13	a	23	LEU
13	a	27	THR
13	a	31	THR
13	a	48	ASP
13	a	49	ASN
13	a	51	VAL
13	a	52	MET
13	a	67	ARG
13	a	85	SER
13	a	103	PHE
13	a	109	THR
13	a	135	GLN
13	a	151	ASP
13	a	152	ASN
13	a	165	ASN
13	a	172	LEU
13	a	174	TYR
13	a	175	LEU
13	a	214	LYS
13	a	221	ARG
14	b	9	THR
14	b	34	LEU
14	b	48	ASN
14	b	72	THR

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Mol	Chain	Res	Type
14	b	85	GLU
14	b	102	GLN
14	b	104	ARG
14	b	111	TRP
14	b	132	LEU
14	b	138	SER
14	b	140	PRO
14	b	171	GLN
14	b	212	LEU
14	b	216	ASN
14	b	226	LYS
15	c	1130	LYS
15	c	1162	VAL
15	c	1165	GLU
15	c	1168	LYS
15	c	1170	LYS
15	c	1227	ASP
15	d	1130	LYS
15	d	1227	ASP
15	e	1174	SER
15	e	1227	ASP
15	f	1130	LYS
15	f	1165	GLU
15	f	1166	SER
15	f	1168	LYS
15	f	1174	SER
15	f	1227	ASP
15	g	1130	LYS
15	g	1166	SER
15	g	1170	LYS
15	g	1227	ASP
15	h	1130	LYS
15	h	1227	ASP
15	i	1174	SER
15	i	1227	ASP
15	j	1130	LYS
15	j	1162	VAL
15	j	1165	GLU
15	j	1168	LYS
15	j	1170	LYS
15	j	1227	ASP
15	k	1130	LYS

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Mol	Chain	Res	Type
15	k	1227	ASP
15	l	1174	SER
15	l	1227	ASP
15	m	1130	LYS
15	m	1165	GLU
15	m	1166	SER
15	m	1168	LYS
15	m	1174	SER
15	m	1227	ASP
15	n	1130	LYS
15	n	1166	SER
15	n	1170	LYS
15	n	1227	ASP
15	o	1130	LYS
15	o	1227	ASP
15	p	1174	SER
15	p	1227	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (259) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	92	ASN
1	A	123	ASN
1	A	126	GLN
1	A	130	GLN
1	A	176	GLN
1	A	184	ASN
1	A	193	HIS
1	A	195	ASN
1	A	209	HIS
1	A	251	GLN
2	B	94	HIS
2	B	139	HIS
2	B	218	ASN
2	B	241	GLN
2	B	244	ASN
3	C	70	ASN
3	C	94	HIS
3	C	96	GLN
3	C	97	ASN
3	C	103	ASN

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Mol	Chain	Res	Type
3	C	120	GLN
3	C	124	GLN
3	C	156	ASN
3	C	177	GLN
3	C	221	ASN
3	C	227	GLN
4	D	94	GLN
4	D	162	GLN
4	D	178	ASN
4	D	209	ASN
4	D	241	GLN
4	D	243	GLN
5	E	99	HIS
5	E	108	ASN
5	E	154	GLN
5	E	168	ASN
5	E	215	ASN
5	E	233	ASN
6	F	100	ASN
6	F	110	HIS
6	F	121	GLN
6	F	152	ASN
6	F	185	ASN
7	G	72	HIS
7	G	86	HIS
7	G	122	HIS
7	G	126	ASN
7	G	194	GLN
7	G	206	ASN
7	G	224	ASN
8	H	38	HIS
8	H	60	GLN
8	H	69	GLN
8	H	157	HIS
9	I	22	GLN
9	I	62	ASN
9	I	66	HIS
9	I	116	HIS
9	I	144	GLN
9	I	160	GLN
9	I	165	ASN
10	J	37	ASN

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Mol	Chain	Res	Type
10	J	71	ASN
10	J	88	GLN
10	J	156	ASN
11	K	37	GLN
11	K	118	GLN
11	K	147	HIS
11	K	191	GLN
11	K	196	GLN
11	K	198	GLN
12	L	9	GLN
12	L	66	HIS
12	L	85	ASN
12	L	133	GLN
12	L	176	ASN
12	L	188	HIS
12	L	190	ASN
12	L	191	HIS
12	L	208	ASN
13	M	3	ASN
13	M	49	ASN
13	M	70	ASN
13	M	80	ASN
13	M	108	HIS
13	M	152	ASN
13	M	158	ASN
13	M	165	ASN
13	M	195	HIS
14	N	3	GLN
14	N	18	ASN
14	N	48	ASN
14	N	62	HIS
14	N	108	ASN
14	N	149	HIS
14	N	152	ASN
14	N	171	GLN
14	N	179	ASN
14	N	211	ASN
14	N	216	ASN
1	O	39	ASN
1	O	92	ASN
1	O	123	ASN
1	O	126	GLN

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Mol	Chain	Res	Type
1	O	130	GLN
1	O	176	GLN
1	O	184	ASN
1	O	193	HIS
1	O	195	ASN
1	O	209	HIS
1	O	251	GLN
2	P	94	HIS
2	P	139	HIS
2	P	218	ASN
2	P	241	GLN
2	P	244	ASN
3	Q	70	ASN
3	Q	94	HIS
3	Q	96	GLN
3	Q	97	ASN
3	Q	103	ASN
3	Q	120	GLN
3	Q	124	GLN
3	Q	156	ASN
3	Q	177	GLN
3	Q	221	ASN
3	Q	227	GLN
4	R	94	GLN
4	R	162	GLN
4	R	178	ASN
4	R	209	ASN
4	R	241	GLN
4	R	243	GLN
5	S	99	HIS
5	S	108	ASN
5	S	154	GLN
5	S	168	ASN
5	S	215	ASN
5	S	233	ASN
6	T	69	HIS
6	T	100	ASN
6	T	110	HIS
6	T	121	GLN
6	T	152	ASN
6	T	185	ASN
7	U	72	HIS

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Mol	Chain	Res	Type
7	U	86	HIS
7	U	122	HIS
7	U	126	ASN
7	U	194	GLN
7	U	206	ASN
7	U	224	ASN
8	V	38	HIS
8	V	60	GLN
8	V	69	GLN
8	V	157	HIS
9	W	22	GLN
9	W	62	ASN
9	W	66	HIS
9	W	144	GLN
9	W	160	GLN
9	W	165	ASN
10	X	37	ASN
10	X	88	GLN
10	X	156	ASN
11	Y	37	GLN
11	Y	118	GLN
11	Y	147	HIS
11	Y	191	GLN
11	Y	196	GLN
11	Y	198	GLN
12	Z	9	GLN
12	Z	66	HIS
12	Z	85	ASN
12	Z	133	GLN
12	Z	176	ASN
12	Z	188	HIS
12	Z	190	ASN
12	Z	191	HIS
13	a	3	ASN
13	a	49	ASN
13	a	70	ASN
13	a	80	ASN
13	a	108	HIS
13	a	152	ASN
13	a	158	ASN
13	a	165	ASN
13	a	195	HIS

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Mol	Chain	Res	Type
14	b	3	GLN
14	b	18	ASN
14	b	48	ASN
14	b	62	HIS
14	b	108	ASN
14	b	149	HIS
14	b	152	ASN
14	b	171	GLN
14	b	179	ASN
14	b	211	ASN
14	b	216	ASN
15	c	1047	HIS
15	c	1072	GLN
15	c	1099	HIS
15	d	1047	HIS
15	d	1072	GLN
15	d	1079	HIS
15	d	1099	HIS
15	e	1047	HIS
15	e	1072	GLN
15	e	1079	HIS
15	e	1099	HIS
15	e	1111	HIS
15	f	1047	HIS
15	f	1072	GLN
15	f	1079	HIS
15	f	1099	HIS
15	g	1047	HIS
15	g	1072	GLN
15	g	1079	HIS
15	g	1099	HIS
15	g	1111	HIS
15	h	1047	HIS
15	h	1072	GLN
15	h	1079	HIS
15	h	1099	HIS
15	h	1111	HIS
15	i	1047	HIS
15	i	1072	GLN
15	i	1079	HIS
15	i	1099	HIS
15	j	1047	HIS

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Mol	Chain	Res	Type
15	j	1072	GLN
15	j	1099	HIS
15	k	1047	HIS
15	k	1072	GLN
15	k	1079	HIS
15	k	1099	HIS
15	l	1047	HIS
15	l	1072	GLN
15	l	1079	HIS
15	l	1099	HIS
15	l	1111	HIS
15	m	1047	HIS
15	m	1072	GLN
15	m	1079	HIS
15	m	1099	HIS
15	n	1047	HIS
15	n	1072	GLN
15	n	1079	HIS
15	n	1099	HIS
15	n	1111	HIS
15	o	1047	HIS
15	o	1072	GLN
15	o	1079	HIS
15	o	1111	HIS
15	p	1047	HIS
15	p	1072	GLN
15	p	1079	HIS
15	p	1099	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	243/252 (96%)	0.30	10 (4%) 41 28	47, 82, 112, 124	0
1	O	243/252 (96%)	0.27	12 (4%) 33 22	47, 82, 112, 125	0
2	B	249/250 (99%)	0.17	8 (3%) 51 38	45, 67, 102, 123	0
2	P	249/250 (99%)	0.03	9 (3%) 46 33	46, 68, 102, 123	0
3	C	243/258 (94%)	0.01	5 (2%) 67 54	32, 60, 108, 122	0
3	Q	243/258 (94%)	0.10	10 (4%) 41 28	32, 62, 108, 122	0
4	D	241/254 (94%)	0.02	5 (2%) 67 54	34, 58, 105, 135	0
4	R	241/254 (94%)	-0.02	8 (3%) 50 37	35, 61, 104, 133	0
5	E	245/260 (94%)	0.13	16 (6%) 22 13	31, 55, 108, 133	0
5	S	245/260 (94%)	0.11	13 (5%) 30 19	33, 57, 108, 134	0
6	F	234/234 (100%)	-0.14	1 (0%) 93 90	34, 58, 78, 111	0
6	T	234/234 (100%)	-0.05	3 (1%) 79 69	36, 59, 79, 111	0
7	G	243/288 (84%)	0.16	4 (1%) 74 64	48, 69, 112, 121	0
7	U	243/288 (84%)	0.27	15 (6%) 24 15	50, 70, 112, 121	0
8	H	196/196 (100%)	0.03	5 (2%) 59 47	46, 66, 91, 98	0
8	V	196/196 (100%)	0.09	6 (3%) 52 40	46, 66, 91, 98	0
9	I	222/222 (100%)	-0.07	4 (1%) 71 60	40, 60, 84, 128	0
9	W	222/222 (100%)	0.00	5 (2%) 64 52	39, 59, 84, 127	0
10	J	204/205 (99%)	-0.38	2 (0%) 84 77	28, 43, 63, 76	0
10	X	204/205 (99%)	-0.37	1 (0%) 91 87	27, 43, 62, 76	0
11	K	198/198 (100%)	-0.22	5 (2%) 61 49	23, 40, 61, 126	0
11	Y	198/198 (100%)	-0.34	3 (1%) 76 65	24, 41, 62, 126	0
12	L	212/212 (100%)	-0.39	0 100 100	17, 37, 55, 72	0
12	Z	212/212 (100%)	-0.49	0 100 100	18, 38, 54, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	222/222 (100%)	-0.29	1 (0%) 91 87	24, 47, 65, 80	0
13	a	222/222 (100%)	-0.26	1 (0%) 91 87	24, 48, 66, 80	0
14	N	233/233 (100%)	-0.10	2 (0%) 85 79	34, 60, 87, 98	0
14	b	233/233 (100%)	0.05	7 (3%) 54 41	36, 61, 87, 98	0
15	c	195/231 (84%)	0.33	10 (5%) 32 20	46, 79, 110, 123	0
15	d	195/231 (84%)	0.18	6 (3%) 52 40	46, 75, 109, 125	0
15	e	195/231 (84%)	0.22	12 (6%) 24 15	40, 70, 104, 122	0
15	f	195/231 (84%)	0.00	3 (1%) 76 65	38, 69, 103, 130	0
15	g	195/231 (84%)	0.15	9 (4%) 36 24	47, 75, 110, 159	0
15	h	195/231 (84%)	0.52	14 (7%) 18 11	55, 85, 119, 168	0
15	i	192/231 (83%)	0.59	16 (8%) 14 8	56, 86, 112, 159	1 (0%)
15	j	195/231 (84%)	0.52	14 (7%) 18 11	61, 96, 124, 134	0
15	k	195/231 (84%)	0.63	23 (11%) 6 4	66, 100, 130, 138	0
15	l	195/231 (84%)	0.49	16 (8%) 14 8	64, 98, 127, 136	0
15	m	195/231 (84%)	0.36	16 (8%) 14 8	56, 96, 129, 140	0
15	n	195/231 (84%)	0.40	19 (9%) 10 7	58, 92, 130, 169	0
15	o	195/231 (84%)	0.41	16 (8%) 14 8	64, 93, 122, 167	0
15	p	192/231 (83%)	0.45	10 (5%) 31 19	57, 93, 119, 165	1 (0%)
All	All	9094/9802 (92%)	0.09	345 (3%) 44 30	17, 66, 113, 169	2 (0%)

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	p	1231	SER	9.7
15	h	1227	ASP	8.7
3	Q	245	THR	8.7
15	h	1231	SER	7.2
3	Q	244	ILE	7.1
3	C	245	THR	6.6
5	S	126	GLY	6.5
15	j	1002	PRO	6.1
5	S	129	GLY	6.1
5	S	125	GLU	5.9
15	h	1226	SER	5.9
15	o	1231	SER	5.5
15	i	1231	SER	5.4

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Mol	Chain	Res	Type	RSRZ
15	p	1229	MET	5.3
4	D	52	LEU	5.3
5	E	128	SER	5.3
5	S	128	SER	5.3
15	c	1159	LEU	5.3
15	p	1227	ASP	5.2
15	l	1179	LEU	5.2
11	K	196	GLN	5.1
5	S	250	GLU	5.1
15	m	1055	TYR	5.1
15	i	1229	MET	4.9
15	m	1159	LEU	4.8
15	k	1055	TYR	4.8
1	A	251	GLN	4.8
15	n	1157	ASP	4.7
15	i	1228	HIS	4.7
11	Y	198	GLN	4.7
15	o	1227	ASP	4.6
11	K	198	GLN	4.6
4	R	51	THR	4.6
15	m	1227	ASP	4.6
15	k	1002	PRO	4.6
15	p	1228	HIS	4.5
5	E	124	GLY	4.5
8	V	11	GLY	4.5
15	l	1055	TYR	4.5
15	o	1229	MET	4.5
15	o	1226	SER	4.4
15	o	1228	HIS	4.4
5	E	247	GLU	4.4
1	O	252	ASP	4.3
15	p	1230	VAL	4.3
7	U	5	THR	4.3
15	k	1057	ARG	4.3
15	k	1159	LEU	4.3
15	o	1159	LEU	4.3
15	k	1182	GLU	4.2
14	b	1	THR	4.2
15	f	1227	ASP	4.2
15	h	1228	HIS	4.2
8	V	10	ASP	4.2
5	E	127	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
15	l	1177	PRO	4.1
5	S	127	ALA	4.1
15	n	1159	LEU	4.1
15	i	1055	TYR	4.1
15	g	1231	SER	4.0
15	m	1231	SER	4.0
15	m	1179	LEU	4.0
15	d	1159	LEU	4.0
5	E	125	GLU	3.9
4	D	51	THR	3.9
2	P	249	ALA	3.9
15	k	1152	ARG	3.8
15	n	1002	PRO	3.8
2	B	52	SER	3.8
15	k	1056	GLY	3.7
15	j	1055	TYR	3.7
15	n	1231	SER	3.7
15	k	1060	ALA	3.7
6	T	1	MET	3.6
15	c	1231	SER	3.6
15	o	1230	VAL	3.6
1	O	249	ALA	3.6
3	Q	42	ASP	3.6
8	H	11	GLY	3.6
15	h	1230	VAL	3.5
11	K	197	ALA	3.5
8	H	10	ASP	3.5
15	m	1183	LEU	3.5
15	i	1179	LEU	3.5
9	W	222	ASP	3.4
15	h	1159	LEU	3.5
15	i	1227	ASP	3.4
15	o	1002	PRO	3.4
7	U	201	LEU	3.4
15	o	1183	LEU	3.4
11	Y	196	GLN	3.3
15	g	1157	ASP	3.3
15	g	1227	ASP	3.3
15	h	1002	PRO	3.3
8	H	8	PHE	3.3
15	m	1057	ARG	3.3
7	G	186	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
4	R	52	LEU	3.3
14	N	203	ASN	3.3
3	C	219	GLY	3.3
5	S	131	GLU	3.3
15	n	1228	HIS	3.2
3	Q	41	SER	3.2
7	U	205	ASP	3.2
5	E	244	LYS	3.2
4	D	242	GLU	3.2
15	n	1229	MET	3.2
15	n	1226	SER	3.2
2	P	39	ALA	3.2
15	n	1158	LYS	3.2
9	I	221	CYS	3.2
15	h	1158	LYS	3.2
15	k	1071	LEU	3.2
15	d	1063	SER	3.1
7	U	220	LEU	3.1
3	Q	221	ASN	3.1
15	n	1053	SER	3.1
5	S	130	GLU	3.1
9	W	219	ASN	3.1
1	A	252	ASP	3.1
5	E	240	ILE	3.1
14	N	1	THR	3.1
15	l	1231	SER	3.1
3	Q	205	ALA	3.1
7	G	207	LYS	3.1
15	h	1055	TYR	3.1
5	E	129	GLY	3.0
15	e	1158	LYS	3.0
15	l	1157	ASP	3.0
3	Q	204	SER	3.0
4	R	205	THR	3.0
15	e	1157	ASP	3.0
7	U	184	GLU	3.0
15	i	1159	LEU	3.0
15	n	1155	VAL	3.0
3	Q	184	MET	3.0
5	S	132	ARG	3.0
15	c	1179	LEU	3.0
1	A	50	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
8	H	9	LYS	2.9
15	o	1055	TYR	2.9
15	j	1157	ASP	2.9
15	d	1180	LEU	2.9
15	k	1143	TYR	2.9
15	i	1003	PRO	2.9
8	V	9	LYS	2.9
15	e	1055	TYR	2.9
15	m	1158	LYS	2.9
15	p	1159	LEU	2.9
15	c	1052	ASN	2.8
15	l	1003	PRO	2.8
15	k	1231	SER	2.8
15	h	1229	MET	2.8
15	m	1061	GLU	2.8
5	S	124	GLY	2.8
7	U	44	GLY	2.8
2	P	250	LEU	2.8
15	e	1231	SER	2.8
15	k	1158	LYS	2.8
15	j	1180	LEU	2.8
15	m	1178	SER	2.8
4	R	40	ASN	2.8
15	e	1002	PRO	2.8
8	V	8	PHE	2.8
3	C	220	ALA	2.8
15	g	1063	SER	2.8
2	B	247	LEU	2.8
5	E	131	GLU	2.8
15	k	1061	GLU	2.8
9	W	220	ILE	2.8
14	b	18	ASN	2.8
13	a	1	GLN	2.8
1	A	222	ASP	2.7
15	e	1159	LEU	2.7
15	j	1067	LEU	2.7
9	W	221	CYS	2.7
15	l	1149	LEU	2.7
15	i	1157	ASP	2.7
1	O	189	SER	2.7
3	C	60	ASP	2.7
4	R	236	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
15	i	1230	VAL	2.7
7	U	207	LYS	2.7
1	A	213	ALA	2.7
1	A	214	LEU	2.7
15	f	1159	LEU	2.7
15	g	1159	LEU	2.7
1	O	39	ASN	2.7
11	K	195	PHE	2.6
15	d	1181	LEU	2.6
15	h	1050	ILE	2.6
15	d	1179	LEU	2.6
15	l	1050	ILE	2.6
15	n	1060	ALA	2.6
15	l	1180	LEU	2.6
7	U	246	ILE	2.6
15	k	1016	TYR	2.6
5	E	207	VAL	2.6
15	i	1002	PRO	2.6
2	P	208	THR	2.6
15	k	1181	LEU	2.6
15	n	1182	GLU	2.6
11	Y	197	ALA	2.6
15	c	1063	SER	2.6
15	p	1002	PRO	2.6
15	j	1047	HIS	2.6
9	W	218	VAL	2.6
2	P	247	LEU	2.5
7	U	217	TRP	2.5
15	k	1183	LEU	2.5
15	g	1228	HIS	2.5
1	A	197	GLU	2.5
5	E	132	ARG	2.5
15	j	1061	GLU	2.5
10	J	191	LYS	2.5
14	b	202	LYS	2.5
1	A	198	SER	2.5
7	G	244	LYS	2.5
15	c	1062	LYS	2.5
3	Q	220	ALA	2.5
4	D	241	GLN	2.5
15	m	1228	HIS	2.5
15	o	1157	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	218	PHE	2.5
15	l	1159	LEU	2.5
2	P	216	ASP	2.5
15	e	1061	GLU	2.5
14	b	16	TYR	2.5
2	B	178	ARG	2.5
15	e	1179	LEU	2.5
15	i	1178	SER	2.5
15	m	1187	ASP	2.5
15	n	1227	ASP	2.5
15	j	1147	GLU	2.4
2	B	177	LYS	2.4
15	c	1067	LEU	2.4
4	R	241	GLN	2.4
6	F	1	MET	2.4
15	i	1182	GLU	2.4
4	R	60	THR	2.4
10	X	194	VAL	2.4
2	B	206	GLY	2.4
15	i	1057	ARG	2.4
9	I	175	VAL	2.4
15	o	1143	TYR	2.4
5	E	133	LEU	2.4
2	B	250	LEU	2.4
2	B	201	GLU	2.4
15	e	1056	GLY	2.4
15	m	1064	PRO	2.4
5	E	130	GLU	2.4
15	n	1057	ARG	2.4
15	k	1227	ASP	2.4
15	l	1187	ASP	2.4
4	D	124	GLY	2.4
8	V	179	THR	2.3
1	O	217	GLU	2.3
15	k	1179	LEU	2.3
9	I	222	ASP	2.3
15	o	1152	ARG	2.3
15	h	1011	ASN	2.3
2	P	201	GLU	2.3
14	b	201	ASP	2.3
15	j	1091	VAL	2.3
15	g	1055	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
5	S	249	ALA	2.3
15	k	1058	ALA	2.3
15	l	1185	GLN	2.3
14	b	47	ASP	2.3
10	J	18	ASP	2.3
15	k	1157	ASP	2.3
15	l	1058	ALA	2.3
2	P	219	PRO	2.3
15	o	1178	SER	2.3
15	m	1182	GLU	2.3
15	i	1183	LEU	2.3
7	U	187	SER	2.3
8	H	12	VAL	2.3
11	K	194	ASP	2.3
15	l	1184	ARG	2.3
5	E	126	GLY	2.3
3	C	236	LYS	2.3
7	U	174	GLU	2.3
15	k	1063	SER	2.2
1	O	188	LYS	2.2
15	o	1003	PRO	2.2
15	k	1059	GLN	2.2
5	S	212	LEU	2.2
15	j	1158	LYS	2.2
8	V	182	GLY	2.2
15	n	1183	LEU	2.2
1	O	191	ILE	2.2
13	M	1	GLN	2.2
7	U	238	ALA	2.2
7	G	185	GLY	2.2
15	j	1068	LEU	2.2
9	I	182	LYS	2.2
15	o	1158	LYS	2.2
3	Q	56	LEU	2.2
15	c	1182	GLU	2.2
1	O	195	ASN	2.2
15	l	1057	ARG	2.2
2	B	174	PHE	2.2
15	e	1228	HIS	2.2
1	O	198	SER	2.2
5	S	248	ALA	2.2
15	p	1003	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
15	e	1183	LEU	2.1
1	A	215	GLY	2.1
15	n	1156	GLU	2.1
6	T	42	THR	2.1
15	n	1189	ASP	2.1
5	E	248	ALA	2.1
1	O	194	ILE	2.1
2	P	52	SER	2.1
15	j	1074	TYR	2.1
1	A	168	ALA	2.1
7	U	242	ALA	2.1
15	d	1187	ASP	2.1
15	i	1036	ILE	2.1
15	n	1063	SER	2.1
15	g	1060	ALA	2.1
7	U	232	GLY	2.1
15	n	1003	PRO	2.1
14	b	198	ALA	2.1
15	j	1019	THR	2.1
4	R	61	PRO	2.1
15	m	1186	ILE	2.0
1	O	231	ASP	2.0
15	c	1124	THR	2.0
15	c	1055	TYR	2.0
15	f	1228	HIS	2.0
15	e	1053	SER	2.0
15	p	1068	LEU	2.0
5	E	236	THR	2.0
15	k	1054	THR	2.0
15	l	1002	PRO	2.0
15	m	1050	ILE	2.0
15	p	1183	LEU	2.0
15	g	1226	SER	2.0
15	h	1157	ASP	2.0
6	T	3	ARG	2.0
7	U	221	SER	2.0
15	h	1003	PRO	2.0
15	j	1231	SER	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.